N_2

1991

3 Б1145. **Лазерная спектроскопия высокого разрешения N_2 и CO в крайней ультрафиолетовой области.** High resolution XUV laser spectroscopy on N_2 and CO /Levelt P., Ubachs W., Hogervorst W. //COMET XII: Eur. Res. Conf. Mol. Energy Transfer, Berg en Dal, 21—26 July, 1991 : Book Abstr.—Nijmegen, 1991 .—С. 33 .—Англ.

На базе наносекундных узкополосных (ширина полосы возбуждения 0,3 $см^{-1}$) импульсных лазеров высокой мощности и методов нелинейной оптики разработан прецизионный (точность 0,04 $см^{-1}$) спектрометр, работающий в крайней УФ-области (90—100 нм), с помощью к-рого методом резонансно усиленной двухфотонной (1 КУФ+1 УФ) ионизации исследованы: ридберговые состояния $c'^1_4\Sigma^+_u$ (v=0) и $o_3{}^3\pi_u$ (v=0) молекулы N_2 возмущенные валентными состояниями $b'^1\Sigma^+_u$ и $b^1\Pi_u$; ридберговые состояния $L4p\pi^1\pi$ (V=0), K $4p\sigma^1\Sigma^+$(v=0), $W^3s\sigma^1\pi$ (v=0 молекулы CO. Обнаружен также новый переход CO при 98,58 нм.

В. М. Ковба

М.П.

(4)

Х. 1993, N3

CO

N_2 1991

Liu Lei, Li Jia-ming.

м.п. J. Phys. B. 1991. <u>24</u>, N 8. С. 1893-1898.

(Сл. ● C_2; III)

N_2

1991

115: 145982z **Two-photon spectroscopy of molecular nitrogen: multiphoton ionization, laser-induced fluorescence, and direct absorption via the a″ $^1\Sigma_g^+$ state.** Lykke, Keith R.; Kay, Bruce D. (Sandia Natl. Lab., Albuquerque, NM 87185 USA). *J. Chem. Phys.* 1991, 95(4), 2252-8 (Eng). A new (2 + 1) resonantly enhanced multiphoton ionization (REMPI) process via the a″ $^1\Sigma_g^+$ state of N_2 with a quantum specific detection sensitivity of ~10^5 mol. cm^{-3} is reported. The resulting spectra are easily analyzed and yield directly the relative rotational and vibrational populations in the ground electronic state of N_2. Addnl., both two-photon direct absorption (TPDA) to, and laser-induced fluorescence (LIF) from two-photon excitation of, the a″ state of N_2 are obsd. These spectroscopies are compared with (1 + 1) REMPI and TPDA via the *E, F* state of H_2.

состояние

a″ $^1\Sigma_g^+$, спектр

C.A. 1991, <u>115</u>, N 14

N_2

1991

5 Д142. Анализ 8f, 9f, и 10f, $v=1$ ридберговских состояний N_2. Analysis of the 8f, 9f, and 10f, $v=1$ Rydberg states of N_2 / McCormack E. F., Pratt S. T., Dehmer J. L., Dehmer P. M. // Phys. Rev. A.— 1991.— 44, № 5.— С. 3007—3015.— Англ.

Метод спектроскопии двойного резонанса из состояния $a1\Pi_g$, $v'=5$ использован для изучения автоионизационного $(X^2\Sigma_g{}^+)$8f, 9f, 10f, $v=1$ состояния N_2. Используемая модель основывается на рассмотрении дальнодействующего взаимодействия остова молекулярного иона с ридберговским электроном и может быть использовано как для описания энергий уровней 8f, $v=1$, так и для определения эффективного квадрупольного момента и поляризуемости $N_2{}^+X'\Sigma_g{}^+$ $v=1$ остова. Анализ состояния 9f, $v=1$ позволил обнаружить новое состояние, считавшееся ненаблюдаемым $(A^2\Pi_u)3d\pi'\Delta_u$, $v=2$. Полученные результаты дают полное представление о деталях однофотонного спектра поглощения N_2 в диапазоне 125 667—126 850 см$^{-1}$.

М·П·

сф. 1992, N5

N_2

1991

11 Б1155. **Анализ** 8*f*, 9*f* **и** 10*f*, $v=1$ **ридберговых состояний** N_2. Analysis of the 8*f*, 9*f*, and 10*f*, $v=1$ Rydberg states of N_2 / McCormack E. F., Pratt S. T., Dehmer J. L., Dehmer P. M. // Phys. Rev. A.— 1991.— 44, № 5.— С. 3007—3015.— Англ.

С помощью ионизац. спектроскопии двойного резонанса исследована автоионизация $(X^2\Sigma_g{}^+)8f$, 9*f* и 10*f* $(v=1)$ состояний N_2 через ряд вращат. уровней $a^1\Pi_g$ $(v'=5)$ состояния. Исследуемые состояния лежат в сложной области спектра, к-рая содержит переходы на высокие колебат. уровни $b'\Sigma_u{}^+$ валентного состояния и ридберговые состояния, сходящиеся к $X^2\Sigma_g{}^+$, $A^2\Pi_u$ в $B^2\Sigma_u{}^+$ состояниям иона. Для интерпретации структуры *f*-состояний и идентификации степени вз-вия с близколежащими состояниями использована модель дальнодействующего вз-вия, основанная на вз-вии ридбергового электрона с поляризуемостью и квадрупольным

И·П·

Х. 1992, № 11

моментом коры иона. N_2^+. Обработкой МНК получены значения энергии невозмущенного $8f$ состояния и эффективные значения величины квадрупольного момента $(3,2\pm0,1)$ и изотропный поляризуемости $(16,1\pm0,4)$ для $X^2\Sigma_g^+$ $(v^+=1)$ состояния иона. Кроме того, наблюдалось новое состояние, возмущающее $9f$ $(v=1)$ состояние, к-рое интерпретировано как $(A^2\Pi_u)3d\pi^1\Delta_u$ $(v=2)$ состояние. Библ. 41. Е. А. Пазюк

N_2 Om 36486 1991

Ondrey G.S., Rose C., et al.,

J. Chem. Phys. 1991, 95, N11,
7823-7827.

Resonant multiphoton ionization
dynamics of N_2 via the

$a\,^1\Pi_g$ ($v=10-14$) states;
preparation of state-selected
N_2^+ $X^2\Sigma_g^+$ ($v^+=0-4$) ions.

N_2

1991

115: 145340p **High-resolution Fourier spectrometry of nitrogen ($^{14}N_2$) infrared emission spectrum: extensive analysis of the $w^1\Delta_u \rightarrow a^1\Pi_g$ system.** Roux, F.; Michaud, F. (Lab. Spectrom. Ionique Mol., Univ. Claude Bernard-Lyon I, 69622 Villeurbanne, Fr.). *J. Mol. Spectrosc.* 1991, 149(2), 441–6 (Eng). Rotational anal. of the $w^1\Delta_u \rightarrow a^1\Pi_g$ system of $^{14}N_2$ was extended to include the vibrational levels of the $w^1\Delta_u$ state ($v = 4 \rightarrow 8$) and the $a^1\Pi_g$ state ($v = 3 \rightarrow 6$), resp. Recently the spectrum were recorded at high resoln. with better exptl. conditions by Fourier transform spectrometry at 4500–6000 cm^{-1} to obtain more exptl. data. The mol. parameters of these states were obtained by a complete fitting procedure. Derived values of equil. consts. were deduced. RKR potential energy curves for the 2 states were constructed, and the Franck-Condon factors were calcd. for the w → a system.

$w^1\Delta_u - a^1\Pi_g$

м.п., факторы Ф-К

C.A. 1991, 115, N 14

N_2 Оп. 36155 1991

Samson J.A.R., Chueng Y.,

фотоэл. спектр

Lee E.-M.,

J. Chem. Phys. 1991, <u>95</u>, N 1, 717-719

N_2 Om·35773 1991

Svensson S., Carlsson-Göthe M.

спектр, et al.,

структура Phys. Scr. 1991, 44, N2,

184-190

Inner Valence ● Satellite

Structure in High Resolution X-ray Excited Photoelectron Spectra of N_2 and CO.

N_2 1991

$(X^1\Sigma_g^+, A^3\Sigma_u^+, \ldots)$

120: 89437q **Calculation on the energy levels and radiation constants of molecules.** Tian, Xingshi (Dep. Phys., Yunnan Univ., Kunming, Peop. Rep. China 650091). *Yunnan Daxue Xuebao, Ziran Kexueban* **1991**, 13(3), 222-8 (Ch). The radiation consts. of mols. are usually indicated by means of the oscillator strength. The method of calcg. the energy levels of electronic states and oscillator strengths of their transition for mols. was put forward. The energy levels of $X^1\Sigma_g^+$, $A^3\Sigma_u^+$, $B^3\Pi_g$, $C^3\Pi_u$ and $D^3\Sigma_u^+$ states and the oscillator strengths of the first, the second and the fourth pos. band systems for the N_2 mol. are calcd. The calcd. values are in good agreement with exptl. values.

C.A. 1994, 120, N 8

N_2

1991

11 Д167. Точные расчеты функции потенциальной энергии и энергии диссоциации N_2 в приближении конфигурационного взаимодействия с набором исходных конфигураций. Acurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of N_2 / Werner Hans-Joachim Knowles Peter J. // J. Chem. Phys.— 1991.— 94, № 2.— С. 1264—1270.— Англ.

(м.п., De)

С использованием методов НИК-КВ и полного пространства активных орбиталей (ПАП ССП) рассчитана ф-ция потенц. энергии молекулы N_2. Исследовались зависимости рассчитанных спектроскопич. постоянных и энергии диссоциации от используемого базиса. Найдено, что энергетически оптимизованные корреляционно-согласованные базисы Даннинга дают лучшие результаты, чем базисы атомных естественных орбиталей той же величины. Расчеты с использованием базиса, вклю·

ф. 1991, N11

чающего ф-ций h-типа, а также учитывающего остовно-остовные и остовно-валентные корреляционные эффекты, дают очень точные значения r_e, ω_e и D_e с ошибками 0,0003 Å, 8 см$^{-1}$ и 0,7 ккал/моль соответственно. Включение базисных ф-ций i-типа уменьшает ошибку в рассчитанном значении энергии диссоциации до 0,3 ккал/моль (0,013 эВ).

Т. Д.

N_2

1991

22 Б1033. **Точные расчеты методом конфигурационного взаимодействия с несколькими исходными конфигурациями функции потенциальной энергии и энергии диссоциации N_2.** Accurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of N_2 / Werner Hans-Joachim, Knowles Peter J. // J. Chem. Phys.— 1991.— **94,** № 2.— С. 1264—1270.— Англ.

Внутренне сгруппир. методом конфигурац. вз-вия с учетом одно- и двукратных возбуждений по отношению к многоконфигурац. исходной волновой ф-ции рассчитана потенциальная кривая основного электронного состояния молекулы N_2. Орбитали получены многоконфигурац. методом ССП в полном активном пространстве. Рассмотрена сходимость энергии диссоциации и др. спектроскопич. постоянных при различных способах

(м.п., Де)

Х. 1991, N 22

расширения базиса. Показано, что при одинаковых размерах корреляционно согласованные базисы Даннинга обеспечивают лучшие результаты, чем базисы натуральных АО. При использовании наибольших базисов, включавших поляризац. ф-ции до h-типа, и при учете остовно — остовных и остовно — валентных корреляц. эффектов ошибки в межъядерном расстоянии, колебат. частоте и энергии диссоциации составили 0,0003 A, 8 см$^{-1}$ и 0,7 ккал/моль, соотв.; включение в базис i-функции снизило ошибку в энергии диссоциации до 0,3 ккал/моль. А. А. Сафонов

N_2

1991

114: 150670e **Accurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of nitrogen.** Werner, Hans Joachim; Knowles, Peter J. (Fak. Chem., Univ. Bielefeld, D-4800 Bielefeld, Fed. Rep. Ger.). *J. Chem. Phys.* 1991, 94(2), 1264-70 (Eng). The potential energy function of the N_2 mol. is calcd. using the internally contracted multireference CI method (CMR-CI) and complete active space SCF (CAS-SCF) ref. wave functions. A full CI calcn. in a DZP basis set is used to est. the errors assocd. with the CMR-CI wave function. The dependence of the computed spectroscopic consts. and the dissocn. energy on the basis set is also investigated. Uncontracted and segmented basis sets are compared with ANO (at. natural orbital) and other generally contracted basis sets. It is found that the energy-optimized "correlation-consistent" basis sets of Dunning yield substantially better results than ANO basis sets of the same size. In the largest calcns., which included up to *h*-type basis functions and also accounted for core-core and core-valence correlation effects, the remaining errors are 0.0003 Å, 8 cm^{-1}, and 0.7

потенц.
ф-ия.
D_0, расчет

C. A. 1991, 114, N 16

kcal/mol for r_e, ω_e, and D_e, resp. The inclusion of an *i*-type basis function reduces the error in the dissocn. energy to 0.3 kcal/mol (0.013 eV).

N_2

1992

9 Б1090. Исследование столкновительного внутримолекулярного связывания состояний $N_2(B^3\Pi_g)$ с $N_2(A^3\Sigma_u)$ и $N_2(W^3\Delta_u)$ в молекулярных пучках. Molecular-beam study of the collisional intramolecular coupling of $N_2(B^3\Pi_g)$ with the $N_2(A^3\Sigma_u^+)$ and $N_2(W^3\Delta_u)$ states /Bachmann R., Li X., Ottinger Ch., Vilesov A. F. //J. Chem. Phys .— 1992 .— 96 ,№ 7 .— С. 5151 — 5164 .— Англ.

Индуцированный столкновениями внутримолек. перенос энергии между возбужденными триплетными состояниями N_2 впервые исследован в условиях молек. пучка. Пучок, содержащий N_2 в $A^3\Sigma_u^+$ и $W^3\Delta_u$-состояниях, взаимодействовал с частицами мишени (H_2, N_2, NO и инертные газы) либо в столкновит. ячейке, либо пресекаясь с др. молек. пучком. В результате вз-вия наблюдалось испускание N_2 в $B^3\Pi_g$-состояние. Установлено, что общая заселенность $N_2(B, V')$ в пучке, вызванная столкновениями, складывается из двух компонент, соотв-щих процессам внутримолек. переноса энергии с квазирезонансных $N_2(A, V')$- и $N_2(W, V')$-состояний. Найдено, что компонента, обусловленная столкновит. связыванием A, V' → B, V',

М·Л

Х. 1993, N. 9

остается постоянной вдоль всего пучка, что связано с большим временем жизни A-состояния. Компонента столкновит. связывания $W, V' \to B, V'$ наоборот уменьшается вдоль пучка. Это наблюдение согласуется с известными временами жизни W, V'-уровней. Для $W, V' \to B, V'$ переноса получены также величины абс. сечений. Эти величины уменьшаются экспоненциально с ростом энергии несоответствия, к-рая зависит от природы сталкивающегося газа. Библ. 37. Е. А. Пазюк

N_3

1992

5 Б1065. Колебательно-вращательный спектр радикала N_3 в $X^2\pi_g$-состоянии. Rovibronic specturm of the N_3 radical in the $X^2\pi_g$ state /Chambaud Gilberte, Rosmus Pavel //J. Chem. Phys .—1992 .—**96** ,№ 1 .—С. 77—89 .—Англ.

С использованием квартичного силового поля, полученного на основе расчетов многоконфигурац. методом ССП в базисе [5s4p3d2f], проведены вычисления колебательно-вращат. спектра N_3 в состояниях, коррелирующих с состоянием симметрии $X^2\pi_g$ равновесной линейной геометрии. По предварит. оценкам энергий низших колебат. уровней в неэмпирич. силовое поле внесены нек-рые поправки. Положения колебательно-вращат. уровней с энергией до 4300 см$^{-1}$ получены вариац. методом с учетом эффекта Реннера—Теллера и спин-орбитального вз-вия. Проанализирована структура ядерных волновых ф-ций. Указано, что колебательно-вращат. спектр хорошо описывается в рамках представлений о ферми-полиадах. Результаты сопоставлены с данными аналогичных расчетов для изоэлектронной системы CO_2^+. А. А. Бучаченко

М.Л.

Х. 1993, N5

N_2

1992

8Д114. Метод генераторных координат Хартри—Фока для молекулярных систем. Расчеты N_2, CO **и** BF **вблизи хартри-фоковского предела.** The generator coordinate Hartree—Fock method for molecular systems. Near Hartree—Fock limit calculations for N_2, CO and BF / Da Costa H. F. M., Simas A. M., Smith V. H. (Jr), Trsic M. // Chem. Phys. Lett.. — 1992. — **192**, № 2—3. — С. 195—298. — Англ.

Generator coordinate Hartree—Fock calculations were performed for the fourteen-electron diatomic molecules N_2, CO and BF. The ground state HF energy and multipole electric moments were calculated. The Griffin-Wheeler HF equations were solved by discretization with the aid of the HONDO program. The Gaussian type basis was of size 26s18p10d7f for each atom. The results are of near numerical HF quality.

М.П.

(+2) ☒

ср. 1993, N8

N_2 1992

Gadre Shridhar R.,
Kulkarni S.A. et al.
J. Chem. Phys. 1992.
м. п. 96, N 7. С. 5253-5260.

(см. ● NH_3 ; $\overline{\underline{III}}$)

N_2 1992

7 Б1185. Фурье-спектроскопия высокого разрешения сверхзвуковых пучков. Инфракрасные полосы системы Германа $C''^5\Pi_{ui} - A'^5\Sigma_g^+$ $^{14}N_2$. High-Resolution Fourier Transform Spectroscopy of Supersonic Jets. The $C''^5\Pi_{ui} \rightarrow A'^5\Sigma_g^+$ Herman Infrared Bands of $^{14}N_2$ /Huber K. P., Vervloet M. //J. Mol. Spectrosc. .—1992 .—**153** ,№ 1—2 .—С. 17—25 .—Англ.

ИК-полосы системы Германа $C''\Pi_{ui} - A'^5\Sigma_g^+$ молекулы $^{14}N_2$ зарегистрированы в испускании при свободном расширении струи с помощью фурье-спектрометра с расширением 0,05 $см^{-1}$. В результате проведенного анализа определены вращат. постоянные и константы спинового вз-вия для нижнего состояния $A'(v=0-4)$, а также значения колебат. термов для нижней компоненты $\Omega=3$ C''-состояниия. Эксперим. значения колебат. энергий и межъядерных расстояний сравнены с результатами неэмпирич. квантовохим. расчетов.

Е. А. Пазюк

М-П-

Х.1994, N7

$^{14}N_2$

1992

$C''\,^5\Pi_u \rightarrow A'\,^5\Sigma_g^+$

ω_e, r_e

117: 35701r High-resolution Fourier transform spectroscopy of supersonic jets. The $C''\,^5\Pi_{ui} \rightarrow A'\,^5\Sigma_g^+$ Herman infrared bands of molecular nitrogen ($^{14}N_2$). Huber, K. P.; Vervloet, M. (Herzberg Inst. Astrophys., Natl. Res. Counc. Canada, Ottawa, ON Can. K1A 0R6). *J. Mol. Spectrosc.* 1992, 153(1-2), 17-25 (Eng). The $C''\,^5\Pi_{ui} \rightarrow A'\,^5\Sigma_g^+$ Herman IR bands of $^{14}N_2$ in emission from a free jet expansion were recorded by Fourier transform spectrometry at an apodized resoln. of 0.05 cm^{-1}. The anal. leads to the detn. of rotational and spin-coupling consts. for the A' lower state and finds term values for the $\Omega = 3$ lowest spin component in the C'' upper state. Exptl. vibrational energies and internuclear distances are compared with the results of ab initio calcns. by H. Partridge et al. (1988).

C. A. 1992, 117, N 4

N–N связь

1992

118: 176290p **Semi-empirical dependence of nitrogen-nitrogen bond energies on equilibrium distances.** Ionov, S. P.; Orlovsky, V. P.; Kirilenko, V. V. (Inst. Obshch. Neorg. Khim. im. N. S. Kurnakova, Moscow, Russia). *Dokl. Akad. Nauk* 1992, 327(4–6), 521–3 [Phys. Chem.] (Russ). A semiempirical method is described for calcg. N–N bond energies $D_0 = k\theta^2$ with $\ln\theta = A_0 + (R_0^2 - R_e^2)/R_0R_e$ in terms of equil. bond lengths R_e, distance in N related to the external orbital max. radial distribution; k and A_0 are consts.

(D_0)

C.A. 1993, 118, N18

N_2

1992

1) **19 Б1270. Прямое наблюдение индуцируемых столкновениями переходов между уровнями a$^1\pi_g$(V=0) и a$^1\Sigma_u^-$(V=0) молекулы N_2 с помощью двойной резонансно усиленной многофотонной ионизационной спектроскопии.** Direct observation of collision induced transitions between the a$^1\pi_g$-(v=0) and a$'^1\Sigma_u^-$(v=0) levels of N_2 via double resonance enhanced multiphoton ionization spectroscopy /Katayama D. H., Dentamaro A. V. //J. Chem. Phys. .—1992 .—97 ,№ 4 .—С. 2820—2822 .—Англ.

М.П.

Методом двойной резонансно усиленной многофотонной ионизации исследованы индуцируемые столкновениями электронные переходы между a$^1\pi_g$(v=0) и a$^1\Sigma_u^-$(v=0) состояниями молекулы N_2 в присутствии атомов He при т-ре жидк. азота. В экспериментах использованы два лазера на красителях: один, накачиваемый Nd:YAG лазером, а второй — эксимерным лазером. Установлено, что

Х. 1993, N 19

хотя переходы, индуцируемые столкновениями $He-N_2$, являются более предпочтительными, в спектре наблюдаются и $E-E$ переходы между молекулами N_2. Данный метод дает возможность изучать высоко лежащие состояния, недоступные с основного состояния. Не установлено корреляции между факторами Франка-Кондона и эффективностью индуцируемых столкновениями переходов. Библ. 30. Е. А. Пазюк

N_2

1992

117: 118895h Accurate proton affinities: ab initio proton binding energies for molecular nitrogen, carbon monoxide, carbon dioxide, and methane. Komornicki, Andrew; Dixon, David A. (Polyatomics Res. Inst., Mountain View, CA 94043 USA). *J. Chem. Phys.* 1992, 97(2), 1087–94 (Eng). A set of large-scale ab initio MO calcns. on the title mols. and their protonated forms has been performed. The aim of the present study has been to help establish very accurate abs. proton affinities for each of these mols. For each mol. a series of calcns. was performed using increasingly larger at. natural orbital (ANO) one-particle spaces. The energetics of protonation were then evaluated using four methods. These include self-consistent-field (SCF), second-order perturbation theory (MP2), the shingles and doubles coupled-cluster (CCSD) ansatz, and the CCSD(T) method, which includes a perturbational est. of connected triple excitations. The final proton affinities all attain chem. accuracy in that they contain <1 kcal/mol error. Present results are in extremely good agreement and consistent with the recently revised abs. proton affinity scale.

(Ap)

теор. расчет

(+3) ☒ CO, CO_2, ● CH_4

C.A. 1992, 117, N 12

N_2 1992

Kutzler F.W., Painter G.S.,

Phys. Rev. B. 1992,

м.л. 45, N 7, С. 3236-3244

(см. Li_2 ; III)

N_2 1992

Ридбер. сост.

117: 79221p XUV-laser spectroscopy on the $c'_4\ ^1\Sigma_u^+$, v = 0 and $c_3\ ^1\Pi_u$, v = 0 Rydberg states of molecular nitrogen. Levelt, Pieternel F.; Ubachs, Wim (Laser Cent., Free Univ., 1081 HV Amsterdam, Neth.). *Chem. Phys.* 1992, 163(2), 263-75 (Eng). The $c_4'\ ^1\Sigma_u^+$, v = 0 and $c_3\ ^1\Pi_u$, v = 0 Rydberg states of N_2 were studied by means of 1 XUV + 1 UV resonance enhanced two-photon ionization. The exptl. resoln. (0.35 cm^{-1}fwhm) combined with a calibration against a visible wavelength I_2 std. results in an order of magnitude better accuracy in the abs. line positions than in previous non-laser based investigations. The effects of homogeneous and heterogeneous perturbations of the Rydberg states by $b'\ ^1\Sigma_u^+$ and $b\ ^1\Pi_u$ valence states are analyzed.

C. A. 1992, 117, N 8

N_2

1992

$(A^3\Sigma_u^+ \rightarrow B^3\Pi_g)$

118: 135115s Properties of superlattices and multiple quantum wells in the presence of a high threading dislocation density. Liu, Tak Yiu (Univ. California, Santa Barbara, CA USA). 1990. 148 pp. (Eng). Avail. Univ. Microfilms Int., Order No. DA9135758. From *Diss. Abstr. Int. B* 1992, 52(7), 3803.

C.A. 1993, 118, N 14

N_2 1992

Mc Lean A.D., Liu B., et al.,

ф-ии потенц-энергии, r_e, w_e, Y, De, расчет

J. Chem. Phys., 1992, <u>97</u> (11), 8459-64

(см. B_2^+; <u>III</u>)

N_2 1992

Rinsland Curtis P.,
Goldman A., et al.

Ик спектр,
„HITRAN database"

J. Quant. Spectrosc.
Radiat. Transfer
1992, 48 (5-6), 693-99.

(cece. CoF_2; III)

Na 1992

Stark G., Smith P.L., et al.,

J. Chem. Phys. — 1992, <u>97</u>, N 7,

м.л. с. 4809–4814

Р.Ж.Х. N 7, 1994, 7Б 1196

N_2 1992

116: 136455y **SCF-Xα-SW calculations for small molecules using the optimization technique of atomic-sphere radii.** Takai, Y.; Johnson, K. H. (Dep. Mater. Sci. Eng., Massachusetts Inst. Technol., Cambridge, MA 02139 USA). *Chem. Phys. Lett.* 1992, 61, 518-23 (Eng). SCF-Xα-SW calcns. of structure parameters, normal-stretching-vibration frequencies and ionization energies of the small mols. N_2, O_2, F_2, CO, CH_2 and NH_3 have been performed using the at.-sphere radii detd. by a technique previously proposed on the basis of optimization of the virial theorem and minimization of total energy. The effectiveness of this optimization technique in the SCF-xα-SW method has been confirmed by the improved agreement between the calcns. and exptl. data for all the cases. An extension of this technique to more complicated mols. is discussed using the H_2CO mol. as a test example.

теор. расчет D_i, структур. параметры, I.

⑮

C.A. 1992, 116, N 14

N_2

1992

Toscano M., Russo N.,

низших
электр.
состоян.;
теорет.
расчет

Z. Phys. D: At. Mol. Clusters. 1992, <u>22</u>(4), 683-92

(см. ● PN; <u>III</u>)

N_2

1993

$(G^3\Delta_g - W^3\Delta_u)$

119: 237035d **A new band system of nitrogen: observation of the molecular nitrogen ($G\ ^3\Delta_g \rightarrow W\ ^3\Delta_u$) transition.** Bachmann, R.; Ottinger, C.; Vilesov, A. F. (Max Planck Inst. Stroemungsforsch., D-37073 Goettingen, Germany). *J. Chem. Phys.* 1993, 99(5), 3262-7 (Eng). The first exptl. observation of the $N_2(G\ ^3\Delta_g \rightarrow W\ ^3\Delta_u)$ transition is reported on here. The emission forms part of the spectrum of the so-called N_2 beam afterglow, a spontaneous luminescence emitted by a mol. beam of N_2 issuing from an intense d.c. discharge. Using a high performance charge-coupled device (CCD) optical multichannel detector, 18 bands of a new band system were obsd. with 2 Å full width at half-max. (FWHM) resoln. in the 350-650 nm region. Three well-resolved v'' progressions were analyzed. From a comparison with the known vibrational spacings in the $N_2(G)$ and $N_2(W)$ states, they could be assigned unambiguously to the $N_2(G \rightarrow W)$ transition. This observation allows the energy of the $N_2(G)$ state to be detd. as T_0 = 89,505 cm^{-1} or 11.10 eV, thereby also fixing the location of the previously obsd. $H(^3\Phi_u)$ state at T_0 = 107,328 cm^{-1} or 13.31 eV.

C.A. 1993, 119, N22

N_2

1993

$c_4'\,^1\Sigma_u^+ - X^1\Sigma_g^+$

$a\,^1\Pi_g - X^1\Sigma_g^+$

121: 144283j Spectroscopic diagnosis of vibrationally-hot nitrogen molecule. Darrach, M; Wang, S; Woolsey, J M; McConkey, J W (Phys. Dep., Univ. Windsor, Windsor, ON Can. N9B 3P4). *Plasma Sources Sci. Technol.* 1993, 2(4), 258-60 (Eng). Electron-impact induced VUV emission measurements of the $c'^1\Sigma_u^+-X^1\Sigma_g^+$ and $a^1\Pi_g-X^1\Sigma_g^+$ systems of N_2 allow significant information about the vibrational character of an RF excited N_2 beam to be obtained. The former system provides a rather accurate direct monitor of the v = 0 population of the ground state, whereas the latter allows conclusions to be drawn about the population in other states as well. The relative quantum efficiency of a CCD-based detection system used in some of the measurements is established also.

C.A. 1994, 121, N12

N_2

1993

(посл. данные в осн-сост.) RKR потенц. кривая

119: 279171a The electronic ground state of molecular nitrogen. Edwards, Simon; Roncin, Jean Yves; Launay, Francoise; Rostas, Francois (DAMAP, Obs. Paris-Meudon, 92195 Meudon, Fr.). *J. Mol. Spectrosc.* 1993, 162(1), 257-67 (Eng). The mol. consts. of the electronic ground state of mol. nitrogen were updated by combining published high-resoln. data with the results from recently recorded high-resoln. vacuum UV emission spectra. These consts. were obtained from a weighted least-squares fit to the Dunham formula with constraints imposed on the higher order terms. An extensive list of rovibrational level energies is given for the first time. These results were used to calc. a new RKR potential curve for this state and comparisons are made with previous studies.

C. A. 1993, 119, N 26

N2 1993

Hubert K.P., Stark G.,
Ito K.,

J. Chem. Phys. 1993, 98, N6,
м.л. с. 4471 – 4477

Вращательная структура в сериях
Хопфилда

р.ж.х. N 3, 1994, 3Б 1130

N_2

1993

119: 58614v Vibrational relaxation in the lowest electronically excited state of molecular nitrogen in solid krypton and xenon. Kuszner, D.; Schwentner, N. (Inst. Experimentalphys., FU Berlin, 1000 Berlin, 33 Germany). *J. Chem. Phys.* 1993, 98(9), 6965–74 (Eng). Vibrational relaxation in the $A^3\Sigma_u^+$ state of N_2 in rare gas matrixes was investigated by selective excitation with an excimer pumped and frequency doubled dye laser system combined with stimulated anti-Stokes Raman scattering. The relaxation is dominated at high N_2 concns. of some percent by nonresonant electronic energy transfer to other randomly distributed N_2 mols. and at low concns. by multiphonon processes. The relaxation by energy transfer can be described with the Foerster–Dexter model and exchange interaction. Time resolved data are compared with calcd. configuration averaged rate consts. The multiphonon processes can compete with energy transfer only if the N_2–N_2 spacings exceed several lattice consts. The multiphonon rate consts. are comparable to the radiative ones in Kr but are much smaller than the radiative ones in Xe. The increase in radiative rate consts. with vibrational quantum no. is explained by a stronger mixing with the host excitons due to a better energy resonance.

(спектр)

C.A 1993 119 - NG

N_2

1993

118: 89828b **Tentative interpretation of the Rydberg series converging to the $A^2\Pi_u$ state of dinitrogen(+) N_2^+.** Lefebvre-Brion, H.; Yoshino, K. (Lab. Photophys. Mol., Univ. Paris-Sud, 91405 Orsay, Fr.). *J. Mol. Spectrosc.* 1993, 158(1), 140–6 (Eng). Assignments are suggested for the strong unidentified bands which appear in the absorption spectrum of N_2 below 83.0 nm. They are proposed to be the $^1\Pi_u$ Rydberg states belonging to series converging to the $A^2\Pi_u$ state of N_2^+.

$^1\Pi_u \rightarrow A^2\Pi_u$
Ридберг·серии

C·A·1993, 118, N10

N_2 1993

Peterson K.A., Kendall R.A.,
et al.,

м.-п.,
теор.
расчет

J. Chem. Phys., 1993,
99, N 12, 9790-805.

(см. B_2; III) ●

$^{14}N_2$

1993

($C^3\Pi_u \to B^3\Pi_g$)

118: 179193v **High-resolution Fourier spectrometry of dinitrogen-14 violet emission spectrum: extensive analysis of the $C^3\Pi_u \to B^3\Pi_g$ system.** Roux, F.; Michaud, F.; Vervloet, M. (Lab. Spectrom. Ionique Mol., Univ. Claude Bernard-Lyon I, 69622 Villeurbanne, Fr.). *J. Mol. Spectrosc.* 1993, 158(2), 270-7 (Eng). Rotational anal. of the $C^3\Pi_u \to B^3\Pi_g$ system of $^{14}N_2$ was extended to include the vibrational levels of the $C^3\Pi_u$ state ($v = 1 \to 4$). The $v = 5$ level is not obsd. Equil. consts. of this state are deduced, RKR potential energy curves for the two states are constructed, and the Franck-Condon factors are calcd. for the $C^3\Pi_u \to B^3\Pi_g$ transition. Except for one in the $v = 1$ level, weak rotational perturbations are localized to a few rotational levels.

C.A. 1993, 118, N 18

N_2

1993

89703g Direct spectroscopic detection of $A'^5\Sigma^+_g$ state of nitrogen molecule. Scripter, Charles; Augustyniak, Edward; Borysow, Jacek (Dep. Phys., Michigan Technol. Univ., Houghton, MI 49931 USA). *Chem. Phys. Lett.* 1993, 201(1–4), 194–8 (Eng). The $A'^5\Sigma^+_g$ state of N_2 was detected for the first time in a direct measurement, using a high-resoln. laser absorption technique within the $C''^5\Pi_u \leftarrow A'^5\Sigma^+_g$ ($v' = 0 \leftarrow v'' = 0$) band. Evidence is given that the quintet state was created by means of an energy pooling reaction from the $A^3\Sigma^+_u$ state in a pure nitrogen pulsed discharge. From the abs. d. measurements of the quintet A' state and its precursor triplet A state, the upper limit for the destruction rate coeff. of the $A'^5\Sigma$ state by a ground state mol. nitrogen was estd. to be 7×10^{-12} cm^3 $mol.^{-1}$ s^{-1}.

($A'^5\Sigma_g^+$,
лазр. спектр
высокого разреш.
$C''^5\Pi_u \leftarrow A'^5\Sigma_g^+$

C.A. 1993, <u>118</u>, N10

N_2

1993

119: 281419f **Resonance-enhanced 2 + 2 photon ionization of nitrogen: The Lyman-Birge-Hopfield band system.** Trickl, T.; Proch, D.; Kompa, K. L. (Max-Planck-Inst. Quantenopt., D-85740 Garching, Germany). *J. Mol. Spectrosc.* 1993, 162(1), 184-229 (Eng). High-resoln. resonance-enhanced multiphoton ionization (REMPI) spectroscopy of a pulsed nitrogen beam is applied to det. the (1, 0) to (4, 0) line positions, ($J'' \leq 2$) of the $a^1\Pi_g \leftarrow X^1\Sigma_g^+$ transition. A strong a.c. Stark effect is obsd. even next to the REMPI threshold pulse energies and is tentatively correlated with certain energy levels near the three-photon energy. At the same time, the REMPI signal, which is not exactly proportional to the a ← X Franck-Condon factors, is dominated by the near-resonant enhancement due to these levels. This is particularly pronounced in the case of the (3, 0) band. In the three other cases, precise zero pulse energy values of the line positions can be detd. by linear extrapolation. The signs of the slopes for these extrapolations are opposite to those expected from the theor. expression for the dynamic Stark shift. The obtained band origins are used to recalibrate the literature data which, so far, have exhibited major mutual disagreement. A Dunham-type least-squares fit of more than 3100 available tabulated spectral line positions yields a greatly improved math. description of this transition for $v' \leq 15$ and $v'' \leq 27$, as well as of a few $A^3\Sigma_u^+$ and $b'^1\Sigma_u^+$ levels. The X-state vibrational

$a^1\Pi_g \leftarrow X^1\Sigma_g^+$

$A^3\Sigma_u^+$,

$b'^1\Sigma_u^+$, и.т.

C.A. 1993, <u>119</u>, N 26

levels cannot be adequately described by a simple $v'' + 1/2$ polynomial. It is, however, found that the application of two sep. polynomials for $v'' \leq 5$ and $v'' > 5$ can remove all discrepancies. There are two conclusions from these calcns. The first is that there is an obvious onset of enhanced anharmonicity of the N_2 ground state for $v'' \geq 5$ which is not obsd. for the isoelectronic CO mol. This effect has already been found in earlier, shorter, and less accurate Dunham expansions. These earlier polynomials, however, do not take into account the sudden change of the vibrational frequency at $v'' = 5$ which must be concluded from two independent expts. by R. E. Miller. This small but distinct change suggests the math. treatment of the vibrational levels in the two ranges specified above. An unambiguous interpretation of the effect is not possible at present. No nearby ${}^1\Sigma_g^+$ state is known which might act as a perturber, and, alternatively, a change of the electronic configuration needs to be quantified by a detailed theor. study. Accurate measurements of the X-state vibrational levels are still rather sparse. The authors' work strongly suggests further expts. need to be done at a ≤ 0.001 cm^{-1} accuracy level that cover the full level range from $v'' = 0$ to at least $v'' = 15$ in order to obtain an even more unambiguous representation of this state and to reveal more details of the rotational structure.

N_2

1994

(теор. расч)

120: 253915s **How large is the effect of 1s correlation on the D_e, ω_e, and r_e of N_2?** Bauschlicher, Charles W., Jr.; Partridge, Harry (Ames Res. Cent., NASA, Moffett Field, CA 94035 USA). *J. Chem. Phys.* 1994, 100(6), 4329-35 (Eng). The effect of N 1s correlation on the spectroscopic consts. [dissocn. energy (D_e), vibrational const. (ω_e), and bond length (r_e)] of N_2 was studied by using the coupled-cluster singles and doubles approach with a perturbational est. of the connected triples [CCSD(T)], and internally-contracted MR-CI (ICMRCI) techniques. At the ICMRCI level, the authors obtained a 1s effect of +1.35 kcal/mol on D_e. However, the effect was smaller when size-extensive methods were used. The 1s effects calcd. at the CCSD(T) and internally-contracted averaged-coupled-pair-functional (ICACPF) levels were in excellent agreement. The authors' best est. for the effect of 1s correlation was +0.8 kcal/mol on D_e, +9 cm^{-1} on ω_e, and -0.002 Å on r_e. Including the authors' est. for the effect of 1s correlation, the authors obtained a D_e of 227.1 kcal/mol by using a correlation-consistent polarized-valence sextuple zeta basis set at the ICMRCI + Q level (where the + Q indicates that the Davidson correction has been included). Basis-set incompleteness, which is estd. to be 0.7 ± 0.2 kcal/mol, is still the major source of error. The CCSD(T) ten-electron results were found to be in excellent agreement with those obtained at the ICACPF or ICMRCI + Q levels of theory.

C.A. 1994, 120, N 20

Na_2 (от. 37775) 1994

Boldyrev A.I., Gonzalez N.,
Simons J.,

$^1\Sigma_g^+$, J. Phys. Chem., 1994,
D,
эксперим., $\underline{98}$, N 40, 9931–44.
теорет.
расчет

N_2

1994

121: 310686q **N_2(B–A) time–resolved Fourier transform emission spectra from a pulsed microwave discharge.** Durry, Georges; Guelachvili, Guy (Lab. Phys. Mol. Appl., Univ. Paris–Sud, 91405 Orsay, Fr.). *J. Mol. Spectrosc.* **1994**, 168(1), 82–91 (Eng). Emission spectra of the electronic transition $B^3\Pi_g \rightarrow A^3\Sigma_u^+$ of the nitrogen mol. have been recorded from a pulsed microwave excited plasma in order to det. the feasibility of high–information time–resolved Fourier spectroscopy. A sequence of 32 time spectra, each one extending from 8676 to 17352 cm^{-1}, obsd. with good signal–to–noise ratio and Doppler–limited spectra resoln. of 0.03 cm^{-1}, has been obtained in a single expt. with a temporal resoln. of 3 μsec. These first high–information time–resolved results from Fourier transform spectroscopy are presented to illustrate the power of this new tool for dynamic studies.

$(B^3\Pi_g \rightarrow X^3\Sigma_u^+)$

C.A.1994, <u>121</u>, N26

N_2

1994

Оп 37612

7 Б1185. f-Ридберговы серии в спектре поглощения N_2. The f Rydberg series in the absorption spectrum of N_2 /Huber K. P., Jungen Ch., Yoshino K., Ito K., Stark G. //J. Chem. Phys. .— 1994 .— **100** ,№ 11 .— С. 7957—7972 .— Англ.

М.Л.

Х.1995, №7

N_2 (ом 37612) 1994

121: 68444v The f Rydberg series in the absorption spectrum of N₂. Huber, K. P.; Jungen, C.; Yoshino, K.; Ito, K.; Stark, G. (Herzberg, Inst. Astrophys., natl. Res. Counc. Canada, Ottawa, ON Can. K1A OR6). *J. Chem. Phys.* 1994, 100(11), 7957–72 (Eng). The nf Rydberg levels of $^{14}N_2$ converging to the X $^2\Sigma_g^+$ ground state of N_2^+ have been studied from n = 4–9 in the high-resoln. absorption spectra of supersonically expanding nitrogen at wavelengths ranging from 843.2 to 802.6 Å (118,600–124,600 cm⁻¹). The best exptl. results, achieving rotational temps. on the order of 20 to 40 K and a resoln. of 0.5 cm⁻¹, were obtained by photographing the jet absorption against the background continuum from a synchrotron radiation source. Complementary data for $^{14}N_2$ and $^{15}N_2$ come from the analyses of spectra recorded under equil. conditions at 70 K with a resoln. of 1 cm⁻¹, using the He continuum as background source. The observations are interpreted with the help of multichannel quantum defect calcns. and lead to the conclusion that, to varying degrees and with the exception of 4f(n=0), all the complexes studied here show the effects of interactions with core excited d and s Rydberg levels built on the A $^2\Pi_u$ first excited state of N_2^+. Also, the 9f(v=0) complex is shown to be perturbed by 10p(n=0), and the strength of the p–f interaction has been detd.

(Ридберг. серии)

C.A. 1994, 121, N6

N_2 Оп. 37601 1994

Kaidee Lee, Dae Young Kim,
Chien-I Ma, and David M.
Hanson,

J. Chem. Phys., 1994, 100 (11),
8550.

Identification of the core
hole excited states

N_2: A failure of the equivalent core approximation.

N_2 1994

Kobayashi Rika,
Amos R. D. et al.

теор.
расчёт
r, α, ω_e,
ν_i

J. Chem. Phys. 1994,
100 (2), 1375-9.

●
(см. HF; III)

N_2

1994

24 Б1129. О столкновительном возбуждении N_2 медленными молекулярными ионами. On the collisional excitation of N_2 by slow molecular ions /Krishnamurthy M., Mathur D. //Int. J. Mass Spectrom. and Ion Process. .—1994 .—**132** ,№ 1—2 .—С. 137—141 .—Англ.

Метод спектроскопии трансляц. энергии высокого разрешения использован для исследования возбуждения молекул N_2 при столкновениях с медленными молек. ионами H_2^+, N_2^+, CO^+, CO_2^+, O_2^+, CS_2^+ (энергия 1,8 кэВ). Наблюдалось возбуждение оптически запрещенных электронных состояний N_2, $A^3\Sigma^+_u$, $B^3\Pi_g$, $B'^3\Sigma^-_u$, $a'^1\Sigma^-_u$. Эксперим. результаты сравниваются с рассчитанными вероятностями переходов. В. М. Ковба

М.П.

Х.1994, N24

N_2

1994

4 Б1021. Неэмпирические расчеты вероятности синглет-триплетных переходов N_2. Ab initio calculations of singlet-triplet transition probabilities of N_2. /Minaev B., Agren H., Norman P., Jonsson D. //8th Int. Cong. Quantum Chem., Prague, June 19—23, 1994; Book Abstr. .—[Praque] ,[1994] .—С. 129 .—Англ.

С использованием методов квадратичного отклика и многоконфигурац. методов ССП изучены дипольно-запрещенные переходы между синглетным основным состоянием $X^1\Sigma_g^+$ и триплетными возбужденными состояниями $W^3\Delta_u$, $B'^3\Sigma_u^-$, $C^3\Pi_u$ и $C'^3\Pi_u$ молекулы азота. И. С.

М-1.

Х. 1995, N4

N_2

1994

> **16 Б1152. Роль $N_2(A'^5\Sigma_g^+)$ в усилении заселенности $N_2B^3\Pi_g$ (v=10) в послесвечении.** Role of $N_2(A'^5\Sigma_g^+)$ in the enhancement of $N_2B^3\Pi_g$ (v=10) populations in the afterglow / Morrill Jeff S., Benesch William M. // J. Chem. Phys. .— 1994 .— **101** , № 8 .— С. 6529—6537 .— Англ.

С разрешением во времени измерен спектр послесвечения азота, возбуждаемый в импульсном разряде. В наблюдаемой первой положит. системе $\underline{N_2}$ (переход $B^3\Pi_g \rightarrow A^3\Sigma_u^+$) обнаружены значительное усиление общей интенсивности и значительные изменения в форме полос переходов с уровня $v'_B=10$ состояния $B^3\Pi_g$. Изменение формы полос объяснено увеличением заселенности нижних вращат. уровней компоненты $\Omega=2$. В спектре наблюдались также полосы инфракрасной системы Германа (переход $C''^5\Pi_u \rightarrow A'^5\Sigma_g^+$, в основном полосы 3—1 и 2—0). Зависящее от времени увеличение интенсивности полос с $v'_B=10$ сильно коррелирует с изменением ин-

М.П.

Х. 1995, N 16

тенсивности полос системы Германа. Это связывается с пересечением потенциальных кривых состояний $A'^5\Sigma_g^+$ и $B^3\Pi_g$ вблизи уровня $v'_B=10$ (данные неэмпирич. расчетов). Предложена простая модель механизма возбуждения спектра послесвечения, включающая перенос энергии $A'^5\Sigma_g^+ \rightarrow B^3\Pi_g$ $(v=10)$ при столкновениях с молекулами азота в основном электронном состоянии. Оценена константа скорости этого процесса $1 \cdot 10$ см³/молекула·с. Библ. 40.

В. М. Ковба

N_2

1994

от· 37637

19 Б1245. **Лазерная спектроскопия возмущенных уровней в N_2 ($B^3\Pi_g$, V=10) и первое экспериментальное определение энергии терма $N_2(A'^5\Sigma_g^+)$.** Laser spectroscopy of perturbed levels in $N_2(B^3\Pi_g$, v=10) and the first experimental determination of the $N_2(A'\ ^5\Sigma_g^+)$ term energy / Ottinger Ch., Vilesov A. F. //J. Chem. Phys. .—1994 .—**100** ,№ 7 .—С. 4862—4869 .—Англ.

М.П.

Х.1994,N19.

N_2

1994

120: 230214y **Fourier transform emission spectroscopy of a He/N_2 supersonic jet in the 2-μm region: a $^1\Pi_g \rightarrow$ a$'^1\Sigma_u^-$ and w$^1\Delta_u \rightarrow$ a$^1\Pi_g$ systems of the $^{14}N_2$ molecule.** Roux, F.; Michaud, F.; Vervloet, M. (Lab. Spectrometr. Ionique Mol., Univ. Claude Bernard Lyon I, 69622 Villeurbanne, Fr.). *J. Mol. Spectrosc.* 1994, 164(2), 510–16 (Eng). Extensive anal. of the a$^1\Pi_g \rightarrow$ a$'^1\Sigma_u$ system of $^{14}N_2$ is reported. The spectrum was recorded by high-resoln. Fourier transform spectrometry at 2500–7500 cm^{-1} using a supersonic jet and a classical microwave discharge. Accurate mol. parameters of the a$'^1\Sigma_u^-$, a$^1\Pi_g$, and w$^1\Delta_u$ states were detd. by fitting simultaneously the whole set of wavenos. of the a → a' and w → a systems. The RKR potential energy curve of the a$'^1\Sigma_u^-$ state was derived, and Franck-Condon factors for the a → a' system were calcd. Predissocn. was obsd. in the a$^1\Pi_g$ (v = 7) level.

(a $^1\Pi_g \rightarrow$ a$'^1\Sigma_u$)

C.A. 1994, <u>120</u>, N 18

N2 1994

Sekine Shigeyuki.,

Denshi gijutsu sogo ken-
м.п. kyujo iho = Bull. Electrotechn
Lab., 1994, 58, N1, c.21-25

р.ж.Х. N9, 1995, 9Б1048

$2^{х}$ атомные молекулы

(N_2, O_2, F_2, Cl_2, HF, HCl, CO)

1994

120: 227410d A new approach to the efficient basis set for accurate molecular calculations: applications to diatomic molecules. Tao, Fu-Ming (Dep. Chem., Harvard Univ., Cambridge, MA 02138 USA). *J. Chem. Phys.* 1994, 100(5), 3645–50 (Eng). The method of the bond function basis set combined with the counterpoise procedure is studied in detail by the complete fourth-order Moeller-Plesset perturbation (MP4) theory, following from a recent communication report [J. Chem. Phys. 98, 2481 (1993)]. This method is applied to calc. mol. dissocn. energies D_e as well as equil. bond distances r_e and harmonic frequencies ω_e of a no. of diat. mols. (N_2, O_2, F_2, Cl_2, HF, HCl, and CO) and the results are compared with those from other methods, without either counterpoise procedure or bond functions or both. The usefulness of the method is shown by the results for all the mols. using a moderately polarized basis set (2p1d for H atom and 2d1f for heavy atoms) augmented with the universal bond functions 3s3p2d. The method has consistently recovered 98%–99% of the exptl. values for D_e, compared to as low as 90% without bond functions. The effect of bond functions is less significant on the predictions of r_e and ω_e, due primarily to the

теор. расчет

D_0, r_e, ω_e

☐

+6

C.A.-1994, 120, N18

inadequacy of the MP4 theory, but the authors' method is still shown to be favored over the other methods. The elec. dipole moments of the polar mols. (HF, HCl, and CO) are also examd. and it is found that the use of bond functions results in a significant improvement of the dipole values. Detailed discussions are given to explain the need for bond functions and the counterpoise procedure. The high linear independence with nucleus-centered basis functions is explained to be responsible for the efficiency of bond functions. The counterpoise procedure is logically justified from the conventional noncounterpoise procedure. Potential problems and limitations assocd. with the proposed method are also discussed.

N_2

1994

122: 67326s **Evidence for predissociation of N_2 a $^1\Pi_g$(v 7) by direct coupling to the $A'^5\Sigma_g^+$ state.** van der Kamp, A.; Siebbeles, Laurens D. A.; van der Zande, Wim J.; Cosby, P. C. (FOM Institute Atomic Molecular Physics, 1098 SJ Amsterdam, Neth.). *J. Chem. Phys.* **1994,** 101(11), 9271–9 (Eng). Predissocn. of the (v = 7–10) levels of the a $^1\Pi_g$ state in N_2 was studied with translational spectroscopy. These levels are produced by the charge-transfer neutralization of a 4 keV energy N_2^+ beam in Na vapor and the dissocn. fragments are monitored by a time- and position-sensitive detector. Lifetimes of 300, 300, 100, and 230 (±20) ns are measured for a $^1\Pi_g$(v = 7, 8, 9, and 10), resp. Quantum mech. calcns. based on Fermi's golden rule give evidence that the predissocn. is caused by direct coupling to the continuum of the $A'\,^5\Sigma_g^+$ state rather than by an indirect mechanism. The a $^1\Pi_g$–$\alpha'^5\Sigma_g^+$ electronic coupling matrix element is 0.44 (±0.03) cm^{-1}. The required change in spin multiplicity suggests that this coupling arises from a spin-spin interaction.

предиссоциации
в $a^1\Pi_g$ (v=7)
состоянием
$A'\,^5\Sigma_g^+$

C.A. 1995, 122, N6

N_2 1995

122: 117751z **Wide band high-resolution time-resolved spectroscopy.** Durry, G.; Guelachvili, G. (Laboratoire de Physique Moleculaire et Applications, CNRS UPR 136, Universite Paris XI, Bat. 350, Centre d'Orsay, F-91405, Orsay, Fr.). *Vib. Spectrosc.* **1995,** 8(2), 255–62 (Eng). The high-resoln. step-scan Fourier transform spectrometer of the Laboratoire de Physique Molecueculaire et Applications was modified to record time-resolved spectra. To reach high temporal and spectral resolns., particular attention was paid to the main difficulties assocd. with the short time available for each data measurement. Solns. to overcome the dynamic-range limitations were proposed and tested. Descriptions of the recording procedures with related simulations are given. To appreciate the high information feasibility of time-resolved Fourier transform spectroscopy, Doppler-limited spectra of the electronic transition B$^3\Pi_g$–A $^3\Sigma^+_u$ of the N mol., emitted from a microwave-excited plasma, were obtained over a range of 7000 cm^{-1}. They show a 2-fold improvement on the total no. of samples in a time-resolved Fourier transform spectroscopy expt.

$(B\ {}^3\Pi_g - A\ {}^3\Sigma_u^+)$

C. A. 1995, $\underline{122}$, N10

N_2

1995

F: N2
P: 3
06.Д.0191. Эталонные расчеты N[2] в приближении полного конфигурационного взаимодействия. Benchmark full configuration interaction calculations on N[2] / Evangelisti S., Bendazzoli G. L. // Nuovo cim. D. - 1995. - 17, N 3. - С. 289-294. - Англ.

В валентном приближении полного конфигурац. взаимодействия (ПКВ) проведены расчеты молекулы N[2] с использованием трехэкспонентного 4s3p-базиса при различных межъядерных расстояниях. Размер пространства ПКВ составлял более 225 млн симметрийно-адаптированных слэтеровских детерминантов. Расчеты, проведенные на компьютере CRAY C90, требовали 1400 с машинного времени на одну итерацию. Определены полные энергии и спектроскопич. постоянные. Полученные результаты могут быть использованы для проверки качества приближенных методов, используемых для исследования электронных корреляций в молекулах.

Х. 1996, N 6

N_2

1995

19 Б110. Применение многочастичной теории возмущений с несколькими исходными конфигурациями в полном активном пространстве для расчета молекулы N_2. Зависимость от рассматриваемого пространства и H_0. Application of complete space multireference many-body perturbation theory to N_2: Dependence on reference space and H_0 / Finley J. P., Freed K. F. // J. Chem. Phys. .— 1995 .— **102** , № 3 .— С. 1306—1333 .— Англ.

Детально рассмотрена многочастичная теория возмущений в полном активном пространстве. Обсужден основной формализм, составные части гамильтониана и фокианов. На примере молекулы N_2 показана зависимость H_{eff} от орбитальных энергий. Сопоставлены результаты расчета r_e, w_e, D_e и E_{eq} для основного состояния молекулы N_2, выполненные методом ССП в полном активном пространстве и в рамках многочастичной теории возмущений; сопоставлены и обсуждены результаты расчета вертикальных ПТ ионизации N_2. Рассмотрены пути дальнейшего уточнения метода расчета эффективного гамильтониана. Библ. 76.

Е. А. Рыкова

М.П.

Х. 1996, N 19

1995

F: N_2
p: 3^α

16Б1175. Расчет методом функционала плотности спектров КР. Предварительные результаты. The prediction of Raman spectra by density functional theory. Preliminary findings / Johnson Benny G., Florian Jan [Chemical Physics Letters] // Chem. Phys. Lett. - 1995. - 247, N 1 - 2. - С. 120-125. - Англ.

РЖХ 1997

Сопоставлены результаты расчетов интенсивностей линий в спектрах КР молекул N[2], HF, C[2]H[6], проведенных методом функционала плотности в локальном приближении (S-VWN) и с учетом градиентных поправок (B-LYP) и неэмпирическим методом ХФ. Показано, что локальное приближение хуже согласуется с эксперим. данными, чем градиентно-скорректированный подход и метод ХФ. Последние дают близкие результаты за исключением молекулы HF, для которой метод ХФ дает менее приемлемые величины. Во всех вариантах расчета учет диффузных поляризационных функций приводит к более точным значениям. Библ. 37.

N_2

1995

124: 40262x Fourier transform (FT) raman spectroscopy of nitrogen at high pressure. McNesby, K. L.; Morris, J. B. (Army Res. Lab., Aberdeen Proving Ground, MD USA). *Report* **1995**, (ARL–TR–718; Order No. AD–A293051), 28 pp. (Eng). Avail. NTIS. From *Gov. Rep. Announce. Index (U. S.)* **1995**, 95(21), Abstr. No. 21–00,634. Rovibrational and rotational Raman spectra of nitrogen gas at 300 K over the pressure range 3–24 MPa (500–3500 psi) were measured using a Fourier–transform (FT) spectrometer employing 1064 nm laser radiation as the scattering source. It is shown that the pressure–induced narrowing and peak shift of the Raman spectrum of N_2 obsd. in these expts. agrees within exptl. error with data obtained by other investigators using different techniques.

Фурье спектр.
комбинац.
рассеяние

С.А. 1996, 124, N4

1995

F: N2
P: 3

16Б1206. Динамика вращательной автоионизации высоколежащих ридберговых состояний азота. Rotational autoionization dynamics in high Rydberg states of nitrogen / Merkt F., Mackenzie S. R., Softley T. P. [Journal of Chemical Physics] // J. Chem. Phys. - 1995. - 103, N 11. - С. 4509-4518. - Англ.

РЖХ 1997

N_2

1995

123: 209381c Rotational autoionization dynamics in high Rydberg states of nitrogen. Merkt, F.; Mackenzie, S. R.; Softley, T. P. (Phys. Theor. Chem. Lab., Oxford Univ., Oxford, UK OX1 3QZ). *J. Chem. Phys.* **1995**, 103(11), 4509–18 (Eng). The decay dynamics of the high Rydberg states of N_2 converging on the first few rotational levels ($N^+ = 0, 1, 2, 3$) of the ground vibronic $X\ ^2\Sigma_g^+$ ($v^+ = 0$) state of the N_2^+ cation have been investigated by delayed pulsed field ionization (PFI) following two-photon enhanced (2 + 1') three-photon excitation via the $a''\ ^1\Sigma_g^+$ ($v' = 0$) state of N_2. The expts. were carried out in the presence of a weak homogeneous dc elec. field and at typical ion densities of 200–2000 ions/mm^3. All Rydberg states in the range of principal quantum no. n = 140–200 exhibit extreme stability against autoionization and predissocn. and some have lifetimes which exceed 30 μs. The decay of the highest Rydberg states beyond n = 200 is induced by external perturbations (field ionization and collisional ionization) and no Rydberg states beyond n = 350 can be obsd. by delayed PFI. The Rydberg states which converge on the $N^+ = 0$ and 1 rotational levels of the ion, and which therefore are not subject to rotational autoionization, decay into

Высокие
Ридберг·сост

C.A. 1995, 123, N 16

neutral products (by a process presumed to be predissocn.) in less than 7 μs in the range $n < 100$. The importance of predissocn. is greatly reduced beyond $n = 100$ and becomes negligible on our exptl. timescale (30 μs) above $n = 140$. The decay of the Rydberg states converging on the $N^+ = 2$ and 3 rotational levels of the ion is more complex. Below $n = 100$, only 30%–40% of the Rydberg population decays by fast rotational autoionization whereas 60%–70% decays by predissocn. The importance of predissocn. decreases rapidly above $n = 100$ and becomes negligible beyond $n = 140$. The decay by rotational autoionization can be obsd. at all n values but becomes noticeably slower beyond $n = 100$. In the range $n = 140$–200 it exhibits a marked biexponential decaying behavior with 30% of the population decaying within a few microseconds and 70% displaying long term stability ($\tau > 30$ μs). The branching between predissocn. and autoionization is explained by the effect of the dc elec. field which mixes strongly the optically accessible p Rydberg series with the high l manifold beyond $n = 100$. The long lifetimes obsd. exptl. indicate that m_l mixing becomes important as soon as l mixing sets in.

1995

F: N2
P: 3
16Б1226. Индуцированное магнитным полем испускание N[2](B A) пучком метастабильных молекул взота и точный терм энергии состояния N[2](A'{5}'СИГМА'[g]{+}). Magnetic-field induced N[2](B A) emission from a beam of metastable nitrogen molecules and precise term energy of the N[2](A'{5}'ЭПСИЛОН'[g]{+}) state / Ottinger Ch., Vilesov A. F. [Journal of Chemical Physics] // J. Chem. Phys. - 1995. - 103, N 23. - С. 9929-9934. - Англ.

РЖХ 1997

Для точной идентификации положения состояния N[2](A'{5}'СИГМА'[g]{+}), которое, как предполагается, возмущает уровень N[2](B{3}'ПИ'[g]), v=10, {3}'ПИ'[2]{e}(12)), выполнены эксперименты по антипересечению в магнитном поле. Перпендикулярно пучку метастибильных молекул азота (состояния A{3}'СИГМА'[u]{+}, A'{5}'СИГМА'[g]{+} и др.) накладывали слабое магнитное поле, которое вызывало дополнительные возмущения уровня v=11 состояния B, связанные со взаимодействием его с уровнем v=2 состояния A'. Регистрировали полосы секвенции 'ДЕЛЬТА' v=3, 11-6 и 10-6 системы B{3}'ПИ'[g] A{3}'СИГМА'[u]{+} в спектре испускания N[2] при различных напряженностях поля. Исследовано влияние на спектры уменьшения заселенностей уровней v=0 и v=2 состояния A' (возмущающих соответственно уровни v=10 и v=11 состояния B) в результате лазерного возбуждения переходов в системе Германа (полосы 2-0 и 4-2, C"{5}П[u] A'{5}'СИГМА'[g]{+}). С высокой точностью (0,02 см{-1}) определено относительное положение исследованных уровней состояний B и A'. Библ. 34.

N_2 Оп 38004 1995

Peterson K.A., Dunning T.H., Jr.,

Do

J. Phys. Chem., 1995, 99, 3898-3901

1995

F: N2
P: 3
16Б119. Теоретические вероятности переходов между B{3}'ПИ'[g]- и A{3}'СИГМА'[u]{+}-, W{3}'ДЕЛЬТА'[u]-, B'{3}'СИГМА'[u]{-}-состояниями N[2]. [Исследование с использованием методов КВ и ССП в полном активном пространстве]. The theoretical transition probabilities between the B{3}'ПИ'[g] and the A{3}'СИГМА'[u]{+}, W{3}'ДЕЛЬТА'[u], B'{3}'СИГМА'[u]{-} states of N[2] / Thummel Helmar T., Partridge Harry, Huo Winifred M. [Chemical Physics Letters] // Chem. Phys. Lett. - 1995. - 247, N 4 - 6. - C. 366-372. - Англ.

Ржх 1997

N_2

1995

Внутрен.
Энергия и
давление
до 8000К,
расчет

124: 38225u **Thermodynamic properties of nitrogen fluid at high temperatures and pressures.** Yakub, E. S. (Odessa State Medical University, Odessa, Ukraine). *High Temp. (Transl. of Teplofiz. Vys. Temp.)* **1995**, 33(5), 687–93 (Eng). The Monte-Carlo method in the atom-atom approxn. was used for calcn. of the internal energy and pressure of mol. nitrogen at temps. of up to 9000 K and densities characteristic of the shock adiabat. Use was made of the at. interaction potential detd. by the scattering of mol. beams. The influence of electron excitation and nonrigidity of mols. was studied. It is shown that it is necessary to take into account the addnl. contribution to the pressure assocd. with the effect of the field of intramol. forces on intramol. motion, which may contribute up to 10% of the total pressure.

C.A. 1996, 124, N 4.

1996

F: N2
P: 3
16Б120. Энергии возбуждения H[2]O, N[2] и C[2] в приближении полного конфигурационного взаимодействия и в рамках метода связанных кластеров. Excitation energies of H[2]O, N[2] and C[2] in full configuration interaction and coupled cluster theory / Christiansen Ove, Koch Henrik, Joorgensen Poul, Olsen Jeppe [Chemical Physics Letters] // Chem. Phys. Lett. - 1996. - 256, N 1 - 2. - C. 185-194. - Англ.

РЖХ 1997

N_2

1996

r_e, ω_e, D_e,
Корреляция

124: 186091n The effect of 1s correlation on D_e, r_e, and ω_e of first-row diatomics. Csaszar, Attila G.; Allen, Wesley D. (Dep. Theoretical Chemistry, Eotvos Univ., H-1518 Budapest, Hung.). *J. Chem. Phys.* 1996, 104(7), 2746-48 (Eng). A collection of high-level D_e, r_e, and ω_e data for first-row diatomics (N_2, O_2, F_2, CO, NO, HF) is presented and which more broadly substantiates the effects of 1s correlation on mol. properties. Partitioning similar to that applied for harmonic frequencies can be cogently constructed for other spectroscopic parameters such as D_e and $\omega_e x_e$, but in the former case the indirect effects are insignificant, consistently less than 0.01 kcal mol^{-1}. Whether the consequences of core correlation for first-row diatomics are characteristic of those for a wide range of heavier systems remains to be demonstrated.

(+5)

C.A. 1996, 124, N14.

N_2

1996

125: 42299j **Identification of slowly diffusing metastable states of the nitrogen molecule.** Fewell, M. P.; Haydon, S. C.; Ernest, A. D. (Department of Physics, University of New England, Armidale, NSW, 2351 Australia). *Chem. Phys.* **1996**, 206(1,2), 257–267 (Eng). Expts. [Haydon et al., Chem. Phys. 206 (1996) 245.] have confirmed the existence of a slowly diffusing metastable state of the nitrogen mol. in addn. to the well-known A $^3\Sigma_u^+$ state. The second state is populated in pre-breakdown discharges and is characterized by a coeff. for diffusion through ground-state nitrogen of about one quarter of that of the A $^3\Sigma_u^+$ state. Recent exptl. work on the structure of the nitrogen mol. provides much evidence bearing on the question of the nature of the second slowly diffusing state. Examn. of a wide variety of possible candidates leads to the conclusion that, on presently available evidence, this state is most likely to be a highly vibrationally excited X $^1\Sigma_g^+$ state.

спектр,
диффузия
метастаб.
состояние,
вероятн. эл.
высоким колеб. $X\,^1\Sigma_g^+$ сост.
сост.

C. A. 1996, 125, N4

N_2

N_2^-

1996

124: 353148v **A bound-state CI approach to nitrogen molecular anions.** Gianturco, F. A.; Schneider, F. (Dep. of Chemistry, Univ. of Rome, 00185 Rome, Italy). *J. Phys. B: At., Mol. Opt. Phys.* 1996, 29(6), 1175–1182 (Eng). We report results of ab initio MRDCI calcns. on the doublet states of different spatial symmetry of the nitrogen mol. anion. The computed ground-state N_2 potential as well as the lowest potential curve of N_2^- were calcd. over a broad range of internuclear distances. Several other resonant states of N_2^- have been detd. at two different internuclear distances by a stabilization procedure. To our knowledge, some of the excited-state $e^- - N_2$ resonances which we found have not yet been reported in the literature. After applying the stabilization method with gradually increased nuclear charges to all of the calcd. anion states we conclude that, despite the appearance of many 'spurious states', the positions of the shape resonance of $^2\Pi_g$ symmetry, of three Feshbach resonances of $^2\Pi_u$ symmetry and of two of $^2\Sigma_g^+$ symmetry have been identified.

потенц.
кривые
основн. сост.,
теорет.
расчет

C.A. 1996, 124, N 26

N_2

1996

124: 353105d **Low-energy electron impact excitation of the nitrogen molecule: optically forbidden transitions.** Gillan, Charles J.; Tennyson, Jonathan; McLaughlin, Brendan M.; Burke, Philip G. (Dep. Applied Math. Theor. Phys., Queen's Univ., Belfast, UK BT7 1NN). *J. Phys. B: At., Mol. Opt. Phys.* 1996, 29(8), 1531–1547 (Eng). Ab initio calcns. are performed on the e^-–N_2 scattering system, at low impact energies, using the R-matrix technique. The X $^1\Sigma_g^+$ ground state and the lowest seven valence excited states, A $^3\Sigma_u^+$, B $^3\Pi_g$, W $^3\Delta_u$, B' $^3\Sigma_u^-$, a' $^1\Sigma_u^-$, a $^1\Pi_g$ and w $^1\Delta_u$, of N_2 are included in the close coupling expansion with each state being represented by a CI wavefunction in a hybrid orbital set. Various approxns. for the representation of the correlation between the target and the incident electron are investigated. Integrated and differential scattering cross sections are presented, and compared to expt., for excitation from the ground level to optically forbidden levels. The results compare favorably with recent expts. in this energy region and remove a no. of problems in the authors' previous work.

теорет. рас-
чет основн. и
возбужд. сост

C. A. 1996, 124, N 26

1996

F: N2
P: 3

18Б1228. Равновесные колебательные свойства азота в основном состоянии при температуре до 35000 К. Equilibrium vibrational properties of ground state nitrogen up to 35,000 K / Hansen C. Frederick // AIAA Journal. - 34, 9. - С. 1843-1846. - Англ.

N_2

1996

11Б1245. Индуцированные столкновениями электронные переходы N_2 с уровней $a^1\Pi_g$ (v=1 и 2). Collision-induced electronic transitions from the N_2 $a^1\Pi_g$ (v=1 and 2) levels / Katayama D. H., Dentamaro A. V., Welsh J. A. // J. Phys. Chem.— 1996 .— **100**, № 19 .— С. 7854—7858 .— Англ. Место хранения ГПНТБ

Методом двойной резонансно усиленной многофотонной ионизации определены скорости тушения для индуцированных столкновениями (He, Ar, N_2) электронных переходов N_2 с уровня v=1 состояния $a^1\Pi_g$ на уровни v=2 и 1 состояния $a'^1\Sigma_u^-$ и с уровня v=2 состояния $a^1\Pi_g$ на уровень v=3 состояния $a'^1\Sigma_u^-$. Для описания полученных экспериментальных результатов использована двухэкспоненциальная модель излучательного распада при столкновительной дезактивации. Библ. 38. В. М. Ковба

М·Л

Х. 1997, №18

N_2 1997

128: 81444j **Near-infrared diode laser spectroscopy of the nitrogen molecule in Rydberg state: analysis of the $c^1\Pi_u - a''^1\Sigma_g^+$, v = 1-0 band.** Kawamoto, Yasunori; Fujitake, Masaharu; Ohashi, Nobukimi (Dep. of Physics, Faculty of Science, Kanazawa University, Kanazawa, Japan 920-11). *J. Mol. Spectrosc.* **1997**, 185(2), 330-335 (Eng), Academic Press. A new singlet-singlet absorption band between Rydberg states of the nitrogen mol. was studied by near-IR diode laser spectroscopy in the 1.3 μm region. An anal. was made for the band to establish line assignments and det. mol. parameters for both the lower and the upper vibronic states. As a result of the anal., this band was assigned to the $c^1\Pi_u - a''^1\Sigma_u^+$ (v = 4) state. The predissocn. in the $c^1\Pi_u$ (v = 1) state was also discussed relating with the line broadening obsd.

$c^1\Pi_u - a''^1\Sigma_g^+$

Ридберг.- сост-

[redacted]

C.A. 1998, 128, N7

N_2

1997

127: 363654h **High−resolution coherent Raman spectra of vibrationally excited $^{14}N_2$ and $^{15}N_2$.** Orlov, M. L.; Ogilvie, J. F.; Nibler, J. W. (Dep. Chem., Oregon State Univ., Corvallis, OR 97331−4003 USA). *J. Mol. Spectrosc.* 1997, 185(1), 128−141 (Eng), Academic. At an effective resoln. of 0.001 cm^{-1}, the authors measured coherent anti−Stokes Raman spectra of elec. discharged $^{14}N_2$ and $^{15}N_2$ in the electronic ground state $X^1\Sigma_g^+$, specifically Q branches of bands with $\Delta v = 1$ up to $v' = 8$ for $^{14}N_2$ and $\psi' = 7$ for $^{15}N_2$, and O and S ranches of the fundamental band of $^{15}N_2$. Account is taken of small wavenumber shifts due to pressure, a.c. Stark, and $|\chi|^2$ interference effects. Sep. fits of the Q−branch data of each isotopic variant, combined with selected data from the literature, yield term coeffs. Y_{kl} and U_{kl} or potential−energy coeffs. c_j that reproduce wavenumbers of measured spectral lines generally within 0.004 cm^{-1}. The value of the harmonic vibrational parameter π_e is 2358.5402(4) cm^{-1} for $^{14}N_2$ and 2278.7913(7) for cm^{-1} for $^{15}N_2$. Efforts to combine spectral data of both isotopic variants to distinguish adiabatic and non−adiabatic effects arising from incomplete sepn. of electronic and nuclear motion in N_2 were unsuccessful.

(CKP)

C.A. 1997, 127, № 26

N_2 1997

Peterson K.A; Wilson A.K.,
et al.,

r_e, ω_e,
теор.
расчет

Theor. Chem. Acc. 1997,
<u>97</u> (1-4), 287-289.

(см. B_2; III)

N_2, N_2^+, N_2^- 1997

Электр. сост., м.п., теор. расчет, сравнение с экспериментом

С.А. 1998, 128, N3

128: 28078s **The nitrogen system Feynman's way.** Sorensen, Thomas E.; England, Walter B. (Department of Chemistry and Laboratory for Surface Studies, University of Wisconsin–Milwaukee, Milwaukee, WI 53201 USA). *Mol. Phys.* **1997**, 92(3), 555–567 (Eng), Taylor & Francis. Feynman's way is applied to the X $^1\Sigma_g^+$, A $^3\Sigma_u^+$, B $^3\Pi_g$, W $^3\Delta_u$, B' $^3\Sigma_u^-$, a' $^1\Sigma_u^-$, a $^1\Pi_g^-$, w $^1\Delta_u$, A' $^5\Sigma_g^+$, G $^3\Delta_g$, C $^3\Pi_u$, C'' $^5\Pi_u$, C' $^3\Pi_u$, and H $^3\Phi_u$ states of N_2; the X $^2\Pi_g$ state of N_2^-; the X $^2\Sigma_g^+$, A $^2\Pi_u$, B $^2\Sigma_u^+$, D $^2\Pi_g$, and C $^2\Sigma_u^+$ states of N_2^+; and the X $^3\Pi_u$, a $^1\Sigma_g^+$, and e $^1\Sigma_u^+$ states of N_2^{+2}. Relative to expt., the av. errors in the spectroscopic consts. for the twenty-three states at 2nd-order (3rd-order) are: D_e 37(38) kJ mol^{-1}, R_e 5.2 (5.1) pm; ω_e 91(88) cm^{-1}; and T_e 49(49) kJ mol^{-1}.

N_2 1997

Wathelet, Valerie;
Champagne, Benoît; et al.;

теорет.
расчет
We

Chem. Phys. Lett. 1997,
<u>275</u> (5, 6), 506-512

(см. H_2; III)

N2 ? Деи 4. 1998

129: 294098g Calibration and benchmarking of model core potentials: applications to systems containing main-group elements. Decker, Stephen A.; Klobukowski, Mariusz; Sakai, Yoshiko; Miyoshi, Eisaku (Department of Chemistry, University of Alberta, Edmonton, AB Can. T6G 2G2). *THEOCHEM* 1998, 451(1-2), 215-226 (Eng), Elsevier Science B.V.. The recently developed model core potentials for the main-group elements were used in a systematic investigation of their reliability and predictive power in the studies of the prospective ligand building blocks for organometallic complexes. The mols. studied include: homonuclear diatomics (Group VB: N_2, P_2, As_2, Sb_2 and the halogens: F_2, Cl_2, Br_2, I_2); heteronuclear diatomics (CO analogs XY, where X = C, Si, Ge, Sn, and Y = O, S, Se, Te; and interhalogen compds.); triat. hydrides AH_2 (OH_2, SH_2, SeH_2, TeH_2), triat. oxides (CO_2 and SO_2), tetraat. hydrides AH_3 (NH_3, PH_3, AsH_3, SbH_3), tetraat. analogs of NF_3, and small hydrocarbons (C_2H_2, C_2H_4, CH_2). Mol. geometries were optimized using a modified Powell method of searches along conjugate directions and the results compared with exptl. data. Electron correlation effects were studied at the MP2 and CISD levels.

теор. расчет
стр-ры и стабиц

122

C. A. 1998, 129, N22

N_2

1998

$(X^1\Sigma_g^+, A^3\Sigma_u^+, B^3\Pi_g)$

теор.-расч

~~структ. и стаб~~

129: 321510u Analytical potential energy function for the electronic states $X\ ^1\Sigma_g^+$, $A\ ^3\Sigma_u^+$ and $B^3\Pi_g$ of N_2 molecule. Gao, Tao; Yang, Yongjian; Wang, Hongyan; Yi, Yougen; Jiang, Gang; Tan, Mingling; Zhu, Zhenghe (Inst. Atomic Molecular Phys., Chengdu Univ. Sci. Technol., Chengdu, Peop. Rep. China 610065). *Yuanzi Yu Fenzi Wuli Xuebao* 1998, 15(3), 329–334 (Ch), Yuanzi Yu Fenzi Wuli Xuebao Bianjibu. The reasonable dissocn. limits for the electronic states $X^1\Sigma_g^+$, $A^3\Sigma_u^+$ and $B^3\Pi_g$ of the N_2 mol. are derived based on the at. and mol. statics (AMRS). The energies, equil. geometries and harmonic frequencies of these three electronic states have been calcd. and compared using the methods of UHF, CID, UCISD and QCISD with the basis set 6−311G*. The whole potential curves for these three electronic states are further calcd. using the QCISD/6−311G* method, and then are least-square fitted to the Murrell−Sorbie function, which are in good agreement with those from spectroscopy data. It is believed that the Murrell−Sorbie function form is suitable not only for the ground states, but low-lying excited states as well.

C. A. 1998, 129, N 24

N_2

1998

потенц. ф-ция основного состояния

129: 140960v **Accurately solving the electronic Schrodinger equation of atoms and molecules using explicitly correlated $(r_{12}-)$ MR–CI: the ground state potential energy curve of N_2. [Erratum to document cited in CA128:313161].** Gdanitz, Robert J. (Fachbereich Physik der Gesamthochschule Kassel, D–34109 Kassel, Germany). *Chem. Phys. Lett.* **1998**, 288(2,3,4), 590–592 (Eng), Elsevier Science B.V.. Tables 1–3 contained typesetting errors although the numerical data were correct; the cor. tables are given.

CA·1998, 129, N11

№2 1998

теорет-
расчет
структур.
парамет.,
ω, ν,
ΔHатом

Moscardo F, et al.,
J. Comput. Chem.
1998, <u>19</u> (16), 1899–1908

(см. He; <u>III</u>)

N_2

1998

128: 263493g High resolution laser spectroscopy beyond 18 eV: the B $^2\Sigma_u^+$ X $^1\Sigma_g^+$ photoelectronic transition of N_2. Palm, H.; Merkt, F. (ETH–Zurich, Laboratorium fur Physikalische Chemie, CH–8092 Zurich, Switz.). *Chem. Phys. Lett.* 1998, 284(5,6), 419–422 (Eng), Elsevier Science B.V.. Coherent, narrow–bandwidth laser radiation was generated beyond 18 eV. The radiation was used to record a rotationally resolved pulsed–field–ionization zero–kinetic–energy photoelectron spectrum of the B $^2\Sigma_u^+$ X $^1\Sigma_g^+$ transition of N_2. Anal. of the rotational structure indicates that the removal of one of the two $2\sigma_u^*$ inner–valence–shell electrons is accompanied by substantial changes in the core rotational angular momentum quantum no.: Rotational branches are obsd. with $\Delta N=N^+-N=\pm1$ and ±3, where N^+ and N represent the core rotational angular momentum of the ion and the neutral, resp. These branches can be explained by the ejection of a photoelectron with dominant $l = 0$ and $l = 2$ character.

$B^2\Sigma_u$ —

— $X^1\Sigma_g^+$

фотоэл. спектр

C.A. 1998, 128, N21

N_2 1998

Plemmons, D.H. et al.,

Appl. Opt. 1998, <u>37</u>(12),

(Фл. спектр) 2493 – 2498

(Call. NH, III)

N_2

1998

with available exptl. data.

Спектр

128: 328219u **The high-resolution vacuum ultraviolet emission spectrum of molecular nitrogen from 82.6 to 124.2 nm: level energies of 10 excited singlet electronic states.** Roncin, Jean-Yves; Subtil, Jean-Louis; Launay, Francoise (Laboratoire Traitement du Signail et Instrumentation, CNRS UMR 5516, 42023 Saint-Etienne, Fr.). *J. Mol. Spectrosc.* **1998**, 188(2), 128-137 (Eng), Academic Press. The high-resoln. emission spectrum of N_2 was photographed in the vacuum UV at 82.6-124.2 nm. The use of a low-pressure Penning-type elec. discharge source led to considerably reduced self-absorption at short wavelengths, making it possible to record $\leq$283 emission bands. All emission bands were rotationally analyzed, 215 novel, and are reported in a sep. publication. Energy values were deduced for the nonpredissociative or only slightly predissociative rovibronic levels in 10 singlet electronic excited states.

C.A. 1998; 128, N26

Теоретические расчета и их
и их коррект-
ции D_e, r_e, ω_e
(вандер-Ваальс
св. систем.
N_2, HF, HCl,
ArHF, HCO^-
$(HF)_2$

N_2

1998

130: 115345m The effect of basis set superposition error (BSSE) on the convergence of molecular properties calculated with the correlation consistent basis sets. Van Mourik, Tanja; Wilson, Angela K.; Peterson, Kirk A.; Woon, David E.; Dunning, Thom H., Jr. (Environmental Molecualr Sciences Laboratory, Pacific Northwest National Lab., Richland, WA 99352 USA). *Adv. Quantum Chem.* 1998, 31, 105–135 (Eng), Academic Press. In many cases, the convergence behavior of mol. properties computed with the correlation consistent basis sets (both std. and augmented sets) is significantly improved if basis set superposition error (BSSE) is taken into account. The effects are most pronounced for pure van der Waals systems like the helium or argon dimers. For these systems the uncorrected D_e, r_e, and ω_e behave very irregularly with increasing basis set size, with the convergence behavior being dramatically improved by use of the counterpoise procedure. Even

(+4)

C. A. 1999, 130, N9

for strongly bound diatomics like N_2, HF, and HCl, the counterpoise correction often significantly improves the convergence behavior of r_e and ω_e. Similar behavior is obsd. in the weakly bound mol. complexes, ArHF, HCO^-, and $(HF)_2$, as well as for the more strongly bound HCO mol. For HCO^-, because of the pronounced lengthening of the CO bond upon mol. formation, the deformation energy must also be taken into account. (c) 1998 Academic Press.

N_2

1998

129: 101294m **Ab initio full configuration interaction calculations of spectroscopic constants of N_2, CO, CO^+, BO, and BO^+ molecules.** Wulfov, A. L. (Institute of Chemistry, Kharkov State University, Ukraine). *J. Struct. Chem.* 1997 (Pub. 1998), 38(6), 982–984 (Eng), Consultants Bureau. Total energies, equil. distances, harmonic frequencies, and dissocn. energies were calcd. for N_2, CO, CO^+, BO, and BO^+ mols. with full allowance for electron correlation effects. Huzinaga–Dunning's std. double–zeta basis set was complemented with six–component d–functions.

М·П·,
ab initio
расчет

㊹

CA 1998,129,N8

1999

F: N2
P: 3

131:304646 Observation of the y1.PI.g- c'41.SIGMA.u+ and k1.PI.g- c'41.SIGMA.u+ systems of N2. De Lange, Arno; Ubachs, Wim Department of Physics and Astronomy, Vrije Universiteit Amsterdam 1081 HV, Neth. Chem. Phys. Lett., 310(5,6), 471-476 (English) 1999 The authors obsd. the .LAMBDA.-doublet of both parity components of the (1, 0) band of the y1.PI.g-c'41.SIGMA.u+ and k1.PI.g-c'41.SIGMA.u+ systems of N2 in an extreme UV (XUV) + IR double resonance expt. The (e) components as well as the (f) components are obsd. up to J = 21 in the ca of the y state and up to J = 17 in the case of the k state. Apart from mutual interaction between y1.PI.g and k1.PI.g, the (e) components underg addnl. perturbations giving rise to predissocn.

1999

om 40983

F: N2
P: 3 131:292669 High-Resolution Fourier
Transform Spectroscopy of 14N2: Analys the (1-0),
(2-1) Bands of the B3.PI.g-W3.DELTA.u System.
Faye, A.; Kou, Q Farrenq, R.; Guelachvili,
G. Laboratoire de Photophysique Moleculaire, CN
Orsay F-91405, Fr. J. Mol. Spectrosc.,
197(2), 147-157 (English) 1999 The extension
of high-resoln. observation of the electronic
emission spectrum of 14N2 toward the IR domain is
presented. To date, rotational of the widely
studied spectrum of the N2 mol. was done in a
spectral doma ranging from 2500 cm-1 to the UV.

The authors have recorded for the 1st the IR part of the 14N2 spectrum from 1250 to 2250 cm-1, using the Fourie transform spectrometer of Laboratoire de Photophysique Moleculaire (LPPM) unapodized resoln. of 0.0043 cm-1. A complete rotational anal. is perfor the (1 0), (2 1), (01), (1 2) bands of the B3.PI.g-W3.DELTA.u system, not included in any previous anal. Spectroscopic parameters for the v = 0, v = 2 levels of the B3.PI.g and the W3.DELTA.u states, consistent with thos previously reported but with improved accuracy, are obtained from the exp wavenumbers by a nonlinear least-squares procedure.

1999

F: N2
P: 3
131:206347 Coupling between the vibrational motion of core-excited and va ionized states of N2. Marquette, A.; Meyer, M.; Sirotti, F.; Fink, R. F. (LURE, Centre Universitaire Paris-Sud, Orsay F-91898, Fr.). J. Phys. B: Mol. Opt. Phys., 32(13), L325-L333 (English) 1999 Fluorescence emission of the N2+ (A 2.PI.u) and N2+ (B 2.SIGMA.u+) state was studied after resonant excitation of the N2 (1s-1-.pi.*) resonance wi monochromatized synchrotron radiation. The vibrational structure of the excited state and of the final ionic state was resolved in the

photoexcit and in the dispersed fluorescence spectra, resp. A detailed anal. of the spectra and a comparison with theor. results show a strong coupling betwe vibrational levels in the core-excited and the ionic state produced via autoionization. The N2+ (A 2.PI.u) potential curve is almost parallel to core-excited state which causes mainly (.DELTA.v = 0) transitions in the autoionization process. For the N2+ (B 2.SIGMA.u+) state, the prodn. via .pi.* resonance leads to the population of higher vibrational states whic only very weakly populated by direct ionization. The calcns. reproduce t obsd. structures and underline the complementary character of fluorescenc photoelectron spectroscopy.

1999

F: N2
P: 3
131:108412 Deformationally self-consistent treatment of high-resolution coherent Raman spectra of 14N2 and 15N2 in the X1.SIGMA.g+ electronic ground state. Molski, Marcin (Department of Theoretical Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Poznan PL 60-780, Pol.) J. Raman Spectrosc., 30(6), 449-452 (English) 1999 The coherent Raman spectra of elec. discharged 14N2 and 15N2 were analyze using the deformationally self-consistent procedure for the treatment of spectral data. By making use of 8 independent unconstrained parameters, 356 measured

C. A. 1999, 131

spectral lines were reproduced with .sigma. = 0.0023 cm-1, .sigma. = 1.96 and F = 8.74 .times. 1013. From a marginally evaluated value of the parameter t0N, related to nonadiabatic rotational effects, t authors predicted a rough value of the rotational g-factor for 15N2 g0 = 0.37(21), near the known exptl. value g0 = -0.2593(5). Fit with the constrained t0N yielded .sigma. = 0.0023 cm-1, .sigma. = 1.96, F = 1.00 .times. 1014, and the set of 7 well evaluated parameters representing the Born-Oppenheimer potential energy function and nonadiabatic vibrational effects.

1999

F: N2
P: 3
132:83921 Near-threshold excitation of the E3.SIGMA.g+ state of N2 by ele impact.

Poparic, G.; Vicic, M.; Belic, D. S.

Studentski trg 16, Faculty of Physics, University of Belgrade Belgrade 11001, Yugoslavia

Phys. Rev. A: At., Mol., Opt. Phys., 60(6), 4542-4545 (English) 1999 Relative differential cross sections, at 0.degree., for electron-impact excitation of the E3.SIGMA.g+ state of the N mol. were measured in the ne threshold energy region. A high-resoln. crossed-beam double trochoidal e spectrometer is used and the cross section is measured directly, by inelastically scattered

C. A. 2000, 132

electrons detection. Measurements are placed on abs. scale by simultaneous measurement of this process and vibrational excitation of the v = 8 level of the ground state of N2, via the 2.PI.g resonance. Integral cross sections are obtained by using relative angula distributions from previous measurements, for energies of 11.94 and 12.14 Obtained results are compared with other available data. □

F: N2
P: 3

1999

132:83921 Near-threshold excitation of the E3.SIGMA.g+ state of N2 by electron impact. Poparic, G.; Vicic, M.; Belic, D. S. Studentski trg 16, Faculty of Physics, University of Belgrade Belgrade 11001, Yugoslavia Phys. Rev. A: At., Mol., Opt. Phys., 60(6), 4542-4545 (English) 1999 Relative differential cross sections, at 0.degree., for electron- impact excitation of the E3.SIGMA.g+ state of the N mol. were measured in the near-threshold energy region. A high-resoln. crossed-beam double trochoidal electron spectrometer is used and the cross section is measured directly, by inelastically scattered electrons detection. Measurements are placed on the abs. scale by simultaneous measurement

C-A. 2000, 132

of this process and vibrational excitation of the v = 8 level of the ground state of N2, via the 2.PI.g resonance. Integral cross sections are obtained by using relative angular distributions from previous measurements, for energies of 11.94 and 12.14 eV. Obtained results are compared with other available data.

1999

F: N2
P: 3
131:220545 Excitation of N2(B3.PI.g) in the nitrogen short-lived afterglo Supiot, P.; Blois, D.; De Benedictis, S.; Dilecce, G.; Barj, M.; Chapput A.; Dessaux, O.; Goudmand, P. Laboratoire de Genie des Procedes d'Interac Fluides Reactifs-Materiaux Fr. J. Phys. D: Appl. Phys., 32(15), 1887-1893 (English) 1999

The excitation of the N2(B3.PI.g) state in microwave discharges ignited flowing N and in their short-lived afterglow was studied. Simultaneous measurements in the post-discharge on this species and the N2+(B2.SIGMA.u through emissions, and also on the electronic ground state of N2 by spont Raman scattering, provide information of their vibrational distribution function. A spatial study was carried out, showing a quite slow evolutio the vibrational populations along the short-lived afterglow, and in parti the 1st proof of a steady vibrational distribution of N2(X1.SIGMA.g+) fro beginning to the bulk of this ionized region. The N2(B3.PI.g) vibrationa distribution is analyzed by a steady-state kinetic model taking into acco the B state excitation processes, i.e. electron collisions and reactions mol. excited states, and quenching. The reaction between the vibrational excited N2(X1.SIGMA.g+) and N2(A3.SIGMA.u+) is the pre-eminent excitation mechanism in the short-lived afterglow.

N_2

2000

ab initio
расчет, м.п.,
см. пост.

133: 169727t **Ab initio computation of forces and molecular spectroscopic constants using plane waves based auxiliary field Monte Carlo with application to N_2.** Baer, Roi (Department of Physical Chemistry and the Lise Meitner Minerva–Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel). *J. Chem. Phys.* 2000, 113(2), 473–476 (Eng), American Institute of Physics. Correlated sampling within the shifted contour auxiliary field Monte Carlo method, implemented using plane waves and pseudopotentials, allows computation of electronic forces on nuclei, potential energy differences, geometric and vibrotational spectroscopic consts. This is exemplified on the N_2 mol., where it is possible to accurately compute forces, dissocn. energies, bond length parameters, and harmonic frequencies.

C-A, 2000, 133, N12

F: N2
P: 3

2000

133:367340 Rotational coherent anti-Stokes Raman spectroscopy (CARS) in nitrogen at high pressures (0.1-44 MPa): experimental and modelling resul Bood, Joakim; Bengtsson, Per-Erik; Dreier, Thomas Department of Combustion Physics, Lund Institute of Technology Lund, Swed. J. Raman Spectrosc., 31(8/9), 703-710 (English) 2000 Pure rotational coherent anti-Stokes Raman scattering (CARS) was studied for pressures .ltoreq.44 MPa in N gas at room temp. An at. filter consis a heated cell with Na vapor was applied for suppression of stray light originating from the narrowband CARS pump laser beam. With increasing pr the rotational CARS spectrum is smoothed gradually, and at .gtorsim.10 MP spectral lines are no longer resolvable. Exptl. data were compared using linewidths calcd. with

3 different models: the energy cor. sudden scaling (ECS), the modified exponential gap model (MEG), and a semi-classical ab model. All 3 models resulted in bad spectral fits when a linear scaling pressure was employed. By using addnl. scale factors for the Raman linew the quality of the spectral fits and also the temp. accuracy were signifi improved. The resulting scale factors indicate a nonlinear pressure depe of the linewidths, and visualize a narrowing of the spectral envelope at highest pressure, i.e. 44 MPa. The results indicate shortcomings in the isolated line models and emphasize the need for new exptl. data on pure rotational Raman linewidths at high d.

2000

F: N2
P: 3
132:99783 Manifestation of Many-Electron Correlations in Photoionization of the K Shell of N2. Cherepkov, N. A.; Semenov, S. K.; Hikosaka, Y.; Ito, K.; Motoki, S.; Yagishita, A. State University of Aerospace Instrumentation St. Petersburg 190000, Russia Phys. Rev. Lett., 84(2), 250-253 (English) 2000 It is demonstrated theor. in the RPA that due to the intershell many-electron correlations the .sigma.* shape resonance in the photoionization of K shells of

C.A. 2000, 132

the N2 mol. appears not only in the 1.sigma.g .epsilon..sigma.u channel as it was believed earlier from single particle calcns., but in both 1.sigma.g .epsilon..sigma.u and 1.sigma.u .epsilon..sigma.g channels. As a confirmation of this phenomenon the exptl. angular distributions of photoelectrons ejected from fixed-in-space N2 mols. can be reproduced theor. only after taking into account many-electron correlations.

F: N2
P: 3

2000

132:300811 Dissociative single and double photoionization with excitation between 37 and 69 eV in N2. Ehresmann, Arno; Machida, Shuntaro; Kitajima, Masashi; Ukai, Masatoshi; Kameta, Kosei; Kouchi, Noriyuki; Hatano, Yoshihiko; Shigemasa, Eiji; Hayaishi, Tatsuji Department of Physics, University of Kaiserslautern Kaiserslautern D-67653, Germany J. Phys. B: At., Mol. Opt. Phys., 33(3), 473-490 (English) 2000, [illegible]

Dissociative single and double photoionization of N2 as a function of the exciting photon energy has been investigated using monochromatized synchrotron radiation in the energy range between 37 and 69 eV by dispersed vacuum-UV fluorescence spectroscopy (80 nm .ltoreq. .lambda.n .ltoreq. 200 nm). Relative partial emission cross

C. A. 2000

sections for NI and NII fluorescence have been recorded as a function of the exciting-photon energy. There is strong evidence that the precursors of dissociative single ionization with one of the fragments being excited are the N2+2.sigma.g-12.SIGMA.g+ state with its closely lying correlation states only. An approx. linear excess energy dependence of the cross sections for the mol. double photoionization into the N22+ D 1.SIGMA.u+ state has been obsd. in the excitation spectrum of D 1.SIGMA.u+ .fwdarw. X .SIGMA.g+ fluorescence in N22+ close to its threshold. Evidence for dissociative double photoionization with excitation has been found.

F: N2
P: 3

133:313945 The basis set convergence of the Hartree-Fock energy for H3+, Li2 and N2. Jensen, Frank Department of Chemistry, SDU, Odense University Odense M 5230, Den. Theor. Chem. Acc., 104(6), 484-490 (English) 2000. By using completely optimized basis functions it is shown that the convergence of the Hartree-Fock energy for the H3+, Li2 and N2 mols. is significantly better described by exponential behavior than by inverse power dependence. This is the case both with respect to the no. of basis functions of a given type and with respect to the highest angular momentum function included. The Hartree-Fock limit for H3+ is estd. to be -1.300372125 hartree.

N_2

m. 40212

2000

Энергии атомизации, расчет

Keld L. Bak, Poul Jørgensen et al.,

Chem. Phys. Lett, 2000, 317, 116 – 122

2000

F: N2
P: 3
133:313918 Renormalized CCSD(T) and CCSD(TQ) approaches: Dissociation of the N2 triple bond.

Kowalski, Karol; Piecuch, Piotr

Department of Chemistry, Michigan State University East Lansing, MI 48824, USA J. Chem. Phys., 113(14), 5644-5652 (English) 2000.

The recently proposed renormalized and completely renormalized CCSD(T) and CCSD(TQ) methods, which can be viewed as generalizations of the noniterative perturbative CCSD(T) and CCSD(TQf) schemes and which result from the more general method of moments of coupled-cluster equations, are applied to the dissocn. of the ground-state N2 mol. It is shown that the renormalized and completely renormalized CCSD(T) and CCSD(TQ) methods provide significantly better results for large N-N sepns. than their unrenormalized CCSD(T) and CCSD(TQf) counterparts.

F: N2
P: 3

2000

132:257612 Partial electron yield spectrum of N2: doubly excited states at the K-shell threshold.

Neeb, M.; Kivimaki, A.; Kempgens, B.; Koppe, H. M.; Maier, K.; Bradshaw, A. M.; Kosugi, N. Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin D-14195, Germany Chem. Phys. Lett., 320(3,4), 217-221 (English) 2000 [illegible] The partial electron yield spectrum of N2 was measured at a kinetic energy corresponding to the Auger decay of doubly excited core-hole states. The spectrum reveals previously unresolved double excitations just below and above the K- shell ionization threshold. Their excitation energies and dissociative nature agree with calcd. potential energy curves of the doubly excited states. [illegible]

C. A. 2000

2000

F: N2

P: 3

132:257441 Predissociation in b1.PI.u,v (v = 1, 4, 5, 6) levels of N2. Ubachs, W.; Velchev, I.; de Lange, A. Department of Physics and Astronomy, Vrije Universiteit Amsterdam 1081 HV, Neth. J. Chem. Phys., 112(13), 5711-5716 (English) 2000 [illegible]

C.A. 2000

[illegible]. In a high-resoln. laser spectroscopic study, using a tunable Fourier-transform limited light source in the extreme UV, the b1.PI.u excited valence state of mol. nitrogen is reinvestigated for vibrational levels v = 1, 4, 5, and 6. From line broadening of individual rotational levels excited state lifetimes were detd.: .tau.(v=1) = 1.1.+-.0.3 ns, .tau.(v=4) = 18.+- .1 ps, .tau.(v=5) = 205.+-.25 ps, and .tau.(v=6) = 350.+-.75 ps. Addnl., the lifetime of the o31.PI.u, v = 0 Rydberg state was detd.: .tau. = 240.+-.50 ps. For the b1.PI.u v = 1 state, improved rotational consts. were detd.

N_2

2001

135: 97682r **Core excitation and autoionising transitions from $^{1,3}\Pi_u$ states of N_2, by near threshold electron impact.** Almeida, D. P.; Dawber, G.; Michelin, S. E.; King, G. C. (Departamento de Fisica, Universidade Federal de Santa Catarina, Ex. de Massa por Colisae Electronica, 88040−900 Florianopolis, Brazil). *Chem. Phys.* **2001**, 269(1−3), 159−165 (Eng), Elsevier Science B.V. The inner−shell excited states, $(1s)^{-1}(2p\pi_u)^{1,3}\Pi$, of N_2 were obsd. by electron−impact excitation, as a function of electron incident energy via their decay, by electronic ejection, to an ionic state of the mol. The relative cross−sections for the formation of the $N_2^+(X\ ^2\Sigma_g)$ final ionic state, via the decay of these triplet and singlet inner−shell excited states, are compared with predictions of a theor. model based on the distorted−wave approxn. Results of the distorted−wave calcns. for the integral cross−sections for the transitions leading to the triplet and the singlet excited states are also presented.

(спектр)

C. A. 2001, 135, N7.

N_2

2001

потенц. кривые

135: 294209t A general coupled cluster study of the N_2 molecule. Krogh, J. W.; Olsen, J. (Department of Chemistry, University of Aarhus, Aarhus, DK–8000 Den.). *Chem. Phys. Lett.* **2001**, 344(5,6), 578–586 (Eng), Elsevier Science B.V. The equil. distance, harmonic frequency and potential curve of the nitrogen mol. are investigated using the cc–

C.A. 2001, <u>135</u>, N20

pVDZ basis and various single− and multi−ref. coupled cluster (CC) methods. Including single and double excitations from all determinants of the smallest active space that ensures correct dissocn., the CC method gives deviations from full CI (FCI) of 0.0001 A for the equil. distance, 1 cm^{-1} for the frequency, and a non−parallelity error (NPE) of 0.0006 E_h for the potential curve. Restricting the single and double excitations from the active space to those that are at most quadruple excited compared to the Hartree−Fock determinant, produces results that are very close to those obtained including all excitations up to quadruple excitations.

F: N2
P: 3

2001

135:37388 **A systematic theoretical investigation of the valence excited states of the diatomic molecules B2, C2, N2 and O2.** Muller, Thomas; Dallos, Michal; Lischka, Hans; Dubrovay, Zsofia; Szalay, Peter G. Institute for Theoretical Chemistry and Structural Biology, University of Vienna, Vienna, Austria. Theor. Chem. Acc. (2001), 105(3), 227-243. in English.

A quant. survey on the performance of multireference (MR), CI with all singles and doubles (CISD), MRCISD with the Davidson correction and MR-av. quadratic coupled cluster (AQCC) methods for a wide range of excited states of the diat. mols. B2, C2, N2 and O2 is presented. The spectroscopic consts. re, ωe, Te and De for a total of 60 states have been evaluated and critically compared with available exptl. data. Basis set extrapolations and size-extensivity corrections are essential for highly accurate results: MR-AQCC mean-errors of 0.001

A, 10 cm-1, 300 cm-1 and 300 cm-1 have been obtained for re, ωe, Te and De, resp. Owing to the very systematic behavior of the results depending on the basis set and the choice of method, shortcomings of the calcns., such as Rydberg state coupling or insufficient configuration spaces, can be identified independently of exptl. data. On the other hand, significant discrepancies with expt. for states which indicate no shortcomings whatsoever in the theor. treatment suggest the re-evaluation of exptl. results. The broad variety of states included in our survey and the uniform quality of the results indicate that the obsd. systematics is a general feature of the methods and, hence, is mol.-independent.

N_2 Noga, Josef; et al., 2001

Датонц., теор. расчет J. Chem. Phys., 2001, <u>115</u>(5), 2022-32

[см. CH_2; <u>III</u>]