C_3 1989

111: 163213w Observation of stimulated emission pumping spectra of jet-cooled thiocyanogen (NCS) and carbon triatomic molecule. Northrup, F. J.; Sears, Trevor J. (Chem. Dep., Brookhaven Natl. Lab., Upton, NY 11973 USA). *Chem. Phys. Lett.* 1989, 159(5-6), 421-5 (Eng). The observation of stimulated emission pumping (SEP) spectra of free-jet-cooled NCS and C_3 is reported. These species were generated by UV laser photolysis of a suitable precursor mol. in a large excess of inert gas in the throat of a supersonic free jet expansion. Individual rotational lines in the cold laser-induced fluorescence excitation spectrum were pumped and stimulated emission induced using two dye lasers pumped by a single excimer laser. The technique should be of general use in measuring vibronic level spacings in the ground electronic state of small free radicals.

(спектр) ☒

(Н) NCS

C.A. 1989, 111, N 18

CCC^{4-} Оп 32059 1989

11 Д78. Неэмпирическое исследование тенденций связывания в 22-электронных системах типа A=B=A. Доказательство для иона $O{=}O{=}O^{2+}$. Ab initio study of bonding trends among the 22-electron A=B=A systems: evidence for $O{=}O{=}O^{2+}$ / Pyykkö Pekka // Chem. Phys. Lett.— 1989.— 156, № 4.— С. 337—340.— Англ.

В рамках метода ССП с использованием базиса АО 6-31 ГФ* рассчитаны равновесные межъядерные расстояния *R* и частоты колебаний ν_i ($i=1, 2, 3$) 22-электронных систем типа A=B=A в основном состоянии. Отмечено, что результаты расчетов согласуются с эксперим. данными для анионов в кристаллах. Проанализированы тенденции изменения параметров *R* и ν_i в сериях молекул: CCC^{4-}, NBN^{3-}—NFN^{+}, $OBeO^{2-}$—OOO^{2+} и FBeF—FNF^{3+}. Показано, что эти величины систематически зависят от заряда ядра центрального атома в каждой серии. Высказано предложение о возможности существования систем OOO^{2+} и FNF^{3+}

М.Л.

☒

⑥

ф. 1989, N 11

в газовой фазе. Потенциал симметричной моды молекулы OOO^{2+} рассчитан методами КВ с учетом одно- и двухкратных возбуждений и теории возмущений Меллера — Плессета (ТВМП) 2-, 3- и 4-го порядков. Результаты этих расчетов, за исключением ТВМП 4-го порядка, подтверждают существование связного состояния у OOO^{2+}. Библ. 26. А. Ю. Ермилов

CCC^{4-}

(От 32059)

1989

111: 84425p Ab initio study of bonding trends among the 22-electron A:B:A systems: evidence for ozone dication ($O{:}O{:}O^{2+}$). Pyykko, Pekka (Dep. Chem., Univ. Helsinki, SF-00100 Helsinki, Finland). *Chem. Phys. Lett.* 1989, 156(4), 337–40 (Eng). Hartree–Fock/6-31G* calcns. of bond lengths and vibrational frequencies are reported for the isoelectronic species CCC^{4-}, NBN^{3-} to NFN^{+}, $OBeO^{2-}$ to OOO^{2+} and FBeFto FNF^{3+}. Systematic trends are found as function of the central nuclear charge. The calcd. R_e and ω_e at this level agree with exptl. values for anions in crystals. The new gas-phase species OOO^{2+} and FNF^{3+} are predicted. Correlated calcns. (MP2–MP4, CISD) are reported for $O{=}O{=}O^{2+}$.

ν_i, r_e, теор-расчет

(76) ☒

C.A. 1989, 111, N10

C_3

От 34276

1989

24 Б4678. Спектроскопия лазеро-индуцированной флуоресценции [кластеров] C_3, охлажденных в [газовой] струе. Laser-induced-fluorescence spectroscopy of jet-cooled C_3 / Rohlfing Eric A. // J. Chem. Phys.— 1989.— **91**, № 8.— С. 4531—4542.— Англ.

Зарегистрированы спектры ФЛ и спектры лазеро-индуцир. ФЛ кластеров C_3, полученных методом лазерного испарения графитовой мишени в импульсную сверхзвуковую газ. струю He, расширяющегося в вакуум. Наряду с хорошо известной кометной системой спектральных полос $C_3(\tilde{A}^1\Pi_u-\tilde{X}^1\Sigma_g^+)$ зарегистрирована система полос в УФ-области перехода ${}^1\Pi_g$ и (или) ${}^1\Delta_u-\tilde{X}^1\Sigma_g^+$. Спектры ФЛ новой системы содержат очень большое число интенсивных полос, к-рые позволяют зондировать переходы на колебат. уровни основного электронного состояния $C_3(\tilde{X}^1\Sigma_g^+)$ с энергиями до 17 000 см$^{-1}$. Измерены 144 колебат. терма этого со-

спектр.

М.П.

Х.1990, №24

стояния в областях колебат. квантовых чисел: $v_1=0$—8, $v_2=0$—37, $v_3=0$—4. Наблюдаемая структура уровней демонстрирует высокую ангармоничность потенциальной ПВ C_3 и необычную внутр. динамику процессов на этой ПВ. В частности, имеются заметные барьеры переходов в линейные структуры с уровней $v_3=2$ и $v_3=4$. Наблюдается также повышение молек. жесткости при возбуждении симм. вал. колебаний. Библ. 46. В. Е. Скурат

C_3 Ом 34276 1989

111: 243181c Laser-induced-fluorescence spectroscopy of jet-cooled carbon triatomic molecule. Rohlfing, Eric A. (Combust. Res. Facil., Sandia Natl. Lab., Livermore, CA 94551 USA). *J. Chem. Phys.* 1989, 91(9), 4531–42 (Eng). A spectroscopic study is presented of jet-cooled C_3 in which laser-induced-fluorescence (LIF) excitation spectra and dispersed-fluorescence (DF) spectra are taken for a new vibronically induced band system ($^1\Pi_g$ and/or $^1\Delta_u$) – $\tilde{X}\,^1\Sigma_g^+$ in the UV. In addn., DF spectra are taken for the well-known cometary band system, $\tilde{A}\,^1\Pi_u$ – $\tilde{X}\,^1\Sigma_g^+$. The DF spectra of the new system are very rich and display strong fluorescence bands in stretch-bend progressions that reach as high as 17,000 cm^{-1} in the $^1\Sigma_g^+$ ground state. The data from the DF spectra of both systems is used to assign vibrational term energies to 144 ground-state levels that cover the range: $0 \le v_1 \le 3$, $0 \le v_2 \le 37$, and $0 \le v_3 \le 4$. The obsd. level structure clearly demonstrates the highly anharmonic nature of the potential energy surface of C_3 and the unusual internal dynamics that occurs upon it. These include pronounced barriers to linearity in the $v_3 = 2$ and $v_3 = 4$ states and an increase in mol. rigidity as the sym. stretch is excited.

$^1\Pi_g(^1\Delta_u) - X^1\Sigma_g^+$

$\tilde{A}\ ^1\Pi_u - X^1\Sigma_g^+$

М·Л·

C.A. 1989, <u>111</u>, N 26

C_3

1989

24 Б1423. Спектроскопия вынужденной лазерной флуоресценции охлажденных в сверхзвуковой струе молекул C_3. Stimulated emission pumping spectroscopy of jet-cooled C_3 / Rohlfing E. A., Goldsmith J. E. M. // J. Chem. Phys.— 1989.— **90**, № 11.— С. 6804—6805.— Англ.

Методом стимулированной Фл с лазерной накачкой исследовано основное $\tilde{X}^1\Sigma_g^+$ состояние $^{12}C_3$. Зарегистрировано 13 электронно-колебательно-вращат. полос $\Sigma_u^+—\Sigma_g^+$ типа с колебат. числами $0 \leqslant V_1 < 8$, $0 < V_2 \leqslant 37$ и $0 < V_3 \leqslant 4$. Из анализа разрешенных по вращат. структуре спектров Фл, лежащих в обл. 33 588 см$^{-1}$, определены колебат. термы G_v, вращат. постоянные B_v и константы удвоения l-типа q_v для состояний с $0 < V_1 < 6$, $1 \leqslant V_2 < 13$ и $V_3 = 3$. Измеренные величины q_v лежат в диапазоне от 0,0055 до 0,0112 см$^{-1}$, что указывает на сильное колебательно-вращат. взаимодействие в $\tilde{X}^1\Sigma_g^+$ состоянии, вызванное большой гибкостью молекулы C_3 (ω_2 ~62 см$^{-1}$).

А. В. Столяров

М.П.

Х.1989, N24

C_3

1989

111: 30666z Stimulated emission pumping spectroscopy of jet-cooled triatomic carbon. Rohlfing, Eric A.; Goldsmith, J. E. M. (Combust. Res. Facil., Sandia Natl. Lab., Livermore, CA 94551 USA). *J. Chem. Phys.* 1989, 90(11), 6804–5 (Eng). Dispersed fluorescence spectra were obtained for excitation of 1,3 vibronic bands of jet-cooled C_3; the assigned vibrational lines span the range $0 \leq v_1 \leq 8$, $0 \leq v_2 \leq 37$, and $0 \leq v_3 \leq 4$. The dispersed fluorescence from, and the stimulated emission pumping through, the $\Sigma_u^+ - \Sigma_g^+$ vibronic band at 33,558 cm^{-1} are reported.

(спектр)

C.A.1989, 111, N4

C_3^+

1989

3 Д46. Альтернативная интерпретация данных по кулоновскому взрыву C_3^+. An alternative interpretation of Coulomb explosion data on C_3^+ / Vager Z., Kanter E. P. // J. Phys. Chem.— 1989.— 93, № 22.— С. 7745—7746.— Англ. Место хранения ГПНТБ СССР

Известные данные (Faibis A. et al. // Phys. Chem.— 1987.— С. 6445) по кулоновскому взрыву C_3^+ интерпретируются авторами исходя из допущения об отсутствии вклада колебательного возбуждения в энергетич. баланс процесса. Показано, что при учете вероятного колебательного возбуждения исходных компонент невозможен однозначный вывод в пользу линейной или кольцевой структуры C_3^+. Уточнение интерпретации может быть получено лишь с помощью дополнительных эксперим. данных.

Г. А. Вомпе

М.Л.

ф. 1990, №3

C_3^+
C_3^-

оп. 34168

1989

Weltner W., Jr., Van Zee R. J.,
Chem. Rev. 1989, 89, N 8,
1713 - 1747.
Carbon Molecules, Ions,
and Clusters.

C_3 1989

Weltner W., Jr., Van Zee R.J.,
Chem. Rev. 1989, 89, N 8,
1713–1747.
Carbon Molecules,
Ions, and Clusters.

Колебат.
и вращат.
св-ва в
основном
состоянии
м.п.

C_3

1990

Электронные состояния, расчет

115: 290078p **Electronic spectra of the carbon (trimer) calculated by RINDO/S method.** Kumar, A.; Singh, S. N.; Singh, S. Nath (Dep. Phys., Magadh Univ., Gaya, India). *Acta Cienc. Indica, Phys.* 1990, 16P(1), 1-6 (Eng). Some transitions in the UV spectra of C_3 were calcd. using RINDO/S methods. Transition energies and some oscillator strengths and Rydberg characters were calcd. The first Rydberg series is predicted to start at 8.42 ev. Comparisons were made with previous expts.

C. A. 1991, 115, N 26.

C_3^+

ОМ 34294

1990

23 Б1063. C_3^+-**катион с изогнутой структурой.** C_3^+ is bent / Grev Roger S., Alberts Ian L., Schaefer III Henry F. // J. Phys. Chem.— 1990.— **94,** № 9.— С. 3379—3381.— Англ.

Методом конфигурац. взаимодействия (КВ) с учетом 1- и 2-кратных возбуждений и методом ССП в полном активном пространстве оптимизированы геометрии и рассчитаны колебат. частоты 4 состояний линейного и изогнутого катиона C_3^+. Использован трёхэкспонентный дважды поляризованный базис. Уточнение энергией проведено методом КВ с учетом 1-, 2-, 3- и 4-кратных возбуждений в двухэкспонентном поляризованном базисе. Найдено, что абс. минимум отвечает $^2B_2$-состоянию изогнутой (C^2_k) конфигурации с углом ССС, близким к 70°. Состояние $^2\Sigma_w^+$ линейной конфигурации является переходным состоянием (ПС), барьер линейности близок к 7 ккал/моль. Состояние $^2A_1$ имеет циклич. структуру и является ПС вырожденной перегруппировками $^2B_2$-состояния, при этом барьер псевдовращения невелик. $^2\Pi$-состояние отвечает довольно высоколежащему метастабильному минимуму.

В. Я. Беспалов

М.П.

Х. 1990, N 23.

C_3^+

1990

5 Д121. Исправления к статье: C_3^+ — нелинейный ион. Erratum: C_3^+ is bent / Grev Roger S., Alberts Ian L., Schaefer Henry F. (III) // J. Phys. Chem.— 1990.— 94, № 24.— С. 8744.— Англ.

См. // ibid.— 1990.— 94.— С. 3381

М.Л.

ф.1991, N5

C_3^+

1990

13 Б1048. [Молекулярный ион] C_3^+ **нелинейный. Исправление ошибки.** C_3^+ is bent: Errata / Grev Roger S., Alberts Ian L., Schaefer Henry F. (III) // J. Phys. Chem.— 1990.— 94, № 24.— С. 8744.— Англ.

Приведены исправленные результаты расчетов разности энергий состояний $^2\Sigma_u^+$ и $^2B_2$ молек. иона C_3^+ (см. // J. Phys. Chem.— 1990.— 94.— С. 3381).

А. В. Немухин

М.Л.

Х.1991, № 13

C_3^+

1990

23 Б1125. **О геометрической структуре катиона C_3^+. Неэмпирическое исследование.** On the geometrical structure of the C_3^+ cation — an ab initio study / Martin J. M. L., Francois J. P., Gijbels R. // J. Chem. Phys.— 1990.— 93, № 7.— С. 5037—5045.— Англ.

Методом связанных кластеров рассчитана потенциальная ПВ основного электронного состояния иона C_3^+. Использован базис сгруппир. гауссовых ф-ций 6-311 ГФ*. Оптимизированы геометрич. параметры шести структур, отвечающих стационарным точкам потенциальной ПВ. Определены гармонич. колебат. частоты и интенсивности переходов ИК- и КР-спектров. Низшую энергию имеет циклич. структура симметрии C_{2v} (состояние $^2B_2$) с равновесным межъядерным расстоянием 1,3242 А и валентным углом 73,06°. Линейная структура (состояние $^2\Sigma^+$) имеет энергию на 2 ккал/моль выше основного состояния. Отмечена низкая величина барьера изомеризации между вырожденными структурами. Предсказаны теплота образования (при 298 К) 194,9±2 ккал/моль и вертикальный и адиабатич. потенциалы ионизации 11,92±0,1 и 11,84±0,61 эВ соответственно.

А. А. Сафонов

Мл-

Х. 1991, N 23

C_3^+

1990

11 Д95. О геометрической структуре катиона C_3^+. Неэмпирический расчет. On the geometrical structure of the C_3^+ cation — an *ab initio* study / Martin J. M. L., François J. P., Gijbels R. // J. Chem. Phys.— 1990.— 93, № 7.— С. 5037—5045.— Англ.

Исследована поверхность потенц. энергии катиона C_3^+ с применением техники связанных кластеров и большой базисной системы. Данные чрезвычайно чувствительны к учету электронных корреляций. В наиболее точном приближении линейная структура (состояние $^2\Sigma^+$) лежит на 2 ккал/моль выше основного, нелинейного состояния. Низкий барьер для изомеризации приводит к большой гибкости иона. Для различных структур рассчитаны гармонич. частоты, а также гармонич. интенсивности для ИК-спектроскопии и спектроскопии комб. рас. Указаны интересные аналогии C_3^+ с B_3 и B_2N. Для C_3 рассчитаны теплота образования при 298,15 К 194,9±2 ккал/моль, вертикальный и адиабатич. потенциалы ионизации (11,92±0,1 эВ и 11,84±0,1 эВ).

Г. К.

М-П·

ф. 1991, N 11

C_3^+.

1990

114: 69415d On the geometrical structure of the carbon triatomic monopositive ion – an ab initio study. Martin, J. M. L.; Francois, J. P.; Gijbels, R. (Dep. SBM, Limburgs Univ. Cent., B–3610 Diepenbeck, Belg.). *J. Chem. Phys.* 1990, 93(7), 5037–45 (Eng). The potential energy surface of the C_3^+ cation was investigated using coupled cluster techniques and large basis sets. The results are particularly sensitive towards the level of electron correlation. Spin contamination even produces a "false stationary point" at the UHV/6-31G* level. C_3^+ has a cyclic $^2B_2$ ground state with predicted geometry r = 1.3242 Å, ϑ = 73.06° (MP2/6-311G*, empirically correlated bond distance). At the highest level of theory considered, the linear structure ($^2\Sigma_u^+$ state) lies about 2 kcal/mol above the ground state: this might imply quasilinearity. There is also a low barrier towards degenerate isomerization: at high temps., C_3^+ will be extremely floppy. Harmonic frequencies (UHF/6-31G*) as well as double-harmonic IR and Raman intensities are given for various structures of C_3^+. Interesting analogies of C_3^+ with B_3 and N_2N are pointed out. The heat of formation at 298.15 K and the vertical and adiabatic ionization potentials of C_3 are predicted as 194.9 ± 2 kcal/mo., 11.92 ± 0.1 eV, and 11.84 ± 0.1 eV, resp.

М.П.,
теор.

C.A. 1991, <u>114</u>, N8

C_3 ОМ 35 055 1990

Northrup E.J., Sears T.J.,

J. Opt. Soc. Amer. B 1990,
<u>7</u>, N 9, 1924-1934

Stimulated- emission
pumping spectroscopy

study of jet-cooled C_3:
pure bending levels and
bend-symmetric-stretch
combination levels of $\tilde{X}\,^1\Sigma_g^+$

C_3^-

1990

7 Д92. Теоретическое исследование C_3, C_3^- и C_3^+. Theoretical study of C_3, C_3^- and C_3^+ / Raghavachari Krishnan // Chem. Phys. Lett.— 1990.— 171, № 3.— С. 249—253.— Англ.

С использованием метода квадратичного конфигурац. взаимодействия при итеративном рассмотрении одно- и двукратных возбуждений и неитеративном пертурбативном рассмотрении тройных возбуждений определены геометрии и колебательные частоты молекулы C_3 и ионов C_3^- и C_3^+. Оптимизация геометрии проведена в приближении Хартри—Фока в базисе 6-31ГФ*. Включались эффекты диффузных и поляризационных ф-ций. В расчетах учитывались корреляц. эффекты только валентных электронов. Получены линейные геометрии для C_3 и C_3^- и изогнутая структура основного состояния (C_{2v}, $^2B_2$) для C_3^+ с углом связи ∼67°. Рассчитаны гермонические колебательные частоты. Определены значения адиабатич. потенциала ионизации и сродства к электрону для C_3, равные, соответственно, 11,7 и 2,0 эВ.

Н. В. В.

М. П.

⊕ ☒

ф. 1991, №7

C_3^+ 1990

Raghavachari Krishnan,

Chem. Phys. Lett. 1990, 171,

М.Л. N3, с. 249–253.

● (см. C_3; III)

C_3^- 1990

Raghavachari Krishnan,

Chem. Phys. Lett. 1990,

М.П. 171, N 3, с. 249-253.

(См. C_3; ~~М.П.~~ III)

C_3

1990

— **16 Б1064. Теоретическое исследование C_3, C_3^- и C_3^+.** Theoretical study of C_3, C_3^- and C_3^+ / Raghavachari Krishnan // Chem. Phys. Lett.— 1990.— 171, № 3.— С. 249—253.— Англ.

Квадратичным методом конфигурац. вз-вия с учетом одно- и двукратных возбуждений (по итерац. схеме), а также трехкратных возбуждений (без итераций по теории возмущений) с валентно-расщепленным базисом 6-31 ГФ* рассчитаны равновесные геометрич. конфигурации и гармонич. частоты колебаний системы C_3, C_3^- и C_3^+. Нек-рые расчеты относит. энергий выполнены с более полными базисами, что в частности, дало оценку адиабатич. сродства к электрону C_3 2,0 эВ, близкую к эксперим. величине (1,98±0,02). Подтверждено, что основным состояниям C_3 и C_3^- отвечают линейные конфигурации, а C_3^+ — изогнутая с углом 67°. Частоты колебаний C_3: 66, 1199 и 2063 см$^{-1}$, C_3^+: 744, 1194 и 1684 см$^{-1}$. Библ. 35.

А. В. Немухин

М.Л.

+2

Х.1991, N16

C_3^-, C_3^+

C_3

1990

113: 178642a Theoretical study of the carbon trimer, and the carbon triatomic mononegative and monopositive ions (C_3, C_3^- and C_3^+). Raghavachari, Krishnan (AT and T Bell Lab., Murray Hill, NJ 07974 USA). *Chem. Phys. Lett.* 1990, 171(3), 249-53 (Eng). The geometries and vibrational frequencies of C_3, C_3^-, and C_3^+ are detd. with the quadratic CI (QCISD(T)) technique using the polarized double-zeta (6-31G*) basis set. Effects of diffuse functions and multiple sets of polarization functions are included by means of single-point calcns. While C_3 and C_3^- have linear geometries, C_3^+ has a bent (C_{2v}, $^2B_2$) ground-state structure with an apex bond angle of ~67°. The adiabatic ionization potential and electron affinity of C_3 are detd. to be 11.7 and 2.0 eV.

геометрия,
ν_i, кв-мех.
расчет

(72) ☒ ● C_3^-, C_3^+

C.A. 1990, 113, N20

C_3^- 1990

Raghavachari Krishnan.

Chem. Phys. Lett. 1990, 171 (3), 249-253.

геометрия, ν_i, кв.-мех. расчёт.

(см. C_3; III)

C_3^+

1990

Raghavachari Krishnan.

Chem. Phys. Lett.
1990, 171, (3), 249-
253.

Геометрия,
Vi, кв-мех.
расчёт

● (см. C_3; III)

C_3

(Om 35054)

1990

113: 180617q **Stimulated-emission pumping spectroscopy of jet-cooled triatomic carbon: antisymmetric stretch-bend levels.** Rohlfing, Eric A.; Goldsmith, J. E. M. (Combust. Res. Facil., Sandia Natl. Lab., Livermore, CA 94551 USA). *J. Opt. Soc. Am. B: Opt. Phys.* 1990, 7(9), 1915-23 (Eng). A study is given of jet-cooled C_3 in which stimulated-emission pumping spectroscopy is used to probe rovibrational levels at energies up to 6930 cm^{-1} in the ground state. Stimulated-emission pumping spectra are reported for pump bands in the $A^1\Pi_u - X^1\Sigma_g^+$ system and for dump transitions that terminate in the bending progressions of states with 2 and 4 quanta of antisym. stretch. These spectra were used to det. the rovibrational term energies over the range $J = 2$ to $J = 12$ for the antisym. stretch-bend levels, 0v2 (v = 0 to v = 8) and 0v4 (v = 0 to v = 14). These data clearly illustrate that the effective bending potentials in the 002 and the 004 states have substantial barriers to linearity.

$A^1\Pi_u - \tilde{X}^1\Sigma_g$

C. A. 1990, 113, N 20

C_3

От 35489 1990

14 Б1371. Перестраиваемая далекая ИК-лазерная спектроскопия охлажденных в пучках углеродных кластеров. Деформационное колебание $\nu_2 C_3$. Tunable Far-IR laser spectroscopy of jet-cooled carbon clusters: The ν bending vibration of C_3 / Schmuttenmaer C. A., Cohen R. C., Pugliano N., Heath J. R., Cooksy A. L., Busarow K. L., Saykally R. J. // Science.— 1990.— **249**, № 4971.— С. 897—900.— Англ.

С высокой точностью на перестраиваемом лазерном спектрометре в далекой ИК-области измерены семь колебательно-вращат. переходов в полосе фундаментального деф. кол. $(0^11\ 0)\ (00^00)$ C_3. Молекулу C_3 получали лазерным испарением графитовой мишени с послед. сверхзвуковым расширением пучка. Получен след. набор молек. постоянных (в $см^{-1}$): $\nu_0 = 63{,}416529$; $B'' = 0{,}4305723$; $B' = 0{,}4424068$; $D'' = 0{,}1472 \cdot 10^{-5}$; $D' = 0{,}2361 \cdot 10^{-5}$; $H'' = 0{,}1333 \cdot 10^{-9}$; $H' = 0{,}267 \cdot 10^{-9}$, $q_e' = 0{,}0056939$, $q_D' = -0{,}0869 \cdot 10^{-5}$, $q_H = 0{,}027 \cdot 10^{-9}$.

Г. В. Чертихин

М. Л.

Х. 1991, N 14

C_3 1990

Szalay Viktor.

колебат. J. Chem. Phys.
уровни, 1990, 92(6), 3633–44.
расчет

(см. HCN/HNC; III)

C_3 1990

Weltner W., Jr.,
Van Zee R. J.
J. Mol. Struct. 1990,
222 (1-2), 201-7.

спектры
в матрицах,
обзор

(см. C_2; ш).

C_3

1991

114: 129622f **Electron affinities of small linear carbon clusters. Coupled cluster calculations with first-order correlation orbitals.** Adamowicz, Ludwik (Dep. Chem., Univ. Arizona, Tucson, AZ 85721 USA). *J. Chem. Phys.* 1991, 94(2), 1241–6 (Eng). Electron affinities of the C_3, C_4, C_5, and C_6 linear clusters are theor. detd. using an ab initio procedure which combines the first-order correlation orbital method and the coupled cluster method. The theor. values 1.58, 3.41, 2.43, and 3.69 e.V. for C_3, C_4, C_5, and C_6, resp., are systematically lower than the exptl. ests. of Smalley et al. (1983) (1.95, 3.70, 2.80, and 4.10 e.V.); however, the trends corresponding to the odd-even numbered chain alternation and to the increase of the size of the cluster are very similar.

Ae

(+3) ☒ C_4, C_5, C_6

C.A. 1991, <u>114</u>, N14

C_3

1991

2 Б1036. **Возбужденные электронные состояния C_3 в методе ССП ПАП.** Electronically excited states of C_3 in the CASSCF approach / Kalcher J., Janoschek R. // J. Mol. Struct. Theochem.— 1991.— 234.— С. 509—514. — Англ.

Многоконфигурационным методом ССП в полном активном пространстве (метод ССП ПАП) рассчитано 15 электронных состояний линейной структуры молекулы C_3 (симметрия $D_{\infty h}$). Использован базис сгруппированных гауссовых ф-ций $(7s3p1d)/[5s3p1d]$. Для нек-рых состояний расчеты проведены также методом конфигурац. взаимодействия с учетом однократных и двукратных возбуждений по отношению к нескольким исходным конфигурациям. Полученные энергии переходов сопоставлены с имеющимися эксперим. и расчетными данными. Описано несколько не наблюдавшихся ранее возбужденных валентных состояний C_3, включая два квинтетных состояния. А. А. Сафонов

М.П.

Х.1992, N2

C_3

1991

1Д169. Электронно-возбужденные состояния C_3 в приближении ПАП ССП. Electronically excited states of C_3 in the CASSCF approach / Kalcher J., Janoschek R. // J. Mol. Struct. Theochem.— 1991.— 234.— С. 509—514.— Англ.

Методами полного активного пространства (ПАП ССП) и конфигурац. взаимодействия (КВ) проведены расчеты основного и электронно-возбужденных состояний линейной молекулы C_3 симметрия $D_{\infty h}$. Представлены основные конфигурации, геометрии C=C и рассчитанные относит. энергии электронных состояний.

М·Л·

ф. 1992, N1

C_3 1991

Оп 36136

115: 37966p Theoretical vibrations of carbon chains C_3, C_4, C_5, C_6, C_7, C_8, and C_9. Kurtz, Joe; Adamowicz, Ludwik (Goddard Space Flight Cent., NASA, Greenbelt, MD 20771 USA). *Astrophys. J.* 1991, 370(2, Pt. 1), 784-90 (Eng). The MBPT(2) procedure with the 6-31 G* basis set was used to study nearly linear C chains. The theor. vibrational frequencies of the mols. C_3 through C_9 are presented and, for C_3 through C_6, compared to exptl. stretching frequencies and their $^{13}C/^{12}C$ isotopomers. Predictions for C_7, C_8, and C_9 stretching frequencies are calcd. by directly scaling the theor. frequencies with factors derived from the exptl.-to-theor. ratios known for the smaller mols.

ν_i, расчет

(tc) ☒

C.A.1991, 115, N4

C_3 1991

Moazzen-Ahmadi N.,
Flatt S.D. et al.,

D_3

Chem. Phys. Lett.,
1991, 186, N 2-3, 291-296

Diode laser ● spectroscopy

of the ν_3 band of $^{13}C_5$.

C_3

1991

7 Д91. Полужесткий деформационный анализ расширенного набора колебательно-вращательных уровней в состоянии $X^1\Sigma_g{}^+C_3$. A semirigid bender analysis of an extensive set of rotation-vibration levels in $X^1\Sigma_g{}^+C_3$ / Northrup F. J., Sears Trevor J. // J. Mol. Spectrosc. — 1991.— **145**, № 1.— С. 74—88.— Англ

Полужесткая деформационная модель использована для определения эффективных деформац. потенциалов для молекулы C_3 в различных низколежащих валентных колебательных состояниях по имеющимся экспериментальным спектроскопич. данным. Показано, что эффективный деформац. потенциал для основного колебательного валентного состояния $v_1=v_3=0$ обладает очень пологим минимумом в линейной конфигурации. При возбуждении симметричного валентного колебания минимум становится более резким, а при возбуждении антисимметричного валентного колебания для эффективного деформац. потенциала появляется барьер, отвечающий линейной конфигурации. Предложено качеств. объяснение данного эффекта, обусловленное зависимостью элементов G-матрицы для валентных колебаний от деформационной переменной. Е. А. Ж.

М.П.

ф. 1991, № 7

C_3

1991

114: 52093z **A semirigid bender analysis of an extensive set of rotation-vibration levels in $X^1\Sigma_g^+$ triatomic carbon.** Northrup, F. J.; Sears, Trevor J.; Kohlfing, Eric A. (Dep. Chem., Brookhaven Natl. Lab., Upton, NY 11973 USA). *J. Mol. Spectrosc.* 1991, 145(1), 74-88 (Eng). The semirigid bender model of P. R. Bunker and B. M. Landsberg (1977) was used to det. effective bending potentials for C_3 in many of the lower stretching vibrational states from recently published exptl. measurements on the ground state of this mol. No barrier to linearity is found in the effective bending potential for either the zero point (v_1 = v_3 = 0) or the equil. stretching states, however, the effective potentials show a very flat min. in both cases. The effective bending develops a much sharper min. as the sym. stretch (ν_1) is excited. By contrast, it develops a barrier at the linear configuration as the antisym. stretching vibration (ν_3) is excited. These observations are qual. rationalized by considering the bending angle dependence of the G-matrix elements for the stretching vibrations.

$X^1\Sigma_g^+$,
колеб. пост
расчет

C.A. 1991, <u>114</u>, N6

C_3

(Om 36065)

1991

114: 155190j A new triplet band system of the carbon trimer: the $b^3\Pi_g$–$a^3\Pi_u$ transition. Sasada, H.; Amano, T.; Jarman, C.; Bernath, P. F. (Herzberg Inst. Astrophys., Natl. Res. Counc., Ottawa, ON Can. K1A 0R6). *J. Chem. Phys.* 1991, 94(4), 2401–7 (Eng). A triplet band system of C_3 was obsd. for the first time in absorption with a distributed-feedback (DFB) diode laser spectrometer and in emission with a Fourier transform spectrometer at around 6500 cm-1. The band was assigned to the $b^3\Pi_g$–$a^3\Pi_u$ system, and the spectroscopic consts. in both the upper and lower states were detd. Near-IR DFB lasers are promising radiation sources for spectroscopy of unstable mols.

$b^3\Pi_g - a^3\Pi_u$

М·Л-

C·A·1991, 114, N16

1991

C_3^+

Э) **20 Б1099. Метод одинарных и двойных связанных кластеров с учетом тройных возбуждений СК 1+2(3) для открытых оболочек на волновых функциях ограниченного метода Хартри—Фока: применение к C_3^+.** The open-shell restricted Hartree—Fock singles and doubles coupled-cluster method including triple excitations CCSD(T): application to C_3^+ / Scuseria Gustavo E. // Chem. Phys. Lett.— 1991.— **176**, № 1.— С. 37—39.— Англ.

Предложен вариант метода связанных кластеров для систем с открытыми оболочками, в к-ром кластерные операторы сохраняют спиновую симметрию исходной волновой ф-ции, полученной ограниченным методом Хартри—Фока. Развитый метод с учетом одинарных и двойных кластерных операторов и включением тройных возбуждений по теории возмущений применен для расчета структуры иона C_3^+. Проведены расчеты энергий изогнутого и линейного изомеров в различных базисах атомных орбиталей и получено, что энергия первого на 6,8 ккал/моль ниже, чем второго. Обсуждено согласие результатов с данными пред. расчетов и влияние учета корреляц. эффектов при наличии хартри-фоковских решений с нарушением симметрии. А. А. Бучаченко

М.Л.

Х.1991, N 20

C_3 Om 36455 1991

Sowa Marianne B.,
Hintz Paul A. et al.

(D_0) J. Chem. Phys. 1991,
95(6), 4719-20.

(см. C_2; III)

C_3^+

1991

Sowa M.B., Hintz P., et al.,

J. Chem. Phys. 1991, 95, N6,

4719–4720.

Dissociation energies for carbon cluster ions (C_{2-15}^+): A

A system whare photodissociation is misleading.

C_3^+

1991

120: 38698t **An ab initio study of the carbon trimer cation using multireference methods.** Taylor, Peter R.; Martin, J. M. L.; Francois, J. P.; Gijbels, R. (Eloret Corp., Palo Alto, CA USA). *NASA Contract. Rep.* 1991, NASA-CR-189026, NAS1.26:189026, 19 pp. (Eng). Avail. NTIS. From *Sci. Tech. Aerosp. Rep.* 1992, 30(12), Abstr. No. N92-21401. The energy difference between the $2\sigma^+_u$ linear and $2B_2$ cyclic structures of the carbon trimer cation were studied using CASSSCF, MRCI, ACPF and QCISD(T) methods. The linear form is 5.2 kcal/mol above the cyclic one.

(теор. расчёт лин. и цикл. структуры)
нижнее эл. сост.

C. A. 1994, 120, N4

C_3^+

1991

2 Б1035. Неэмпирическое исследование катиона C_3^+ с использованием методов с несколькими исходными конфигурациями. Ab initio study of the C_3^+ cation using multireference methods / Taylor P. R., Martin J. M. L., Francois J. P., Gijbels R. // J. Phys. Chem. — 1991.— 95, № 17.— С. 6530—6534.— Англ.

Для расчета разности энергий линейной (состояние $^3\Sigma_u^+$) и циклич. (состояние $^2B_2$) структур иона C_3^+ использован ряд методов с несколькими исходными конфигурациями: многоконфигурац. метод ССП в полном активном пространстве, метод конфигурац. взаимодействия (КВ) с учетом однократных и двукратных воз-

М.П.

Х. 1992, N 2

буждений по отношению к нескольким исходным конфигурациям и усредненный метод функционала связанных электронных пар, а также квадратичный метод КВ с одноконфигурац. исходной волновой ф-цией. Использован базис сгруппированных гауссовых ф-ций (10s6p2d1f)/[5s3p2d1f]. Найдено, что глобальному минимуму энергии C_3^+ отвечает циклич. структура; линейная структура, лежащая на 5,2 ккал/моль выше по энергии, по-видимому, отвечает не переходному состоянию, а локальному минимуму. Отмечена высокая чувствительность энергии изомеризации C_3^+ к кач-ву волновой функции. А. А. Сафонов

C_3^+

1991

7 **1Д168. Неэмпирическое исследование катиона C_3^+ с использованием многоссылочных методов.** Ab initio study of the C_3^+ cation using multireference methods / Taylor P. R., Martin J. M. L., François, J. P., Gijbels R. // J. Phys. Chem.— 1991.— **95**, № 17.— С. 6530—6534.— Англ.

Исследована разность энергий линейной ($^2\Sigma_u^+$) и циклич. ($^2B_2$) структур катиона C_3^+ с использованием широких базисов [$5s3p2d1f$] и многоссылочных методов с учетом электронной корреляции, включая метод полного активного пространства ССП, метод НИК-КВ и метод усредненного функционала связанных пар, а также метод квадратичного конфигурац. взаимодействия. Лучшая оценка, включающая поправки на неполноту базиса, дает разность энергий между циклич. формой и вышележащей линейной формой: $5{,}2\ ^{+1{,}5}_{-1{,}0}$ ккал/моль.

М.Л.

ф.1992, N1

C_3^+

1991

структура,
расчет

115: 99707p Ab initio study of the carbon (C_3^+) cation using multireference methods. Taylor, Peter R.; Martin, J. M. L.; Francois, J. P.; Gijbels, R. (ELORET Inst., Palo Alto, CA 94303 USA). *J. Phys. Chem.* 1991, 95(17), 6530–4 (Eng). The energy difference between the linear $^2\Sigma_u^+$ and cyclic $^2B_2$ structures of C_3^+ has been investigated by using large [5s3p2d1f] basis sets and multireference electron correlation treatments, including complete active space SCF (CASSCF), multireference CI(MRCI), and averaged coupled-pair functional (ACPF) methods, as well as the single-ref. quadratic CI [QCISD(T)] method. Our best est., including a correction for basis set incompleteness,is that the linear form lies above the cyclic form by $5.2_{-1.0}^{+1.5}$ kcal/mol. The $^2\Sigma_u^+$ state is probably not a transition state but a local min. Reliable computation of the cyclic/linear energy difference in C_3^+ is extremely demanding of the electron correlation treatment used: of the single-ref. methods previously considered, CCSD(T) and QCISD(T) perform best. The MCRI+Q(0.01)/[4s2p1d] energy sepn. of 1.68 kcal/mol should provide a comparison std. for other electron correlation methods applied to this system.

C. A. 1991, 115, N10

C_3^+

1991

23 Б1101. Изучение методом связанных кластеров основного состояния C_3^+. A coupled-cluster study of the ground state of C_3^+ / Watts John D., Stanton John F., Gauss Jürgen, Bartlett Rodney J. // J. Chem. Phys.— 1991.— 94, № 6.— С. 4320—4327.— Англ.

Различными вариантами методов ССП и связанных кластеров, наиболее точным из к-рых явился метод связанных кластеров, полностью учитывающий вклады от одно-, двух- и трехкратных возбуждений, рассчитаны энергии и частоты норм. кол. в двух стационарных точках потенциальной ПВ молекулы C_3^+, имеющих симметрию $^2B_2$ и $^2\Sigma_u^+$ (линейная конфигурация). В расчетах использованы три различных базиса сгруппир. гауссовых орбиталей, наиболее полным из к-рых был трехэкспонентный базис [10*s*6*p*2*d*/5*s*3*p*2*d*]. Предсказана нелинейная равновесная геометрич. структура молекулы. Показано, что варианты метода связанных кластеров, лишь приближенно учитывающие вклады от связанных трехкратных возбуждений, приводит к существенно заниженным значениям разности энергий между указанными конфигурациями молекулы. Обсуждены трудности, возникающие при описании конфигурации с

М.П.

Х. 1991, №23

симметрией $^2B_2$ в приближении ССП и связанные с нарушением симметрии волновой ф-ции ограниченного метода ССП для открытых оболочек и с существованием в этом случае двух различных решений в неограниченном приближении Хартри—Фока. Предложен способ преодоления этих трудностей. В. Б. Павлов-Веревкин

C_3^+

1991

Г **11 Д96. Изучение основного состояния C_3^+ методом связанных кластеров.** A coupled-cluster study of the ground state of C_3^+ / Watts John D., Stanton John F., Gauss Jürgen, Bartlett Rodney J. // J. Chem. Phys.— 1991.— 94, № 6.— С. 4320—4327.— Англ.

Проведен расчет структуры и гармонич. частот $^2B_2$ состояния C_3^+ и энергии этого состояния относительно состояния с линейной геометрией $^2\Sigma^+$. Применялись методы самосогласованного поля, связанных кластеров, включая модель одиночного, двойного и тройного возбуждений. Расчет разности энергий $^2\Sigma_u^+ — ^2B_2$ указывает на изогнутую форму молекулы в основном состоянии. Обсуждаются точности различных используемых приближений. Методы связанных кластеров, которые только приближенно включают эффекты, связанные с тройным возбуждением, дают слишком малую величину разности энергий. Поэтому последние предсказания этим методом квазилинейной структуры C_3^+ являются спорными. Г. К.

М.Л.

ф. 1991, N 11

C_3

1992

$(X^1\Sigma^+)$

теорет.-
расчет
потенц.
поверхности

117: 198951m Calculation of the complete-active-space self-consistent-field potential-energy surface, the dipole-moment surfaces, the rotation-vibration energies, and the vibrational transition moments for the carbon trimer $C_3(X^1\Sigma_g^+)$. Jensen, Per; Rohlfing, Celeste McMichael; Almlof, Jan (Phys. Chem. Inst., Justus Liebig Univ., W-6300 Giessen, Germany). *J. Chem. Phys.* 1992, 97(5), 3399-411 (Eng). The present work reports an ab initio calcn. of the potential-energy surface and corresponding dipole moment surfaces for the C_3 mol. employing the full valence complete-active-space self-consistent-field method with a very large basis set. On the basis of the ab initio results we have calcd. the rotation-vibration energies in the lower part of the energy spectrum with the MORBID (Morse oscillator rigid bender internal dynamics) method, and we find that the present ab initio potential-energy surface reproduces qual. the variation of the bending energy-level pattern with excitation of the stretching modes. We conclude from the ab initio results obtained in the present work, and from a fitting to exptl. data carried out with the MORBID computer program, that the equil. structure of C_3 is linear. We have used the ab initio dipole

C.A. 1992, 117, N 20

moment calcd. in the present work to compute the vibrational transition moments for selected vibrational transitions of $^{12}C_3$, obtaining transition moments of 0.44 and 0.35 D, resp., for the ν_2 and ν_3 bands. The ab initio dipole moment values have further been used to calc. the line strengths, integrated absorption coeffs., and peak absorption coeffs. of the low-J transitions in the ν_2 and ν_3 bands; the results of the theor. intensity calcn. are in keeping with the recent exptl. observations.

C_3 1992

Maclagan Robert G.A.R.
Sudkeaw Pravit.

(D_0)

Chem. Phys. Lett. 1992,
194 (3), 147–51.

(См. C_2S; III)

C_3^+ 1992

Ortiz J.V.,

J. Chem. Phys., 1992, 97, N10,

м.л. с. 7531-7536

(см. C_3; ● III)

C_3^- 1992

Ortiz J.V.,

J. Chem. Phys. 1992, 97, N10,

М.Л. с. 7531-7536

● (см. C_3; $\underline{III}$)

C_3

1992

11Д164. Расчеты адиабатических энергий электронных связей в C_3 в рамках теории электронного пропагатора. Electron propagator calculations on the adiabatic electron binding energies of C_3 / Ortiz J. V. // J. Chem. Phys.. — 1992. — **97**, № 10. — С. 7531—7536. — Англ.

New techniques of electron propagator theory (EPT) are applied to C_3, C_3^+, and C_3^-. Gradients of second-order EPT ionization energies and electron affinities are combined with gradients of second-order many-body perturbation theory for the neutral to produce gradients of the ion total energies. Optimized geometries of the ions, vibrational frequencies, and adiabatic electron binding energies are calculated with these methods. A renormalized self-energy is used to produce improved vertical and adiabatic ionization energies and electron affinities.

М.Л.

(+2) $\boxed{\text{XI}}$ C_3^+, ● C_3^-

Ф. 1993, N 11–12

C_3

1992

10 Б1065. Расчет методом электронного пропагатора адиабатических энергий связи электрона в C_3. Electron propagator calculations on the adiabatic electron binding energies of C_3 /Ortiz J. V. //J. Chem. Phys .— 1992 .— 97 ,№ 10 .— С. 7531—7536 .— Англ.

В рамках формализма электронного пропагатора предложен метод вычисления пр-ных энергии ионизации. При совместном использовании с градиентами энергии многочастичной теории возмущений для исходного состояния предложенный подход позволяет оптимизировать геометрич. параметры ионов градиентным методом. Оптимизированы геометрич. параметры и рассчитаны колебат. частоты и адиабатич. энергии связи электрона на C_3, C_3^+ и C_3^-. Получены адиабатич. потенциал ионизации и сродство к электрону C_3 11,9 и 1,8 эВ соотв.

А. А. Сафонов

М·1·

☒

+2

Х. 1993, N 10

C_3

1992

118: 46198d **Electron-propagator calculations on the adiabatic electron binding energies of the carbon trimer.** Ortiz, J. V. (Dep. Chem., Univ. New Mexico, Albuquerque, NM 87131 USA). *J. Chem. Phys.* 1992, 97(10), 7531-6 (Eng). New techniques of the electron propagator theory (EPT) are applied to C_3, C_3^+, and C_2^-. Gradients of 2nd-order EPT ionization energies and electron affinities are combined with gradients of second-order many-body perturbation theory for the neutral to produce gradients of the ion total energies. Optimized geometries of the ions, vibrational frequencies, and adiabatic electron binding energies are calcd. with these methods. A renormalized self-energy is used to produce improved vertical and adiabatic ionization energies and electron affinities. For the cation, the $^2B_2$ state with C_{2v} symmetry and the $^2\Sigma$ state with $C_{\infty v}$ symmetry are very close in energy. The optimized $^2\Sigma_u$ structure is a transition state with an imaginary frequency of σ_u symmetry that lies 2.8 kcal/mol above the $^2B_2$ state. The adiabatic ionization energy is calcd. to be 11.9 eV. The anion in the $^2\Pi_g$ state lies 1.8 eV below the neutral in these calcns.

структура, ν_i, I, D, теор. расчет

(+2) ☒

C.A. 1993, 118, N6

C_3^+, C_2^-

C_3^+ 1992

Ortiz J.V.,

структура, ν_i, I, D, энергет. теор. расчёт

J. Chem. Phys. 1992, <u>97</u>(10), 7831-6.

●

(см. C_3 ; <u>III</u>)

C_3

1993

119: 258756e A hot band LIF study of the $A^1\Pi_u - X^1\Sigma_g^+$ transition in C_3 carbon molecule. Baker, Jacob; Bramble, Simon K.; Hamilton, Peter A. (Department of Chemistry, Queen Mary and Westfield College, Mile End Road, London, UK E1 4NS). *Chem. Phys. Lett.* 1993, 213(3-4), 297-302 (Eng). Laser-induced fluorescence excitation spectra of the $A^1\Pi_u - X^1\Sigma_g^+$ electronic transition have been recorded in the laser wavelength range 386-463 nm using a novel source of rotationally cold but vibrationally excited C_3. A large no. of new transitions are obsd. and the authors report here on some prominent vibrational progressions appearing in the spectra which are assigned to (n'00-n''00) vibronic transitions. A tentative assignment of the (001-001) transition is also given which locates for the first time the $A^1\Pi_u$(001) level.

($A^1\Pi_u - X^1\Sigma_g^+$)
лазерно-флуоресц.

C. A. 1993, 119, N 24

C_3

1993

118: 261303q **Multireference CI study of the electron affinity of C_3.** Fueno, Hiroyuki; Ikuta, Shigeru (Comput. Cent. Tokyo Metrop. Univ., 1-1 Minami-Ohsawa, Hachioji-shi, Tokyo, Japan 192-03). *Chem. Phys. Lett.* 1993, 204(3-4), 320-2 (Eng). The bond lengths of C_3 and C_3^- are evaluated to be 1.295 and 1.311 Å, resp., using the SDCI method with Davidson's correction. That of C_3 is in good agreement with the exptl. data, 1.297 Å. The electron affinities obtained using the SDCI+Q and MR-SDCI+Q methods are 2.02 and 1.89 eV, resp. These values are identical with the recent data (2.00 eV) in C_3^- obtained by photoelectron spectroscopy.

(r_e)
(теор. расчет)

☒ (1) C_3^-

C. A. 1993, 118, N 26

C_3

1993

119: 82335a **Infrared diode laser spectroscopy of the ν_3 fundamental and $\nu_3 + \nu_2 - \nu_2$ sequence bands of carbon trimer-3^{13}C ($^{13}C_3$) and of the ν_3 fundamental band of carbon trimer-^{13}C (^{12}C ^{12}C ^{13}C).** Moazzen-Ahmadi, N.; McKellar, A. R. W. (Dep. Phys., Univ. Lethbridge, Lethbridge, AB Can. T1K 3M4). *J. Chem. Phys.* **1993**, 98(10), 7757–62 (Eng). Gas-phase IR spectra of ^{13}C-substituted C_3 mols. were studied in the region of the ν_3 vibration at ~5 μm, using a tunable diode laser spectrometer and a hollow-cathode discharge in a flowing mixt. of acetylene and He. Three bands were obsd. and assigned: the ν_3 fundamentals of $^{13}C_3$ and of ^{12}C ^{13}C, and the $\nu_3 + \nu_2 - \nu_2$ sequence band of $^{13}C_3$. The obsd. band origins are consistent with previous matrix-isolation spectroscopy of substituted C_3. The rotational and centrifugal distortion parameters are consistent with previous gas-phase work on $^{12}C_3$, and they also reflect the highly anharmonic nature of the bending vibration in this mol. The ν_3 band of ^{12}C ^{13}C, measured here for the 1st time, provides a sensitive means to measure ^{13}C abundances in astrophys. sources contg. C_3.

(ИК., ν_3)

C. A. 1993, 119, N 8

C_3

1993

120: 15064u Matrix isolation infrared spectroscopy in cluster science. Nakata, Munetaka (Fac. Gen. Educ., Tokyo Univ. Agric. Technol., Fuchu, Japan 183). *Bunko Kenkyu* 1993, 42(2), 79–93 (Japan). A review with 53 refs. describing formation, spectral discrimination, structure, reactivities and stabilization in matrixes of mol. cluster ions of O, N, C, NO, CO, and CO_2 and of C_3, C_4, C_5, C_6, and C_8 carbon clusters. IR. E. Shikata

ИК в
матрице
обзор

☒

(+4)

C. A. 1994, 120, N2

C_3

1993

119: 36533r FT-IR studies of optically pumped triatomic carbon in rare gas matrixes. The vibrational and electronic absorption spectrum of the $\tilde{a}^3\Pi_u$ state. Smith, Alice M.; Agreiter, Juergen; Engel, Cornelia; Bondybey, Vladimir E. (Institut fuer Physikalische und Theoretische Chemie, Technische Universitaet Muenchen, W-8046 Garching, Germany). *Chem. Phys. Lett.* 1993, 207(4-6), 381-9 (Eng). Through a double resonance technique, the Fourier transform(FT) IR absorptions of the lowest-lying triplet state of C_3 were obsd. in argon and neon matrixes. The long lived $\tilde{a}^3\Pi_u$ state is populated by an intersystem crossing from the excited $\tilde{A}^1\Pi_u$ state. The difference spectra obtained with and without C_3 $\tilde{A}^1\Pi_u$ laser excitation exhibit a large depletion of the electronic ground state and a simultaneous appearance of the vibrational and electronic $\tilde{a}^3\Pi_u$ absorption spectra. The $\tilde{b}^3\Pi_g \leftarrow \tilde{a}^3\Pi_u$ spectrum extends from ~6500-8400 cm⁻¹ and shows an extensive vibrational structure. The assignments of the two stretching vibrations of the $\tilde{a}^3\Pi_u$ state are verified through a harmonic force field fit to nine isotopic frequencies.

$b^3\Pi_g \Leftarrow a^3\Pi$

Фурье ИК спектр

C.A. 1993, 119, N 4

C_3

1993

120: 119685p **The $\nu_1 + \nu_3$ combination mode of the carbon trimer in argon and krypton matrixes: evidence for a bent structure.** Szczepanski, Jan; Vala, Martin (Dep. Chem., Univ. Florida, Gainesville, FL 32611-2046 USA). *J. Chem. Phys.* 1993, 99(10), 7371-5 (Eng). The $\nu_1 + \nu_3$ combination mode of laser-ablated C_3 was obsd. in Ar and Kr matrixes for all 6 possible $^{12}C/^{13}C$ isotopomers. The ν_1 totally sym. mode frequencies were detd. by difference with the known ν_3 asym. stretching frequencies, cor. for anharmonicity effects. A comparison of certain isotopomer pairs reveals that C_3 is bent in these matrixes. A normal coordinate anal. using 4 force consts. resulted in an excellent fit of the 12 obsd. frequencies (ν_1 and ν_3 for 6 isotopomers). From the fit, a value for the ν_2 bending mode frequency of 82 cm^{-1} was obtained. This is in agreement with the value obtained from the C_3 phosphorescence spectrum. The mol. bending angle which was detd. as 160.0° (in Ar and Kr) matches with the predicted value from ab initio theory (161.6°) and from a fitting of a Morse oscillator-rigid bender potential to gas phase vibrational frequencies (162.5°). The influence of the matrix environment on the vibrational force consts. and frequencies of C_3 is discussed.

$\nu_1 + \nu_3$ в
(матрице)
структура
угловая 160°

С.А. 1994, 120, N10

C_3^+

1993

120: 86628s **Triple excitations in coupled-cluster theory: energies and analytical derivatives.** Watts, John D.; Bartlett, Rodney J. (Dep. Chem., Univ. Florida, Gainesville, FL 32611-2085 USA). *Int. J. Quantum Chem., Quantum Chem. Symp.* 1993, 27(Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods, 1993), 51-66 (Eng). A review with 77 refs. is presented of the authors' recent work which deals with some aspects of the inclusion of connected triple excitations in single ref. coupled-cluster theory. The authors first consider basic aspects of the theory and computational cost, noting the need for accurate and economical approxns. to the complete coupled-cluster single, double and triple excitation method (CCSDT). Several such approxns. are now available, including the CCSD +

мол. пост.

$^2\Sigma_u^+$

☒ (Н) BeO(М) (теор. расчет)

C.A. 1994, 120, N8

T(CCSD) and CCSD(T) methods. The authors have now efficiently implemented anal. deriv. methods for these and related methods for open-shell ref. determinants, including restricted open-shell Hartree–Fock for CCSD(T). Some results with large basis sets are presented for the HCO radical which further demonstrate the reliability of these methods for the spectroscopic characterization of small open-shell species. The remainder of this article deals with several applications of the complete CCSDT method, a new implementation of which the authors have recently completed. Like the authors' previous work, this is for general single ref. determinants, although the authors have now incorporated Abelian symmetry. The authors present a comparison with full CI data for CH_3; a study of the N_2 potential curve using restricted and UHF refs.; a comparison of the dipole moments and polarizabilities of BeO; and a study of the harmonic force field of $^2\Sigma_u^+$ C_3^+. These studies also provide assessments of the accuracy of the approx. schemes for including T_3. Finally, the authors present some timing data for some CCSDT calcns. with the authors' new implementation.

C_3

1994

121: 238782y **Comment on "The $\nu_1 + \nu_3$ combination mode of C_3 in Ar and Kr matrixes: evidence for a bent structure" [J. Chem. Phys. 99, 7371(1993)].** Almlof, J.; Jensen, P.; Northrup, F. J.; Rohlfing, C. M.; Rohlfing, E. A.; Sears, T. J. (Dep. Chem., Univ. Minnesota, Minneapolis, MN 55455 USA). *J. Chem. Phys.* 1994, 101(6), 5413 (Eng). A polemic in response to the title paper by J. Szczerpanski and M. Vala; evidence for the linear structure of C_3 is described.

спектр в матрице $\nu_1 + \nu_3$, структура

C.A. 1994, <u>121</u>, N20

C_3

1994

122: 117934m **Laser-induced fluorescence spectroscopy of the $\tilde{A}\ ^1\Pi_u - \tilde{X}\ ^1\Sigma_g^+$ transition in jet-cooled C_3.** Balfour, Walter J.; Cao, Jianying; Prasad, C. V. V.; Qian, Charles X. W. (Dept. Chem., Univ. Victoria, Victoria, BC Can. V3W 3P6). *J. Chem. Phys.* **1994**, 101(12), 10343-9 (Eng). C_3 radicals were produced in a plasma of Re with methane doped in He and cooled in a supersonic free jet expansion. More than 50 vibronic bands in the laser induced fluorescence spectrum of the $\tilde{A}\ ^1\Pi_u - \tilde{X}\ ^1\Sigma_g^+$ electronic transition were recorded in the region 370–415 nm at 0.4 cm⁻¹ resoln. The observations include bands identified by Gausset et al. (1965) and many bands not previously characterized. Rotational analyses were made for a majority of the bands and the no. of located Renner–Teller levels of the $\tilde{A}$ state was considerably extended. The (002) level is tentatively identified. A comparison of the exptl. detd. energy level pattern in the $\tilde{A}$ state with theor. predictions suggested a no. of revisions to previous assignments and evidence is presented to contradict suggestions from earlier work that the (020) level of the $\tilde{A}$ state is perturbed.

$(A^1\Pi_u - X^1\Sigma_g^+)$

лазервозб.
флуоресц.

C.A. 1995, 122, N10

C_3

ОМ. 37603

1994

Martin J.M.L.,
Taylor P.R.,

М.Л.,
ab initio J. Phys. Chem., 1994,
расчет, 98, 6105–6109.
термохим.

Ab initio study of the
Isoelectronic Molecules BCN,

BNC and C_3 Including Anharmonicity.

C_3

1994

Б/ **10 Б1020. Крупномасштабные неэмпирические расчеты молекулы C_3.** Large-scale ab initio calculations for C_3 /Mladenović M., Schmatz S., Botschwina P. //J. Chem. Phys. .— 1994 .— **101** ,№ 7 .— С. 5891—5899 .— Англ.

Методом связанных кластеров с учетом одно-, двух- и трехкратно возбужденных конфигураций выполнены расчеты молекулы C_3 в различных конфигурациях. Найдено линейное строение C_3 с $R_e = 1{,}2945$ Å. Показано, что использование расширенных базисных наборов и включение в расчет трехкратно возбужденных конфигураций имеет большое значение для количеств. описания плоской потенциальной поверхности молекулы. По сравнению с наилучшими известными расчетами C_3 в приближении метода ССП достигнуто на порядок лучшее согласие рассчитанных х-к колебат. спектра молекулы с эксперим. данными.

Е. А. Рыкова

Мп·

Х·1995, N10

C_3

1994

ab initio
расчет ν_i,
структур.
параметр.,
D_0

121: 238650d Large-scale ab initio calculations for C_3. Mladenovic, M.; Schmatz, S.; Botschwina, P. (Inst. Physikalische Chemie, Univ. Goettingen, D-37077 Goettingen, Germany). *J. Chem. Phys.* **1994,** 101(7), 5891–9 (Eng). Large-scale calcns. by the single, double, and perturbative triple excitation coupled cluster [CCSD(T)] method have been carried out for C_3. A linear equil. geometry with R_e = 1.2945 Å was obtained. The use of large basis sets and the inclusion of connected triple substitutions is crucial for an accurate representation of the extremely shallow bending potential. Rovibrational term energies were calcd. from a three-dimensional CCSD(T) potential (basis: 177 contracted Gaussian-type orbitals) by the discrete variable representation (DVR). Compared with the best previous ab initio calcns. [P. Jensen et al., J. Chem. Phys. 97, 3399 (1992)] agreement with expt. is improved by almost an order of magnitude. The errors in the wave nos. of the fundamentals are −7.7 (ν_1), 0.9 (ν_2), and 0.6 (ν_3) cm^{-1}, resp.

C.A. 1994, 121, N20

C_3

1994

20 Б1095. Энергии связи электрона в линейных кластерах C_3, C_5, C_7 и C_9. Electron binding energies of linear C_3, C_5, C_7, and C_9 clusters /Ortiz J. V., Zakrzewski V. G. //J. Chem. Phys. .— 1994 .— **100** ,№ 9 .— С. 6614—6619 .— Англ.

На основе электронного пропагатора вычислены вертикальные энергии ионизации и сродство к электрону кластеров C_3, C_5, C_7, C_9. Получены оценки адиабатич. величин сродства ~~к электрону~~, к-рые хорошо согласуются с эксперим. данными. Найдено связанное возбужденное состояние C_9^-.

В. Е. Скурат

М-П-

㊸ X

Х. 1994, N20

C_3

1994

120: 307916p Electron binding energies of linear C_3, C_5, C_7, and C_9 clusters. Ortiz, J. V.; Zakrzewski, V. G. (Dep. Chem., Univ. New Mexico, Albuquerque, NM 87131 USA). *J. Chem. Phys.* **1994**, 100(9), 6614–19 (Eng). Electron propagator calcns. are performed on the vertical ionization energies and electron affinities of linear C_3, C_5, C_7, and C_9 clusters with a variety of correlation approxns. and basis sets. Ests. of adiabatic electron affinities are made as well, and are in excellent agreement with expt. A bound, excited state of C_9^- has been found. Correlation effects are large for the electron affinity calcns. and for many vertical ionization energies. The Koopmans description of final states is valid for the Feynman–Dyson amplitudes, but for many cationic states there is considerable shakeup character.

структура,
энергии
связи

C_5, C_7, C_9

(+3) ☒

C. A. 1994, 120, N 24

C_3

1994

121: 238783z Response to "Comment on: 'The $\nu_1 + \nu_3$ combination mode of C_3 in Ar and Kr matrixes: evidence for a bent structure'" [J. Chem. Phys. 101, 5413(1994)]. Szczepanski, J.; Vala, M. (Dep. Chem., Univ. Florida, Gainesville, FL 32611-7200 USA). *J. Chem. Phys.* **1994,** 101(6), 5414 (Eng). A polemic in response to the title article by J. Almlof et al.

спектр в матрице $\nu_1 + \nu_3$, структура

C·A·1994, 121, N 20

$^{13}C_3$

1995

123: 126039w Fourier transform emission spectroscopy of triplet $^{13}C_3$. Civis, Svatopluk; Tokaryk, D. W. (Steacie Inst. Molecular Sciences, Natl. Res. Council Canada, Ottawa, Can. K1A 0R6). *J. Mol. Spectrosc.* 1995, 172(2), 543–51 (Eng). We describe the construction of a liq.-nitrogen-cooled multireflection emission cell. A combination of very small gas input apertures and very rapid evacuation through a combination of mech. and booster pumps provedes for a rapid replenishment of discharge-formed material in the cell. This cell is an excellent source for the study of the C_3 radical in the triplet manifold with a Fourier transform spectrometer. The strongest feature corresponds to the (000)–(000) band of the $b^3\Pi_g \rightarrow \tilde{a}^3\Pi_u$ electronic transition, which for $^{12}C_3$ was obsd. and analyzed by Sasada et al. We have obsd. this band for $^{13}C_3$, and report the line positions and anal. in this paper.

Фурье спектр

$b^3\Pi_g \rightarrow a^3\Pi_u$

C.A. 1995, 123, N10

C_3^{2+}

1995

122: 170536j Ab initio study of the dication carbon trimer C_3^{2+}. Hogreve, H. (International Centre For Theoretical Physics, I-34100 Trieste, Italy). *J. Chem. Phys.* **1995,** 102(8), 3281–91 (Eng). Motivated by the recent exptl. observations of multiply pos. charged fullerene ions C_n^{k+}, n = 56, 60, 70, k = 1 – 7, the doubly charged trimer C_3^{2+} is investigated by multireference CI computations. Studying the lowest potential energy surfaces of various electronic states, several local min. are found that entail not only metastability of the system, but the involved large and wide barriers render C_3^{2+} almost stable against dissociative tunneling. The present computations predict a linear configuration as the most favorable one for C_3^{2+}, with a $^1\Sigma_u^+$ ground state and an energy slightly below the min. found for the lowest triplet state $^3\Sigma_u^+$ or occurring in C_{2v} geometry (state $^1A_1$). Stability and addnl. properties of C_3^{2+} are discussed and compared with those of other trimer dications. Moreover, this study includes accurate data for low-lying states of the dimer ions C_2^+ and C_2^{2+} that are of relevance for the dissocn. channels of C_3^{2+}.

ab initio
расчет
структуры,
мин. низш.
электр. сост.

(+2) ☒

C. A. 1995, 122, N14

C_2^+, C_2^{2+} (-расчет
эл. сост. низших

C_3^{2+}

1995

24 Б1109. Неэмпирическое изучение дикатиона тримера углерода C_3^{2+}. Ab initio study of the dication carbon trimer C_3^{2+} / Hogreve H. // J. Chem. Phys. .— 1995 .— **102** , № 8 .— С. 3281—3291 .— Англ.

Многоссылочным методом конфигурац. взаимодействия исследован дикатион тримера углерода C_3^{2+}. На потенциальных поверхностях различных низколежащих электронных состояний обнаружены несколько локальных минимумов. Предсказано, что линейная конфигурация наиболее предпочтительна для C_3^{2+} в основном состоянии ${}^1\Sigma_g^+$. Самое нижнее триплетное состояние ${}^3\Sigma_u^+$ имеет геометрию C_{2v}. Получены также точные данные и для димерных ионов C_2^+ и C_2^{2+}. Библ. 66. Г. К.

М.П.

Х. 1995, N 24

C_3

1995

123: 211849e New vibronic bands of the laser-vaporized C_3 cluster. Determination of the ν_3 fundamental in the $\tilde{A}\ {}^1\Pi_u$ state. Izuha, Mitsuaki; Yamanouchi, Kaoru (Department of Pure and Applied Sciences, College of Arts and Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo, Japan 153). *Chem. Phys. Lett.* **1995**, 242(4,5), 435–42 (Eng). The laser-induced fluorescence (LIF) spectrum for the $\tilde{A}\ {}^1\Pi_u-\tilde{X}\ {}^1\Sigma_g^+$ band of laser-vaporized C_3 was measured under jet-cooled conditions. By careful inspection of the rotationally resolved LIF spectrum, eight vibronically allowed transitions exhibiting a ${}^1\Sigma_u^+-{}^1\Sigma_g^+$ type rotational structure were identified. This finding led to the detn. of the vibrational energy for the $(v_1, v_2, v_3) = (0, 1^+, 1)$ level of the $\tilde{A}$ state, from which the fundamental wavenumber of the ν_3 anti-sym. mode is ≈539 cm^{-1}, which is considerably smaller than any of the previous ests., 650, 808 and 890 cm^{-1}. In the high-resoln. (≈0.08 cm^{-1}) measurements for the hot-band region, ${}^1\Pi_g-{}^1\Sigma_u^+$ type bands exhibiting a characteristic feature for the transitions from the $\tilde{X}(0, 0, 1)$ level were identified. By assigning the $\tilde{A}(0, 0, 1)-\tilde{X}(0, 0, 1)$ band, the ν_3 fundamental was directly detd. to be 541.7(1) cm^{-1}, in excellent agreement with the above prediction from the vibronically allowed ${}^1\Sigma_u^+-{}^1\Sigma_g^+$ transitions.

$(A^1\Pi_u - X^1\Sigma_g^+)$

м.п.

C.A. 1995, 123, N16

C_3 Om: 38125 1995

Keith R. Lykke,

Phys. Rev. 1995, A52, N2, 1354-1357

Fragmentation ~~of~~ C_{60}: Experimental detection ~~of~~

C_1, C_2, C_3 and C_4 by XUV postionization.

C_3

ОМ 38087

1995

122: 199704y Ab initio study of the optical spectra of C_3, C_5, and C_7 chains. Kolbuszewski, M. (Steacie Inst. Molecular Sci., Natl. Res. Council Canada, Ottawa, ON Can. K1A 0R6). *J. Chem. Phys.* **1995**, 102(9), 3679–84 (Eng). Multireference CI calcns. on the low lying singly excited states of linear C_3, C_5, and C_7 clusters are reported. The $^1\Sigma_u^+$ state of C_3 has a term energy >8.0 eV. The calcd. vertical term energies of the low lying electronic states of these C chains are consistent with the photoelectron spectra of their parent neg. ions. The predicted term energies are also compatible with the matrix spectra of C vapor. An assignment of strong spectral features in those spectra at ≈1950, 2227, and 2471 Å to the $^1\Sigma_u^+ \leftarrow X\ ^1\Sigma_g^+$ transition in C_5, C_7, and C_9, resp., is proposed. A possible relation of C chains to diffuse interstellar bands is discussed.

ab initio рас
чет низших
эл. состоян.

C_5, C_7

(+2) ☒

C. A. 1995, 122, N 16

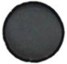
C_3 (от. 37971) 1995

Martin J.M.L., Taylor P.R.,

J. Chem. Phys., 1995, <u>102</u>, N20, 8270 – 8273.

Accurate ab initio total atomization energies of the

C_n clusters ($n = 2-10$)



C_3^- 1995

124: 67215w Large−scale coupled cluster calculations for the linear carbon anions C_3^-, C_4^-, C_7^- and C_{10}^-. Schmatz, Stefan; Botschwina, Peter (Institut fuer Physikalische Chemie, Universitaet Goettingen, Tammannstr. 6, D−37077 Gottingen, Germany). *Int. J. Mass Spectrom. Ion Processes* **1995**, 149/150, 621−9 (Eng). Large−scale open−shell coupled cluster calcns. are carried out for the linear carbon anions C_3^-, C_4^-, C_7^- and C_{10}^-. Accurate equil. geometries (0.001 Å accuracy) are established for C_3^- and the lowest four doublet states of C_4^-. The vibrational structure of the photoelectron spectrum of C_7^- are calcd. within a three−dimensional anharmonic model. The vertical excitation energies of C_{10}^- are predicted to be 1.36 eV ($^2\Sigma^+_u$ and $^2\Sigma^+_g$ states) and 1.51 eV ($\tilde{C}^2\Pi_g$). Inclusion of connected triple substitutions has a large effect of 0.5 eV on the excitation energies of the $^2\Sigma$ states.

re, энергии
возбужд.,
теор. расчет

(+3) ☒ C_4^-, C_7^-, C_{10}^-

C.A. 1996, 124, N 6.

C_3

1995

123: 240522y **Infrared emission spectra of C_3: the Renner effect in the $\tilde{a}^3\Pi_u$ and $\tilde{b}^3\Pi_g$ electronic states.** Tokaryk, D. W.; Civis, Svatopluk (Steacie Inst. Molecular Sciences, Natl. Res. Council, Ottawa, Can. K1A 0R6). *J. Chem. Phys.* **1995**, 103(10), 3928–41 (Eng). Five new triplet bands of $^{12}C_3$, and 3 corresponding bands of $^{13}C_3$, were obsd. in emission at 6000–6600 cm^{-1} with a Fourier transform spectrometer. Rotational anal. shows that these bands arise from excited bending vibrations of the $\tilde{b}^3\Pi_g \rightarrow \tilde{a}^3\Pi_u$ electronic transition, and that all components of the (010) vibrational level of the $\tilde{b}^3\Pi_g$ state exhibit unusual perturbations. Renner parameters for both electronic states were extd. from an anal. of the spin–orbit parameters of the (000) $^3\Pi$, (010) $^3\Delta$, (020) $^3\Phi$, and (030) $^3\Gamma$ levels. The Renner effect is large in both electronic states ($\epsilon' = +0.447$, $\epsilon'' = +0.566$). Approx. bending vibrational frequencies are obtained ($\omega_2' \approx 345$ cm^{-1}, $\omega_2'' \approx 505$ cm^{-1}).

ИК

$a^3\Pi_u$, $b^3\Pi_g$ –
Реннер-эффект

C.A. 1995, 123, N 18

1996

24Б1714. Инфракрасная полупроводниковая лазерная спектроскопия C_3. Полоса ν_3 в электронном состоянии $\tilde{a}^3\Pi_u$. Infrared diode laser spectroscopy of C_3: The ν_3 band of the $\tilde{a}^3\Pi_u$ electronic state / Hwang C. H., Klassen S. A., Moazzen-Ahmadi N., Tokaryk D. W. // Chem. Phys. Lett.— 1996.— **250**, № 3-4.— С. 273–278.— Англ.

Измерена (перестраиваемый полупроводниковый лазерный спектрометр) вращательная структура полосы ν_3 молекулы C_3 в долгоживущем электронном состоянии $\tilde{a}^3\Pi_u$. Молекулы $C_3(\tilde{a}^3\Pi_u)$ получали в условиях разряда через поток смеси ацетилена и гелия. Начало полосы при 1449, 5255 $см^{-1}$. Приведены значения вращательных постоянных (B, D, H), параметров тонкой структуры (A, λ) и параметров удвоения l-типа (o, q). В. М. Ковба

М.П.

Х. 1997, N24

C_3

1996

124: 245210a **Infrared diode laser spectroscopy of C_3: the ν_3 band of the $\tilde{a}\ ^3\Pi_u$ electronic state.** Hwang, C. H.; Klassen, S. A.; Moazzen-Ahmadi, N.; Tokaryk, D. W. (Department of Physics, University of Lethbridge, Lethbridge, Alberta, Can.). *Chem. Phys. Lett.* **1996**, 250(3,4), 273–8 (Eng). The rotationally resolved IR spectrum of the ν_3 band of the long-lived $\tilde{a}\ ^3\Pi_u$ electronic state of C_3 was obsd. at 1428–1473 cm^{-1} using a tunable diode laser spectrometer. Metastable C_3 was produced in a discharge through a flowing mixt. of C_2H_2 and He. The obsd. band consists of 3 R and 3 P branches, which show staggering due to Λ-type doubling and nuclear spin statistics. The band origin of 1449.5255(22) cm^{-1} is close to the value of 1455.3 cm^{-1} detd. previously from matrix isolation expts.

(ν_3 в $\tilde{a}\ ^3\Pi_u$)

C. A. 1996, 124, N 18

C_3

1996

125: 126299x Infrared Spectroscopic Studies of Carbon Clusters Trapped in Solid Parahydrogen. Miki, Masaaki; Wakabayashi, Tomonari; Momose, Takamasa; Shida, Tadamasa (Graduate School of Science, Kyoto University, Kyoto, Japan ITY KYOTO). *J. Phys. Chem.* **1996**, 100(30), 12135−12137 (Eng). Small C clusters produced by laser ablation of a C rod are trapped in solid parahydrogen at 4.8 K. IR spectra show C_3, C_5, C_9, and a few new clusters. The obsd. vibrational spectra with multiplet structures are tentatively assocd. with hindered rotation of the clusters. Temp. dependence of the IR spectra reveals the diffusion of C_3 and C_5 clusters in the crystal at ~8 K, while no diffusion of C_9 and the larger clusters is noticed. Any hydrocarbons which might be produced by reactions between the C clusters and the substrate H_2 mols. are not obsd. both during the deposition and after the thermal annealing.

ИК в
матриц
параводород.

+2

C_5, C_9

C.A. 1996, 125, N10

C_3

1997

127: 72399a **Observation of new bands in the $A^1\Pi_u - X^1E_g^+$ laser induced fluorescence spectrum of C_3.** Baker, Jacob; Bramble, Simon K.; Hamilton, Peter A. (Dep. Chemistry, Queen Mary Westfield College, London, UK E1 4NS). *J. Mol. Spectrosc.* 1997, 183(1), 6−11 (Eng), Academic. The authors report on over 10 new bands of two vibronic types $\Pi_u - E_g^+$ and $\Pi_g - E_u^+$ in the $A^1\Pi_u - X^1E_{g+}$ laser induced fluorescence spectrum of C_3 in the wavelength range 386−463 nm. A fast elec. discharge in the expansion region of a supersonic jet of CO produces rotationally cold but highly vibrationally excited C_3, although the low frequency bending mode appears to be fully quenched. The vibronic symmetries of the upper and lower states involved in the transitions are in general unambiguously assigned from the rotational assignment but the apparent lack of ordered vibrational structure in the $\Pi_g - E_u^+$ type transitions makes vibrational assignments for many of these bands ambiguous. Self consistent preliminary assignments for -30 of the $\Pi_g - E_{u+}$ bands allows new vibrational levels in the A state to be characterized.

$(A\,^1\Pi_u - X\,^1\Sigma_g^+)$

м·л

C.A. 1997, 127, N 5

C_3

1997

128: 40805j **Can the red rectangle molecular emission bands be assigned to C_3?** Glinski, Robert J.; Nuth, Joseph A., III (Astrochemistry Branch, Code 691, Goddard Space Flight Center, National Aeronautics and Space Administration, Greenbelt, MD 20771 USA). *Astrophys. Space Sci.* **1997**, 249(1), 143–149 (Eng), Kluwer. A review with 34 refs. discussed the current information on the unique group of visible emission bands known as the Red Rectangle bands (RRBs). A lab. spectrum exactly matching these bands is not yet available; however, there is sufficient reason to hypothesize phosphorescence from C_3 as the source. The points in favor of the C_3/RRB hypothesis can be summarized as follows: (1) The RRBs are found in the spatial location where carbonaceous grains are being impinged upon by a bipolar outflow. (2) C_3 is known to accompany circumstellar carbon grains and may constitute a 'magic' fragment in the UV photofragmentation of C_n clusters. (3) the authors' recent observation of the spin–forbidden CO Cameron emission bands in this object suggests that charged particle impact excites triplet states. (4) The energy of the lowest triplet state of C_3 is known to be very close to that of the RRBs. (5) The RRBs display a vibrational spacing that is quant. consistent with C_3, including a rare neg. anharmonicity.

спектр.
обзор

C.A. 1998, 128, N 4

C_3^-

1997

126: 204893y Vibrational Spectroscopy of Small Matrix−Isolated Linear Carbon Cluster Anions. Szczepanski, Jan; Ekern, Scott; Vala, Martin (Department of Chemistry and Center for Chemical Physics, University of Florida, Gainesville, FL 32611 USA). *J. Phys. Chem. A* **1997**, 101(10), 1841−1847 (Eng), American Chemical Society. C cluster anions were generated, deposited in an Ar matrix, and studied spectroscopically. A new method involving a dual laser beam−induced Ar plasma using Y or W metal and graphite targets is introduced for the efficient prodn. of matrix−isolated C cluster anions. New bands found in the IR spectra of the deposited plasma mixt. were assigned to asym. stretching modes of the C_3, C_5, C_6, C_7, and C_9 anions. D. functional theory calcns. (B3LYP/6−31G* level) support the attribution of these bands to linear C cluster anions. Calculational results indicate that reactions between linear anionic clusters and linear neutral clusters are highly exothermic and that aggregation between anions and even−membered neutrals are more highly exothermic than between anions and odd−membered neutrals. The anion IR bands are photosensitive at irradn. wavelengths shorter than a certain threshold value. These values are ~0.5 eV higher than the corresponding vertical detachment energies of the vapor phase C_n^- species. The possibility that longer chain C anions are present in the C−rich circumstellar envelopes of C stars is discussed.

Di,
ИК спектр

(44)

C. A. 1997, 126, N 15

C_3^- (Om. 39013) 1997

Jan Szczepanski et al.,

стр-ра J. Phys. Chem., A 1997, 101,
7039-42.

C_3 (От. 39010) 1997

Lakhlifi A., Dahoo R. et al.;

теорет. расчт Chem. Phys., 1997, <u>222</u>, 241-257

A theoretical study of C_3 molecule trapped in rare gas matrices: Influence of bent

or linear configuration
on the infrared spectra.

C_3^+

1997

127: 100085r **A comparative ab initio study of the C_3^+, SiC_2^+, Si_2C^+ and Si_3^+ cations.** Lavendy, H.; Robbe, J. M.; Flament, J. P.; Pascoli, G. (Lab. dynamique moleculaire photonique, CNRS URA 779, Centre d'etudes recherches lasers applications, Univ. Lille 1, 59655 Villeneuve, Fr.). *J. Chim. Phys. Phys.-Chim. Biol.* **1997**, 94(4), 649–664 (Eng), Elsevier. The C_3^+, SiC_2^+, Si_2C^+ and Si_3^+ cations have been investigated at an ab initio high quality electronic correlation level of theory and with d. functional methods. Equil. structures, vibrational frequencies and relative energies have been detd. for cyclic and linear isomers. We have found that the homoat. C_3^+ and Si_3^+ are unambiguously cyclic while the heteroat. systems present very low barriers to linearity.

ab initio
расчет,
структура,
ν_i, D_e

㊸ ☒

C. A. 1997, 127, N 7

C_3

1997

127: 72335b Calculation of rotation–vibration energy levels in ground state C_3 by a Born–Oppenheimer–type separation of the vibration motions. Spirko, V.; Mengel, Markus; Jensen, Per (J. Heyrovsky Inst. Phys. Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Rep. CZ–18223). *J. Mol. Spectrosc.* **1997**, 183(1), 129–138 (Eng), Academic. The MORBID (Morse Oscillator Rigid Bender Internal Dynamics) model [P. Jensen, J. Mol. Spectrosc. 128, 478–501 (1988)] was used to det. effective bending potentials and reduced masses for C_3 in the lowest stretching vibrational states by performing a Born–Oppenheimer sepn. of the bending and stretching motions. These calcns. were based on a potential energy function obtained in a least–squares fit (using the MORBID program) to exptl. data for C_3. For the lowest stretching states of C_3, the vibration energies obtained from the effective Hamiltonians are in a very close agreement with their numerically exact counterparts (i.e., the energies detd. variationally in the MORBID approach), indicating a high accuracy of the Born–Oppenheimer sepn. employed.

Кол. вр.
уровни
энергии

С. А. 1997, 127, № 5

C_3^-

1997

127: 254545c **C_3^- Carbon Cluster Anion: Structure and Asymmetric Stretching Mode Frequency.** Szczepanski, Jan; Wehlburg, Christine; Vala, Martin (Department of Chemistry, University of Florida, Gainesville, FL 32611 USA). *J. Phys. Chem.* A **1997**, 101(38), 7039–7042 (Eng), American Chemical Society. C cluster anions were formed by a combination laser ablation/plasma generation method and then deposited in Ar matrixes and studied via FTIR spectroscopy. A full isotopic study of the C_3^- anionic cluster is reported. All 6 isotopomeric bands of the ν_3 antisym. stretching mode at 1721.8 cm^{-1} (all ^{12}C isotopomer) were obsd. and used together with a normal coordinate calcn. to deduce that C_3^- in Ar matrixes is linear. This is in agreement with previous high-level ab initio calcns. and with new d. functional theory (DFT) and ab initio (MP2) results. Frequency shifts for all 6 C_3^- isotopomers calcd. by DFT and MP2 approaches match the obsd. shifts. Evidence is presented that the C_3^- anionic clusters are formed by electron capture and not by fragment aggregation.

(структ. данн)

C.A.1997, 127, N18

C_3 OM 38858 1997

127: 72354g **Laser spectroscopy of C_3: Stimulated emission and absorption spectra of the A $^1\pi_u$−X $^1\Sigma^+_g$ transition.** Tokaryk, D. W.; Chomiak, D. E. (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON Can. K1A 0R6). *J. Chem. Phys.* 1997, 106(18), 7600−7608 (Eng), American Institute of Physics. Several bands of the A $^1\pi_u$−X $^1\Sigma^+_g$ transition of C_3 were obsd. between 24868 and 25140 cm^{-1} in a liq.−N cooled discharge through methane and He. The spectra were taken with a frequency−doubled continuous−wave Ti:sapphire ring laser. Bands were obsd. either in stimulated emission or in absorption. The stimulated emission spectra include the bands 020−000 $^1\pi^{(-)}_u$−$^1\Sigma_g$, 020−020 $^1\pi^{(-)}_u$−$^1\Sigma^+_g$, 020−020 $^1\pi^{(-)}_u$−$^1\Delta_g$, and 020−020 $^1\Phi_u$ −$^1\Delta_g$. Anal. shows that entanglement of the 020−000 $^1\pi^{(-)}_u$−$^1\Sigma^+_g$ band with the previously unanalyzed 020−020 $^1\Phi_u$−$^1\Delta_g$ band led to flaws in past rotational analyses of the A 020 $^1\pi^{(-)}_u$ level. The absorption spectra include two bands for which the positions of the Q branch heads are reported previously [Can. J. Phys. 45, 4103(1967)]. The 1st band is the 002−100 $^1\pi_u$−$^1\Sigma^+_g$ band, as suggested by Balfour et al. [J. Chem. Phys. 101, 10,343(1994)], and show that the 2nd is the 102−200 $^1\pi_u$−$^1\Sigma^+_g$ band.

$(A^1\Pi_u - X^1\Sigma_g^+)$

C.A. 1997, 127, N5

C_3

1998

спектр в матрице

129: 87461e **Laser–induced emission spectroscopy of matrix–isolated carbon molecules: Experimental setup and new results on C_3.** Cermak, Ivo; Forderer, Markus; Cermakova, Iva; Kalhofer, Stefan; Stopka–Ebeler, Helmut; Monninger, Gerold; Kratschmer, Wolfgang (Max–Planck–Institut fur Kernphysik, Postfach 103980, D–69029 Heidelberg, Germany). *J. Chem. Phys.* **1998**, 108(24), 10129–10142 (Eng), American Institute of Physics. The authors have studied small C mols. using a matrix–isolation technique. The authors' exptl. setup is described. The C clusters were produced by evapg. graphite and trapping the C–vapor mols. in solid Ar, where mol. growth could be induced by controlled matrix annealing. To identify the produced mols., absorption spectroscopy in the UV–visible and IR spectral ranges was applied. Addnl. characterization of the excited and ground states of the mols. was obtained from emission and excitation spectra. The mols. were excited by a pulsed dye laser system and the emission spectra were recorded with a high–sensitivity photodiode–array spectrometer. The authors

C. A. 1998, 129, № 7

present the authors' measurements on linear C_3. The A $^1\Pi_u$ excited state of linear C_3 was populated by the electronic transition A $^1\Pi_u$ X $^1\Sigma_g^+$, and the corresponding excitation spectra of the C_3 fluorescence (A $^1\Pi_u$ X $^1\Sigma_g^+$) and phosphorescence (a $^3\Pi_u$ X $^1\Sigma_g^+$) were studied. Comparison of excitation and absorption spectra yielded information on site effects due to the matrix environment. Emission bands in the fluorescence and phosphorescence spectra up to vibrational energies of 8500 cm^{-1} could be obsd. The radiation lifetime of the A $^1\Pi_u$ excited state of C_3 in solid Ar is shorter than 10 ns. The phosphorescence transition a $^3\Pi_u$ X $^1\Sigma_g^+$ decays in ~10 ms and its rise indicates fast vibrational relaxation within the triplet system. The authors' data support a linear ground state geometry for C_3 also in solid Ar.

C_3 Om 39395 1998

129: 222675v New $\tilde{A}$–$\tilde{X}$ vibronic bands of laser–vaporized C_3. Izuha, Mitsuaki; Yamanouchi, Kaoru (College of Arts and Sciences, Department of Pure and Applied Sciences, The University of Tokyo, 3–8–1 Komaba, Meguro–ku, Tokyo, Japan 153–8902). *J. Chem. Phys.* 1998, 109(5), 1810–1818 (Eng), American Institute of Physics. The laser–induced fluorescence (LIF) spectrum for the $\tilde{A}\,^1\Pi_u$–$\tilde{X}\,^1\Sigma_g^+$ band of C_3 was obsd. under jet–cooled conditions. From our previous report [Chem. Phys. Lett. 242, 435(1995)], in which the ν_3 fundamental in the $\tilde{A}\,^1\Pi_u$ state is 541.7(1) cm^{-1} through the first identification of the $\tilde{A}(0,0,1)$–$\tilde{X}(0,0,1)$ hot–band transition, we extended the measurements of the ν_3 related key bands; the high–resoln. spectra ($\Delta\nu$~0.08 cm^{-1}) of eight vibronically allowed Σ_u^+–Σ_g^+–type transitions and two Π_g–Σ_u^+ hot–band transitions were measured, and their rotational structures were analyzed. The detd. band–origin wave nos. and the symmetries of the rotational structures led to firm assignments of the vibrational levels in the $\tilde{A}\,^1\Pi_u$ state. Using the vibrational level energies of the $\tilde{A}(0,0,v_3)(v_3 = 1–3)$ levels, the anharmonic potential along the ν_3 mode in the $\tilde{A}\,^1\Pi_u$ state has double min. with a barrier height of 284.3 cm^{-1} at the linear configuration.

Спектр

$\tilde{A}\,^1\Pi_u - \tilde{X}\,^1\Sigma_g^+$

C. A. 1998, 129, N 17

C_3

2000

134: 170260n Severely perturbed vibrational structure in the 266−310 nm electronic transition of C_3. Izuha, Mitsuaki; Yamanouchi, Kaoru (Department of Chemistry, School of Science, The University of Tokyo, Bunkyo−ku, Tokyo, Japan 113−0033). *J. Chem. Phys.* **2000**, 113(24), 10999−11008 (Eng), American Institute of Physics. The laser induced fluorescence (LIF) of C_3 are measured under jet−cooled conditions in the wide UV region of 266−310 nm, and 173 vibronic bands are identified. Among them, 77 and 68 vibronic bands exhibit Σ−Σ type and Π−Σ type rotational structures, resp.. From the rotational anal., the band−origin wave nos. and the rotational consts. of the upper Σ and Π vibronic levels and K−type doubling parameters for the Π vibronic levels are detd. The rotational consts. for the Σ and Π vibronic levels exhibit, resp., similar distributions with almost the same mean values, $B' = 0.395(14)$ and $0.398(17)$ cm^{-1}, indicating that the Σ and Π vibronic levels have the same electronic origin and that the av. C−C bond distance of the upper electronic state in the obsd. energy range is ~1.331(25) Å, which is longer than the electronic ground $\tilde{X}\ ^1\Sigma_g^+$ state by 0.054(25) Å.

(Спектр, м.п.)
лазериндуц.
флуоресц. −
в широкой
ультрафиол.
обл.

C.A. 2001, 134, №12

The convolution and Fourier–transform analyses are performed sep. for the spectra composed only of $\Sigma-\Sigma$ type and $\Pi-\Sigma$ type vibronic bands to derive ests. of the vibrational fundamentals in the upper electronic state. The low ν_1 fundamental of 940(60) cm^{-1} derived from these analyses and the seemingly regular ν_1 progression in the convoluted spectra indicate that the bright character is carried primarily by the transitions to the vibrational levels in the $^1\Delta_u$ electronically excited state and is distributed into a large no. of the originally dark transitions to the vibrational levels in the $^1\Pi_g$ electronically excited state, resulting in the exceedingly complex vibronic band system.

2000

F: C3-
P: 3

133:356741 Spectroscopy of excited states of carbon anions above the photodetachment threshold. Lakin, Nicholas M.; Guthe, Felix; Tulej, Marek; Pachkov, Michail; Maier, John P. Institut fur Physikalische Chemie, Universitat Basel Basel, Switz. Faraday Discuss., 115(Molecular Photoionisation), 383-393 (English) 2000 Electronic transitions of C3- and C5- to states lying above the electron affinity of the neutral (EA) were recorded in the gas phase by laser photodetachment spectroscopy. The excited states are identified by comparison with absorption spectra for the mass-selected ions deposited in Ne matrixes and with ab initio calcns. The C2.SIGMA.u+-X2.PI.g transition and 2 higher energy band systems are obsd. for C3-, corresponding to excitation energies >1.5 eV above the EA. In the case of C5- the strongest features, at ~0.6 eV above the EA, are attributed to close lying 2.DELTA.g-X2.PI.u and 2.SIGMA.g--X2.PI.u transitions. The dominant configurations in these states identify them as long-lived Feshbach resonances. Lifetimes for these resonances in C3- are between 200 fs and 3 ps from the band widths.

C_3^- ОМ · 40359 2010

Naaman A., Bhushan K.G. et al.,

м.л. J. Chem. Phys., 2000, 113, N 11, 4662 – 4667

C_3 2000

Rey C., et al.,

abinitio
расчет
стр-ры
и
стабильн.

Phys. Rev. B: Condens. Matter Mater. Phys. 2000, 62 (19), 12640 – 43.

(см. №2; III)

F: C3+ 2000
P: 3

132:142209 Autoionizing states in electron-impact ionization of C3+. Scot M. P.; Teng, Huaguo; Burke, P. G. Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast Belfast BT7 1NN, U J. Phys. B: At., Mol. Opt. Phys., 33(2), L63-L70 (English) 2000 Results are reported on electron-impact ionization of C3+ in the energy range 290-350 eV obtained by the R-matrix with pseudo-states method (RMPS Pseudo-states and autoionizing states were explicitly included in the R-m expansion to take fully into account for the first time the interaction b the direct and indirect ionization processes. The calcd. resonance struc the ionization cross section is in good agreement with the expt. of Mulle al.; there is a small discrepancy in the normalization of the cross secti between theory and expt.

C.A. 2000, 132

2000

F: C3-
P: 3
132:200604 Electronic transitions of C3- above the photodetachment threshold. Tulej, M.; Fulara, J.; Sobolewski, A.; Jungen, M.; Maier, J. P Institute for Physical Chemistry, University of Basle Basel CH-4056, Switz. J. Chem. Phys., 112(8), 3747- 3753 (English) 2000 The A 2.DELTA.u .ltwarw. X 2.PI.g, B 2.SIGMA.u- .ltwarw. X 2.PI.g, and C 2.SIGMA.u+ .ltwarw. X 2.PI.g electronic transitions of C3- obsd. in a Ne matrix

C-A. 2000, 132

and in the gas phase, although the energy of the exc electronic states involved in these transitions is 1-1.5 eV above the photodetachment threshold. The excited Feshbach states are sufficiently long-lived that some of the bands in the gas-phase photodetachment spectr exhibit rotational structure. Assignment of the transitions is made from rotational anal. or profile simulations and theor. calcns. The b 4.PI.u 2.PI.g transition is also weakly obsd. The presence of such discrete ban though in the continuum, provides a means of detection for anions in the interstellar medium.

C_3^-

ОМ 40698

2001

134: 183734v A theoretical study of the Renner–Teller effect in the $X^2\Pi_g$ state of C_3^-. Leonard, C.; Panten, D.; Lakin, N. M.; Chambaud, G.; Rosmus, P. (Department of Chemistry, University of Cambridge, Cambridge, UK CB2 1EW). *Chem. Phys. Lett.* **2001**, 335(1–2), 97–104 (Eng), Elsevier Science B.V. Three–dimensional potential energy functions for the A" and A' components of the $X^2\Pi_g$ state of C_3^- were generated ab initio using the internally contracted multi–ref. CI method. The spin–orbit const. in this state was calcd. from a CAS–SCF wavefunction. These data were used to solve the linear/linear Renner–Teller problem variationally for J = 1/2, 3/2 and 5/2. Rovibronic levels for K=0, 1 and 2 were detd. for energies up to about 3800 cm^{-1}. The very large splitting between A" and A' was found to give rise to a strong mixing for the rovibronic Π and Δ bending states. The results are compared with those obtained exptl. and for similar mol. systems.

Реннер–Тел
лор эффект
в $X^2\Pi_g$ сост.

С. А. 2001, 134, N13

C_3 От. 41307 2002

Monninger G. et al.,
J. Phys. Chem. 2002, A106,
N24, 5779-5788.
Vacuum Ultraviolet Spectroscopy of the Carbon Molecule

C_3 in Matrix Isolated State: Experiment and Theory.

C_3^+

(От. 41460)

2002

$(\tilde{X}\,^2B_2)$

Wang R. et al.,
J. Mol. Struct. (Theochem), 2002, 587, 25-31.

стр-ра,
потенц.
энергия,
теор. рас.

C_3^- (ОМ 41460) 2002

($X^2\Pi_g$) Wang R. et al.,

стр-ра, J. Mol. Struct. (Theochem)
потенц. 2002, 587, 25-31.
Энергии,
теор.
расчет

C_3 см. 419/4 2003

J. Robert, M. Joyeux

теор. расчёт J. Chem. Phys. 2003, <u>119</u>, №16, 8761.

колеб. спектр. Canonical pertrubation theory versus

$\omega_1 = 1225$ см$^{-1}$ Born-Oppenheimer-type separation

$\omega_2 = 63$ см$^{-1}$ of motions: The vibrational dyna-

$\omega_3 = 2040$ см mics of C_3