

H502



Aniray & R.

1969

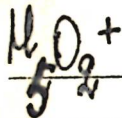
(J.P.)

J. Chem. Phys., 1969,
50, 5, 2012



($\text{C}_{60}\text{H}_{40}^+$)III

1970



Coul. n.

(50382d) Vibrational spectroscopy of the H_2O_2^+ ion (proton dihydrate). Hypothesis of a force field of generalized valence. Chemouni, Elie; Fournier, Michel; Roziere, Jacques; Potier, Jacqueline (Lab. Acides Miner., Fac. Sci., Montpellier, Fr.). *J. Chim. Phys. Physicochim. Biol.* 1970, 67(3), 517-21 (Fr). Spectra of H_2O_2^+ and D_2O_2^+ were identified in the cryst. compds. $\text{HClO}_4 \cdot 2\text{H}_2\text{O}$ and $\text{DClO}_4 \cdot 2\text{D}_2\text{O}$ at -180° . Assignments are given on the basis of a trans structure with sym. H bonding. Normal coordinate anal. by the Wilson method is made. Comparison of some of the force consts. for H_2O_2^+ (Bu class vibrations) with those of H_2O^+ are made. The bending vibration of end OH's (1680 cm^{-1}) is strongly coupled with the asym. vibration of the bridge. RCOQ

C.A. 1970.73.10

1970

 H_2O^+
52

ссыл. лист.

21 Б200. Колебательная спектроскопия иона H_5O_2^+ (дигидратированного протона). Исследование в предположении обобщенного валентного силового поля. Che-mouni Elie, Fournier Michel, Rozière Jacques, Potier Jacqueline. Spectroscopie de vibration de l'ion H_5O_2^+ (dihydrate du proton). Etude dans l'hypothèse du champ de force de valence généralisé. «J. chim. phys. et phys.-chim. biol.», 1970, 67, № 3, 517—521 (франц.; рез. англ.)

Исследованы ИК-спектры поглощения $\text{HClO}_4 \cdot 2\text{H}_2\text{O}$ (I) и $\text{DClO}_4 \cdot 2\text{D}_2\text{O}$ (II) при -180° в области $400—3600 \text{ см}^{-1}$. Отнесение наблюдавшихся ИК-спектров поглощения I, II проведено с учетом того, что согласно рентгенографич. данным (РЖХим, 1969, 14Б377) I и II имеют структуру типа $\text{H}_5\text{O}_2 + \text{ClO}_4^-$, т. е. в тв. состоянии в крист. решетке I, II присутствует дигидрати-

У. 1970. 21

ванный протон H_5O_2^+ (III) (D_5O_2^+ (IV)). В крист. состоянии I, II имеют пространственную группу $R\bar{3}m$ (D_{2h}^{16}) с четырьмя молекулами в элементарной решетке. Ионы ClO_4^- и III имеют локальную симметрию C_s и C_i соотв. Для изолированного иона III предположена симм. структура с атомом Н в центре симметрии (точ. группа симметрии C_{2h}). Вычислены силовые коэф. общего валентного силового поля изолированного иона III (все силовые коэф. взаимодействия угла со связью полагались равными нулю). Вычислено распределение потенциальной энергии для класса B_u иона III. Наблюдавшиеся частоты и вычисленные силовые коэф. иона III сопоставлены с соотв-щими величинами для иона H_3O^+ (точ. группа симметрии C_{3v}). Деф. кол., концевых ОН-групп $\nu_{12}(B_u) = 1680 \text{ см}^{-1}$ иона III сильно взаимодействует с асимм. вал. кол. Н-мостика $\nu_{11}(B_u) = 1770 \text{ см}^{-1}$ (1420 см^{-1} для IV).

А. Александров

XI 1078

1970

HF_2^- , H_5O_2^+ (номер. поверхность)

Kollman P.A., Allen L.C.
J. Amer. Chem. Soc., 1970, 92,
N21, 6101-7

10 (см. HF_2^-) III

$H_2OHOH_2)^+$

XI - 1079

1970

Кв. мех.
расчет

(91476f) SCF MO LCGO [linear combinations of gaussian orbitals] studies on hydrogen bonding. The system $(H_2OHOH_2)^+$. Kraemer, Wolfgang P.; Diercksen, Geerd H. F. (Max-Planck-Inst. Phys. Astrophys., Munich, Ger.). *Chem. Phys. Lett.* 1970, 5(8), 463-5 (Eng). The min. energy geometry of the $(H_2OHOH_2)^+$ system has a linear, symmetric H-bond with an equil. O-O distance 2.39 Å and a binding energy 32.24 kcal/mole relative to the systems H_2O and H_3O^+ in agreement with literature exptl. value (36 kcal/mole). Parts of the energy surface of the system were studied within the SCF MO LCGO framework with a Gaussian basis set to approx. the energy function. A very flat potential curve of the proton in the H bond makes possible a rather large proton shift (~ 0.3 Å) without any considerable change in energy. By continuous formation and splitting of the system or of longer chain structures of the same type), a proton can migrate relatively easily through an aq. soln. This may explain the high proton mobility in such solns.

FBJN

C.A. 1970. 73. 18

4502
(H₂OHON₂)⁺

XI - 1079

1970

10 Д133. Исследование водородной связи методом самосогласованных МО в виде линейных комбинаций гауссовых орбиталей. Система (H₂OHON₂)⁺. Крамерс Wolfgang P., Дирексен Geerd H. F. SCF MO LCGO studies on hydrogen bonding. The system (H₂OHON₂)⁺. «Chem. Phys. Lett.», 1970, 5, № 8, 463—465 (англ.)

Методом Рутана в сжатом базисе из гауссовых орбиталей (по 11 ф-ций s-типа и 7 — p-типа для атомов О и по 6 — s-типа для Н, сжатых до 5 и 4 соответственно для О и 3 для Н, с дополнительным включением 2 поляризационных ф-ций d-типа для каждого атома О и p-типа для Н) исследовано электронное строение двух геометрич. конфигураций системы (H₂OHON₂)⁺. Орбитальные экспоненты поляризационных ф-ций предварительно оптимизировались для Н₂О. Миним. энергией

(расчет)

09. 1970. 1079

обладает конфигурация с линейной симметричной Н-связью с равновесным расстоянием $O-O$ 2,39 Å, энергией связи 32,24 ккал/моль относительно $H_2O + H_3O^+$ (эксперим. значение 36 ккал/моль). Отмечено, что потенц. кривая для осуществляющего Н-связь центрального протона обладает очень слабо выраженным минимумом, ввиду чего возможно его отклонение от положения равновесия примерно на 0,3 Å без заметного изменения энергии.

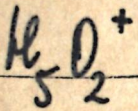
В. Л. Лебедев

11 XI 410 1970
 H_2O (Ap) $(OH^-, H_3O^+, H_5O_2^+, H_7O_3^+, H_9O_4^+,$
 $etc., n.n., - (H_3O_2^-, H_5O_3^-, H_7O_4^-))$

Paz M. de, Ehrenson, S., Friedman L,
J. Chem. Phys, 1970, 52, 47, 3362-3368 (cm)
Study of the H^+ and OH^- hydroxyl
ions by the CNDO/2 method.

Proc, 1970, 80, 165 $W(OH^-; \bar{H})$
1017

1970

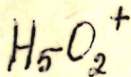


V_i

604
11-409

5116283 Spectroscopic study of perchloric acid dihydrate $H_5O_2^+ClO_4^-$. Pavia, Andre C.; Giguere, Paul A. (Centre Rech. Atom. Mol., Univ. Laval, Quebec, Can.). *J. Chem. Phys.* 1970, 52(7), 3551-4 (Eng). The ir and Raman spectra of the $H_5O_2^+$ ion have been obsd. in the cryst. dihydrate of $HClO_4$ at -180° . Existence of $H_5O_2^+$ ions in that crystal, 1st detected by x-ray diffraction, is further confirmed by the absence of certain characteristic bands of the H_3O^+ and H_2O species. The spectra are consistent with a centrosym. $H_2O-II-OH_2$ structure of trans configuration approximating the C_{2h} point group. In the deuterated compd. the ir spectra indicate the same structure for the $D_5O_2^+$ ion. Interference from the strong bands of ClO_4^- prevented identification of all the fundamentals of $H_5O_2^+$.
RCJQ

C.A. 1970. 72. 22

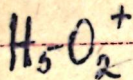


XV - 3203

1972

(Vi) - 81760n Raman and infrared spectroscopic studies of hydrochloric acid dihydrate. Vibrational spectra of the H_5O_2^+ ion. Roziere, J.; Potier, J. (Lab. Acides Miner., Univ. Sci. Tech. Languedoc, Montpellier, Fr.). *J. Mol. Struct.* 1972, 13(1), 91-103 (Fr). An ir and Raman study of cryst. $\text{HCl} \cdot 2\text{H}_2\text{O}$ was made at 50-4000 cm^{-1} . This confirms the occurrence of the H_5O_2^+ ion and allows the assignment of its fundamental vibrations. A comparison with the known spectra of H_5O_2^+ salts with different anions shows that the formation of external H bonds perturbs the central short H bond vibrations.

C. H. 1972. 47.12



поверх.
поверхн.
и

3 Д140. Полуэмпирическое изучение водородной связи в дигидратированном ионе водорода H_5O_2^+ . Anderson George R., Jiang George J. A semiempirical study of hydrogen bonding in the diaquohydrogen ion, H_5O_2^+ . «J. Phys. Chem.», 1973, 77, № 21, 2560—2563 (англ.)

На основе предложенной ранее модели водородной связи (см. РЖФиз, 1973, 11Д278) построена потенциальная поверхность и рассчитаны частоты колебаний для дигидратированного протона $[\text{H}_2\text{OHOH}_2]^+$. Рассматриваемый ион хорошо изучен экспериментально и кроме того для него имеются неэмпирич. расчеты потенц. поверхности. Все эти данные использованы для определения параметров потенциальной поверхности H_5O_2^+ . Рассчитанные на основе полуэмпирич. потенциальных функций частоты колебаний иона хорошо согласуются с результатами исследований ИК-спектров. Найдено, что полученные параметры потенц. поверхности не сильно меняются при переходе к другим соединениям с водородной связью, что позволяет их применять для расчета малоисследованных соединений с водородной связью.

А. И. Дементьев

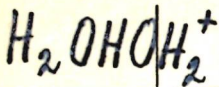
1973

1473-IX

9.1974
13

NL - 5741

1973



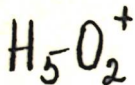
149627y Semiempirical study of hydrogen bonding in the diaquohydrogen ion, H_5O_2^+ : Anderson, George R.; Jiang, George J. (Dep. Chem., Bowdoin Coll., Brunswick, Maine). *J. Phys. Chem.* 1973, 77(21), 2560-3 (Eng). The $\text{H}_2\text{OHCH}_2^+$ ion is a H bonded species of considerable stability and is one for which both exptl. and theor. data are available. In this study, H-bonding properties of H_5O_2^+ are computed by means of a semiempirical model for linear H bonds reported earlier and the results are compared and discussed. Agreement is found to be favorable particularly with respect to vibration frequencies. Furthermore, the model potential energy function contains semiempirical parameters which are not found to change appreciably from 1 system (reported earlier, HF_2^-) to another (H_5O_2^+). These results suggest that perhaps the model for H bonding is sufficiently general to be applied to other H-bonded species for which fewer exptl. data are available.

номен.

ноб. х.и.

кб. мех. паерем.

C. A. 1973, N26, 79



XI - 3989

1973

7073m Tunneling in the proton transfer between two water molecules. Flanigan, Marie C.; De la Vega, Jose R. (Dep. Chem., Villanova Univ., Villanova, Pa.). *Chem. Phys. Lett.* 1973, 21(3), 521-4 (Eng). SCF CNDO calcs. were performed for the species H_5O_2^+ at several positions of the intervening proton and at interoxygen distances of 2.65, 2.70, and 2.75 Å. The energy profile was fitted to a potential energy function contg. a quadratic term plus a Gaussian. The eigenvalues and eigenvectors were obtained by using the variational method with the eigenfunctions of the parabolic potential as basis set. The results indicate that at 2.65 Å the top of the barrier is below the 1st energy level and that at 2.75 Å the 1st 2 energy levels are below the top of the barrier with the splitting of the symmetric-antisymmetric pair of 0.00132 at. units indicating that tunneling occurs at a frequency of 10^{14} reciprocal sec.

m.n.

pacrem

C.A. 1974. 80 n2

$[H_5O_2]^+$

1973

1 Д128. Влияние корреляционных эффектов на энергетические кривые переноса протона. Катион $[H_5O_2]^+$. Meyer Wilfried, Jakubetz Werner, Schuster Peter. Correlation effects on energy curves for proton transfer. The cation $[H_5O_2]^+$. «Chem. Phys. Lett.», 1973, 21, № 1, 97—102 (англ.)

Неэмпирическим методом ССП МО ЛКАО в расширенном гауссовом базисе и методом ССП МО ЛКАО в валентном приближении ППДП в обоих случаях с учетом конфигурационного взаимодействия рассчитаны потенц. кривые для движения протона для структур $[H_5O_2]^+$ (I) 4 типов симметрии. Обнаружено, что энергетич. барьер для симметричного потенциала с 2 минимумами очень чувствителен к учету корреляции. Так, при расстоянии O—O 2,74 Å он оценен в 9,5 и 7,0 ккал/моль при расчетах без учета и с учетом корреляционных эффектов. Данные метода ППДП качественно согласуются с неэмпирическими. Отмечено, что корреляционные вклады индивидуальных электронных пар для движения протона в I и для диссоциации одной связи O—H в $[H_3O]^+$ аналогичны. Проведено детальное обсуждение обоих процессов.

расчет
потенц.
крив.

ф 1974
N 1

40925.8718
TC, Ch, Ph

40892
 $H_5O_2^+$

1974
13-6426

Bates J.B., Toth L.M.

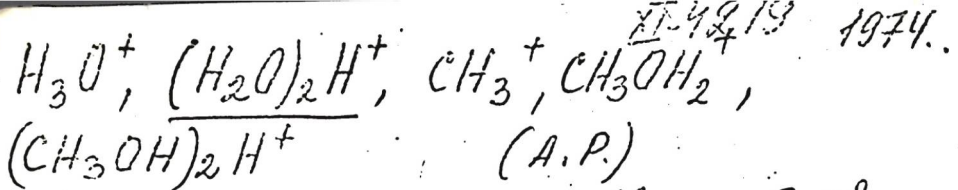
Vibrational spectra of $H_5O_2^+$ ion in crys-
talline $YN O (C O)_2 \cdot H_2O$.

"J. Chem. Phys.", 1974, 61, N 1, 129-137

(англ. 0139171)

162 165 104

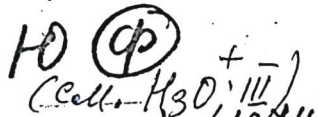
ВИНИТИ



Heinen H. J., Roellgen F. W.,
 Beckey H. D.,
 Z. Naturforsch., Teil A, 1974, 29(5),
 773-81.

Appearance potentials of field ions

C.A. 1974. 31/12. 70013C



$H_5O_2^+$

1975

Picotin G.

(Di)

" Adv. Mol. Relax Processes
1975, I, N3, 177-188 (univ)

(cu HSBCh₆; III)

70218.3710

Ch, TC

дог. кл. 3.6
54997 GR

$H_5O_2^+$

1976

* 4-16838

Schiöberg Dag, Zundel Georg.

$H_5O_2^+$ and other easily polarizable hydrogen bonds in aqueous solutions of

H_2SO_4 : "Z. Phys. Chem." (BRD), 1976,

№102, N 5-6, 169-174

(англ., рез. нем.)

0812 ПКК

773 775

804

ВИНИТИ

$H_5O_2^+$ обзор [оттиск 5905] 1974.
(сер. сборник викариу едурканов)
Sunner J.

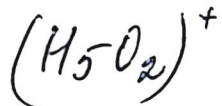
мон-мол.
р-ция,
монументы

Reactions of gas-
-phase ions studied
by the charge trans-
fer technique.
Lund, ● 1974. (Sweden)

$H_5O_2^+$ 6644 1978
Janoschen R. et al.

exp. 1238 - 1245

Calculated and Observed
Isotope Effects with
Easily Polarizable
Hydrogen and Deuterium
Bonds.



Lomnick 8447 / 1979

Feinel G.

Chem. Phys. Lett.

1979, 65 (2), 324-26

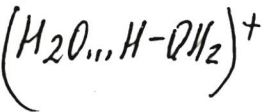
γ₀₋₀

возбужд.

связь

номер.

привес



оттиск 10098 1980

Desmeules P. J., et al.

интермол.
взаимод.
энергии
связей
квант. мех.

J. Chem. Phys., 1980, 72
(9), 4731-48

$H_3O_2^+$

1983

99: 202777p Calculation of infrared spectra of $H_3O_2^+$ and $H_3O_2^-$ groups. Yuhnevich, G. V.; Kokhanova, E. G. (USSR). Zh. Prikl. Spektrosk. 1983, 39(4), 617-21 (Russ). The frequencies of the harmonic vibrations of $H_3O_2^+$ and $H_3O_2^-$ ions were calcd. The forms of vibrations, the intensities of absorption bands and relative shifts of these bands caused by partial isotopic substitutions were obtained. The calcns. show that, besides the already known bands, the $H_3O_2^+$ ion absorption and scattering spectra should have bands near 400 cm^{-1} and 700 cm^{-1} , resp.

ν_i , ν_k ν_{cryst}

~~⊗~~ (7) $H_3O_2^-$

C.A. 1983, 99, N24

$H_5O_2^+$

1983

6 Б1204. Расчет инфракрасных спектров группировок $H_5O_2^+$ и $H_3O_2^-$. Юхневич Г. В., Коханова Е. Г. «Ж. прикл. спектроскопии», 1983, 39, № 4, 617—621 (рез. англ.)

Вычислены частоты гармонич. кол. ионов $H_5O_2^+$ и $H_3O_2^-$, образующихся в кристаллогидратах и водн. р-рах сильных к-т и оснований. Найдены формы этих колебаний, интенсивности соотв-щих им полос поглощения и относит. смещения этих полос, возникающие при частичном дейтерировании ионов. Расчет показал, что, кроме уже обнаруженных полос, ион $H_5O_2^+$ должен иметь в спектрах поглощения и рассеяния полосы, соотв. около 400 и 700 cm^{-1} . Резюме

ν_i ;

(4) 12

Х. 1984, 19, N 6

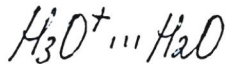
$H_5O_2^+$

[om. 18991] 1984

Толубев Н.С.

сверное-
нее

Жел. риз., 1984, 3,
N 5, 772-774.



1984

102: 101009q Theoretical determination of the potential surface for the system $H_3O^+ \cdots H_2O$ [diaquahydrogen(1+)] at intermediate and large intermolecular distances. Kochanski, E. (Univ. Louis-Pasteur, Strasbourg, Fr.). *Nouv. J. Chim.* 1984, 8(10), 605-10 (Eng). To obtain a relation for calcg. the potential-energy surface of $H_5O_2^+$ [diaquahydrogen(1+) ion], ab-initio calcns. with Gaussian wave functions were done on (a) the total energy of H_3O^+ [oxonium ion], (b) the intermol. potential (including the dispersion contribution) between H_3O^+ and H_2O [water mol.], and (c) the stabilization energy of $H_5O_2^+$, with respect to $H_3O^+ + H_2O$, for 2 different mol. structures of $H_5O_2^+$.

ab initio
racem
homerus.
нобгхх.

c. A. 1985, 102, N12



1984

Kearley Gordon J.,
Fitch Andrew N., et al.

$H_5O_2^+$ can.
noce.

J. Mol. Struct., 1984,
125, N 3-4, 229-241.

(H_3O^+ ; III)

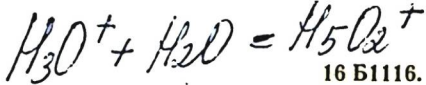
$H_5O_2^+$

1984

структура

100: 109356e SCF-LCGO calculations of the nonrigid structure of dioxonium ion. A basis for a structural analysis of $H_5O_2^+$ in crystals. Potier, A.; Leclercq, J. M.; Allavena, M. (Lab. Acides Miner., USTL, 34060 Montpellier, Fr.). *J. Phys. Chem.* 1984, 88(6), 1125-30 (Eng). The structure of the $H_5O_2^+$ cation was detd. by ab initio LCAO-SCF calcs. using as basis set functions (11s,7p) and (4s) on O and H, resp., augmented by *d* and *p* polarization functions. A minimization of the total energy was performed with respect to the 3 angular coordinates and to the O...O distance followed by a full optimization using the gradient method. As expected from exptl. data, the $H_5O_2^+$ system has a rather flexible structure whose symmetry elements reduce to a C_2 axis. Terminal H_2O mols. may execute large-amplitude motions of rotation and oscillation around the O...O direction at room temp. These results bring some support to the interpretation of the spatial arrangement of both H_2O mols. in the vicinity of the central proton as depending essentially on the direction of their lone pairs, and to a possible bending of the H bridge ($-OHO \simeq 178^\circ$). The various structures of $H_5O_2^+$ exhibited in solid medium are in the range of the predicted structures.

e.A.1984, 100, N 14



1984

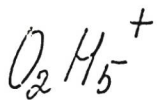
16 Б1116. Неэмпирический расчет термодимических данных для газофазного кластерообразования $\text{H}_3\text{O}^+ + \text{H}_2\text{O} = \text{H}_5\text{O}_2^+$. Ab initio calculation of the thermochemical data on the $\text{H}_3\text{O}^+ + \text{H}_2\text{O} = \text{H}_5\text{O}_2^+$ gas-phase clustering. Yamabe Shinichi, Minato Tsutomu, Hirao Kimihiko. «J. Chem. Phys.», 1984, 80, № 4, 1576—1578 (англ.)

Неэмпирическим методом ССП МО ЛКАО в различных базисах с использованием станд. ур-ний статистической термодинамики оценены ΔH° и ΔS° для газофазной реакции $\text{H}_3\text{O}^+ + \text{H}_2\text{O} = \text{H}_5\text{O}_2^+$. Вклад электронной корреляции учтен методом конфигурац. взаимодействия (КВ). Все геометрич. параметры оптимизированы. Миним. базис ОСТ-3 ГФ существенно переоценивает ΔH° и ΔS° , хотя и приводит к правильной геометрии иона H_3O^+ . Базисы, дополненные поляризац. ф-циями, приводят к ΔH° и ΔS° , сравнимым с их эксперим. значениями. Корреляц. вклад равен ~ 3 ккал/моль. Вклад энергии нул. кол. и т-рных эф-

ком., см.,
 $\Delta H, \Delta S, \Delta G$;

X. 1984, 19, N 16

фактов менее значителен. Наиболее значения термодинамических данных, полученные для исследованной реакции, равны: $\Delta H^\circ = -35,5$ ккал/моль, $\Delta S^\circ = -28,8$ э. е. и $\Delta G = -26,9$ ккал/моль ($T = 298,15$ К). И. Н. Сенченко



[Om. 22 492]

1985

Del Bene J.E., Frisch M.J.,
Pople J.A.,

теорет.
расчет
структур

J. Phys. Chem., 1985,
89, N 17, 3669-3674.



1985

4 Б1269. Влияние механической и электрооптической ангармоничности на колебательные спектры ионов. Юхневич Г. В., Тараканова Е. Г. «Применение колебат. спектров к исслед. неорган. и координац. соедин. 10 Всес. науч. совещ. Тез. докл.». Б. М., 1985, 12

Проведен анализ ряда систем с сильными Н-связями для проявления в их колебат. спектрах ангармонич. составляющей. Рассчитаны колебат. спектры ионов H_5O_2^+ и H_3O_2^- . Результаты расчетов показали, что ангармонизм колебаний этих ионов велик, что приводит к изменению ряда их частот на десятки %. В то же время общая картина спектра остается неизменной.

Из резюме

расчет
колебат.
спектров

(4) 17

X. 1986, 19, N 4

$H_5O_2^+$

DM. 21360

1985

10 Д85. Расчет колебательных спектров ионов $H_5O_2^+$ и $H_3O_2^-$ в ангармоническом приближении. Calculation of vibrational spectra of $H_5O_2^+$ and $H_3O_2^-$ ions in anharmonic approximation. Yukhnevich G. V., Kokhanova E. G., Pavlyuchko A. I., Volkov V. V. «J. Mol. Struct.», 1985, 122, № 1-2, Suppl.: «Theochem», 1985, 23, № 1-2, 1—13 (англ.)

расчет
колебательных
спектров

Полуэмпирическим методом ППДП выполнен расчет квадратичных, кубических и квартичных силовых коэф. и первых и вторых частных производных дипольного момента по внутренним колебательным координатам для водородных мостиков. О...Н...О в ионах $H_5O_2^+$ и $H_3O_2^-$. Из полученных величин силовых коэф. и электроопт. параметров вычислены частоты и интенсивности ИК-полос поглощения этих ионов. Результаты расчета согласуются с эксперим. данными. Отмечено, что наблюдаемое снижение частоты валентного колебания ОН-связи при образовании Н-связи связано со снижением величины валентной силовой постоянной F_{11} , положительный коэф. взаимодействия F_{12} не дает заметного вклада в частоту.

М. Р. Алиев

(4) 

ф. 1985, 18, № 10

$H_5O_2^+$

am. 21360

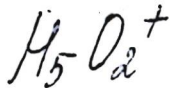
1985

18 Б1252. Расчет колебательных спектров ионов $H_5O_2^+$ и $H_3O_2^-$ в ангармоническом приближении. Calculation of vibrational spectra of $H_5O_2^+$ and $H_3O_2^-$ ions in anharmonic approximation. Yukhnevich G. V., Kokhanova E. G., Pavlyuchko A. I., Volkov V. V. «J. Mol. Struct.», 1985, 122, № 1—2, Suppl.: «Theochem», 23, № 1—2, 1—13 (англ.)

Методом ППДП рассчитаны потенциальные поверхности (ПП) O...H...O мостиковых связей в ионах $H_5O_2^+$ (I) и $H_3O_2^-$ (II), контуры к-рых свидетельствовали о почти идеальной симметрии ионов и сильном пожит. динамич. взаимодействиях связей O...H. На основе аппроксимации ПП рядом Тейлора 4-й степени вычислены силовые константы связей, оценены силовые константы и коэф. эл. ангармоничности углов, соседних к H-связям. Спектры I, II рассчитанные с учетом мех. и эл. ангармоничностей, хорошо согласуются с эксперим. Поглощение ниже 3300 см^{-1} отнесено к обертонам и составным частотам. Наиболее интенсивные полосы в характерной для I, II обл. ($\sim 1000\text{ см}^{-1}$) расположены в последовательности $\nu_{\gamma^*} > \nu_{\rho_{as}} > \nu_{\tau}$. Н. Л. Арюткина

расчет
колебательных
спектров

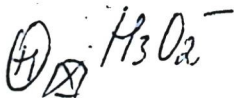
X. 1985, 19, N 18



(Om. 21360) 1985

103: 44955q Calculation of vibrational spectra of H_5O_2^+ and H_3O_2^- ions in anharmonic approximation. Yuhnevich, G. V.; Kokhanova, E. G.; Pavlyuchko, A. I.; Volkov, V. V. (N.S. Kurnakov Inst. Gen. Inorg. Chem., 117071 Moscow, USSR). *THEOCHEM* 1985, 23(1-2), 1-13 (Eng). The potential surfaces of 2-dimensional O...H...O bridges were calcd. by the CNDO method for H_5O_2^+ and H_3O_2^- ions with a modified potential of the at. frameworks. Approximating the surfaces by a 4th power Taylor series, the force parameters up to the 4th order were computed for the bonds forming H bridges. The force const. and the elec. anharmonicity coeffs. of the angles adjacent to H bonds were estd. Vibrational absorption spectra calcd. for isolated ions with due regard to the elec. and mech. anharmonicity are in good agreement with the exptl. data.

неоп. параметр
сил. неоп.,
D₁;



C.A. 1985, 103, N6

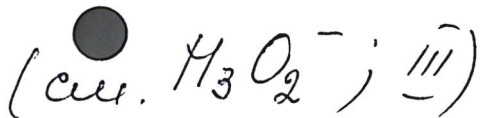


1986

Burshtein K. Ya.,
Isaev A. N.

каталог
поверхн.,
теор.
расчет

Zh. Strukt. Khim.
1986, 27(3), 3-7.



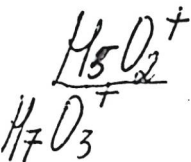
1986

11 Д73. Неэмпирическое исследование колебательных спектров гидратов ионов $\text{H}^+(\text{H}_2\text{O})_2$ и $\text{H}^+(\text{H}_2\text{O})_3$. An ab-initio study of the vibrational spectra of the ion hydrates $\text{H}^+(\text{H}_2\text{O})_2$ and $\text{H}^+(\text{H}_2\text{O})_3$. Williams G. R. J. «J. Mol. Struct. Theochem.», 1986, 138, № 3—4, 333—340 (англ.)

Неэмпирическим методом ССП МО ЛКАО в базисе 4-31ГФ рассчитана равновесная геометрия и колебательные частоты (в гармонич. приближении) ионов H_5O_2^+ (I) и H_7O_3^+ (II). Полученные результаты сопоставлены с данными проведенных ранее расчетов $(\text{H}_2\text{O})_2$ (III). Показано, что наиболее выгодными являются структуры $\text{H}^+(\text{H}_2\text{O})_2$ для I и $\text{H}_3\text{O}^+(\text{H}_2\text{O})_2$ для II симметрии D_{2d} и C_{2v} соответственно. Идентифицирован ряд общих колебательных мод. Основные различия в колебательных частотах связаны с наличием мостиковых атомов. Для I и II увеличение ионности связей и упрочнение мостика $\text{O}-\text{H}-\text{O}$ в сравнении с III проявляется в увеличении колебательных частот.

В. Л. Лебедев

ср. 1986, 18, № 11 (см. H_5O_2^+ ; III)



(см. л.)

(4)

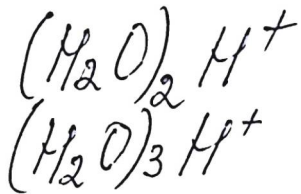


1986

105: 85520d An ab-initio study of the vibrational spectra of the ion hydrates (protonated dimer and trimer of water). Williams, G. R. J. (Electron. Res. Lab., Def. Sci. Technol. Organ., Adelaide, 5001 Australia). *THEOCHEM* 1986, 31(3-4), 333-40 (Eng). The vibrational spectra of the ions $H_5O_2^+$ and $H_7O_3^+$ were calcd. using ab initio MO theory in the harmonic approxn. The calcns. indicate that the structures of the two ions are best represented as $H^+(H_2O)_2$ and $H_3O^+(H_2O)_2$, resp. The vibrational frequencies of the two ion hydrates are analyzed in terms of their resp. structures and compared with the previously reported vibrational spectrum of the neutral water dimer. The general IR absorption characteristics of the two ion hydrate clusters and those of the neutral $(H_2O)_2$ cluster are discussed.

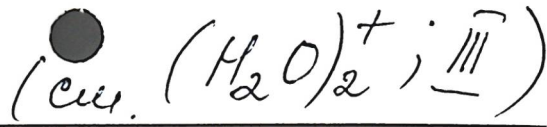
(KOME. CACKMP)
Di

C.A. 1986, 105, N10



(28167) 1987
Shiromaru H.,
Shirohara H.,
et al.

Chem. Phys. Lett., 1987,
141, N1-2, 7-11.



$H_3O^+ \cdot H_2O$

no. 29182

1988

Briznyuk A. A., Voi-
tyuk A. A.

meop.
pacrēm

J. Mol. Struct. Theo-
Chem., 1988, 164, №3-4,
● 343-349.

$(H_5O_2)^+$

1988

109: 237482r Internal rotation in the diaquahydrogen(1+)
($H_5O_2^+$) ion: a quasielastic neutron scattering study of
12-tungstophosphoric acid hexahydrate. Pressman, Helen A.;
Slade, Robert C. T. (Dep. Chem., Univ. Exeter, Exeter, UK EX4
4QD). *Chem. Phys. Lett.* 1988, 151(4-5), 354-61. (Eng).
Variable temp. quasielastic neutron scattering studies are used to
investigate motions in 12-tungstophosphoric acid hexahydrate
($H_3PW_{12}O_{40} \cdot 6H_2O$). A two-fold reorientation (180° flip) of "terminal
waters" within centrosym. $H_5O_2^+$ ions has been identified and the
results of a previous NMR study reinterpreted. The activation
energy and Arrhenius prefactor for the reorientation are 14 kJ mol⁻¹
and 6×10^{-13} s, resp.

V_0 , meap.
Nacem

c.A. 1988, 109, N26

$H_5O_2^+$

1988

Паракамова Е. Г.

м. п.

Ис. прикл. спектроскопии.
1988. 49, № с. 636-642.

(с.  $H_3O_2^-$; III)

$H_5O_2^+$
(P-P)

1989

(UK)

/ 111: 66864b IR spectrum of diaquahydrogen ($H_5O_2^+$) ion in acid solutions. Maiorov, V. D.; Librovič, N. B. (Inst. Khim. Fiz. im. Semenova, Moscow, USSR). *Izv. Akad. Nauk SSSR, Ser. Khim.* 1989, (4), 967-8 (Russ). IR spectrum of $H_5O_2^+$ ion was obtained by subtracting the overlapping bands from the attenuated total internal reflection IR spectra of an aq. soln. of $MeSO_3H$. A broad absorption band was found with the max. at $\sim 2350\text{ cm}^{-1}$ that was not attributed to $H_5O_2^+$ before.

C.A. 1989, 111, N 8

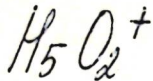
$H_5O_2^+$

Im 32154

1989

111:140949b Incoherent inelastic neutron scattering studies of proton conducting materials trivalent metal acid sulfate hydrates. Part I. The vibrational spectrum of dihydrated proton ($H_5O_2^+$). Jones, Deborah J.; Roziere, Jacques; Penfold, Jeffrey; Tomkinson, John (Lab. Acides Miner., Univ. Sci. Tech. Languedoc, 34060 Montpellier, Fr.). *J. Mol. Struct.* 1989, 195, 283-91 (Eng). To clarify certain aspects concerning the assignment of bands in the vibrational spectrum of the dihydrated proton $H_5O_2^+$, the incoherent inelastic neutron scattering spectra of three inorg. compds. contg. this ion were recorded. The spectrum of $HClO_4 \cdot 2H_2O$, obtained at 77 K, unambiguously reflects one type of ordered $H_5O_2^+$ ion, and contains no contribution from the counterion. Those of the layer structured proton conductors $HFe(SO_4)_2 \cdot 4H_2O$ and $HIn(SO_4)_2 \cdot 4H_2O$, recorded at 20 K, are consistent with the presence of $H_5O_2^+$ as the only mobile protonic species. The spectra were fully assigned in terms of vibrations, librations, and translations of $H_5O_2^+$.

корисам-
ночно ет.



1990

114: 215012p Study of the geometrical configuration, internal rotation and the proton transfer process for diaquahydrogen(1+) (H_5O_2^+). Zhu, Zhixian; Ming, Yaqiang; Wang, Demin (Dep. Tech. Phys., Beijing Univ., Beijing, Peop. Rep. China). *Jisuanji Yu Yingyong Huaxue* 1990, 7(4), 303-14 (Ch). The geometrical configuration of H_5O_2^+ is optimized by using the STO-3G basis sets. It belongs to the D_{2d} point group. The length of the H bond is 2.29 Å. The calcd. results show H_5O_2^+ can rotate freely around the H bond and its barrier of rotation is 0.404 kcal/mol, and the dipole moment and charge distribution on each atom are invariable. The proton transfer process on the H bond has no influence on the geometrical configuration of the system.

geom. conf.,
rotation

C.A. 1991, 114, N 22

$H_5O_2^+$

(Om. 35978)

1991

компьютерная
расчёт

115: 120541s Structure and properties of diaquahydrogen(1+) ($H_5O_2^+$). Peeters, D.; Leroy, G. (Lab. Chim. Quantique, Univ. Cathol. Louvain, B1348 Louvain-la-Neuve, Belg.). *J. Chim. Phys. Phys.-Chim. Biol.* 1991, 88(4), 411-20 (Eng). An anal. of the $H_5O_2^+$ system was performed using a quantum-chem. approach. Optimized geometries were obtained from more and more elaborate basis sets as SCF as well as post-SCF (MP2 and CI) levels of sophistication. While the system's symmetry is C_s near the Hartree-Fock limit, it becomes C_2 once correlation is introduced. A vibrational anal. of this structure is further realized at MP2 level. The latter combined to a full MP4 calcn. performed with the best basis set allows to obtain some thermodyn. insight to the formation reaction.

C.A. 1991, 115, N12

$H_5O_2^+$

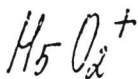
1991

4 Д347 ДЕП. Собственные колебания иона $H_5O_2^+$
/ Тараканова Е. Г., Юхневич Г. В.; Ред. Ж. прикл.
спектроскопии.— Минск, 1991.— 13 с.: ил.— Библиогр.:
16 назв.— Рус.— Деп. в ВИНТИ 03.01.91, № 49—
В91

Рассчитан спектр иона $H_5O_2^+$ с учетом динамиче-
ского и электрооптич. ангармонизма колебаний. Полу-
ченные результаты согласуются с известными эксперим.
данными. На основании проведенного расчета дана
интерпретация колебательных полос иона $H_5O_2^+$ в
спектрах неупругого рассеяния нейтронов и ИК-погло-
щения. Показано, что основной причиной возникнове-
ния непрерывного поглощения в спектре иона $H_5O_2^+$
является электрооптич. ангармонизм колебаний симмет-
ричной водородной связи. Автореферат

М.П.

ср. 1991, № 4

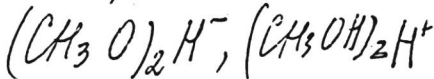
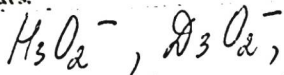
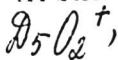


1991

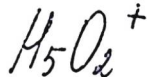
116: 94334a Nature of the high-intensity bands of combination vibrations of $(A...H...A)^+$ complexes. Yakhnevich, G. V.; Tarakanova, E. G. (Inst. Obshch. Neorg. Khim. im. Kurnakova, Moscow, USSR). Dokl. Akad. Nauk SSSR 1991, 320 (5), 1137-41 [Chem.] (Russ). The continuous absorption in the IR spectra of a bisolvated proton $(A...H...A)^+$ is due to a high no. of intense bands of combination vibrations and overtones found in the region 3500-1000 cm^{-1} . Approx. 95% of the total absorption in the $O...H...O$ bridge combination-vibration bands can be attributed to the electrooptical anharmonism of vibrations. The calcs. of the frequencies and intensities of the bands of fundamental vibrations, combination vibrations with the total quantum no. 3, and overtones up to the 5th order were performed for $H_3O_2^+$, $D_3O_2^+$, $(MeOH)_2H^+$, $H_3O_2^-$, $D_3O_2^-$, and $(MeO)_2H^-$ complexes.

(Di)

(75)



c.A. 1992, 116, N 10



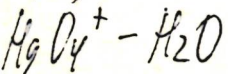
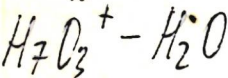
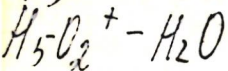
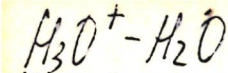
1992

118: 67216y An initio study on the effect of attaching a hydrogen molecule to the diaquahydrogen(1+) ($(H_5O_2)^+$) ion. Bosch, Enric; Moreno, Miquel; Lluch, Jose M. (Dep. Quim., Univ. Auton. Barcelona, Bellaterra, Spain 08193). *J. Chem. Phys.* 1992, 97(9), 6469-71 (Eng). Ab-initio energy calcs. (using the Moeller-Plesset perturbation theory up to fourth order with the 6-31G(D, P) basis set) were done for the $H_5O_2^+$ ion with and without a hydrogen mol. attached to it. In agreement with exptl. results, a C_2 structure, which gives rise to only two high O-H stretching frequencies, was predicted to be the only min. of the isolated ion; whereas when H_2 was present, again only one min. was found which can be roughly assigned to be of the C_2 -type structure. This structure was predicted to have four active O-H stretching frequencies, again in agreement with the exptl. spectrum.

(meop. fauen)

C.A. 1993, 118, 48

1993



120: 62827e Stepwise solvation enthalpies of protonated water clusters: collision-induced dissociation as an alternative to equilibrium studies. Dallek, N. F.; Honma, Kenji; Armentrout, P. B. (Dep. Chem., Univ. Utah, Salt Lake City, UT 84112 USA). *J. Am. Chem. Soc.* 1993, 115(25), 12125-31 (Eng). Abs. reaction cross sections for interaction of $H_3O^+(H_2O)_x$ ($x = 1-5$) with xenon are detd. from thermal energies of 20 eV (CM) by using guided ion beam mass spectrometry. In all cases, the primary product is endothermic collision induced dissociation (CID) to lose one water mol. At higher energies, addnl. water mols. are lost successively, indicating that evapn. is the primary pathway for dissociation. The proper interpretation of the primary CID thresholds is considered in detail and the adjustment of these values to enthalpies at std. conditions is discussed. When the effects of multiple ion-mol. collisions, internal energy of the clusters, and dissociation lifetimes are properly accounted for, the following bond dissociation energies (in eV) are detd.: $D_0[H_3O^+ - H_2O] = 1.35 \pm 0.06$, $D_0[H_5O_2^+ - H_2O] = 0.86 \pm 0.06$, $D_0[H_7O_3^+ - H_2O] = 0.71 \pm 0.06$, $D_0[H_9O_4^+ - H_2O] = 0.52 \pm 0.06$, and $D_0[H_{11}O_5^+ - H_2O] = 0.51 \pm 0.08$. These results are in very good agreement with enthalpies of solvation detd. by equil. methods.

So, meop.
(paren)

C.A. 1994, 120, N 6

$H_5O_2^+$

1993

Sun Fernin, Li Jinsan
et al.

суд.
носеет,
Di

Gaodeng Xue Xiao Hua-
xue Xue Bao 1993, 14(11),
1560-4.

●
(суд. H_3O^+ ; III)

$H_5O_2^+$

1994

121: 213553m The protonated water dimer: extensive theoretical studies of $H_5O_2^+$. Xie, Yaoming; Remington, Richard B.; Schaefer, Henry F., III. (Cent. Computational Quantum Chem., Univ. Georgia, Athens, GA 30602 USA). *J. Chem. Phys.* 1994, 101(6), 4878-84 (Eng). Ab initio quantum mech. methods have been applied to the $H_5O_2^+$ system, for which expts. are beginning to appear. These methods include basis sets up to triple- ζ plus double polarization plus f functions (TZ2Pf) and levels of correlation up to coupled cluster including single, double, and perturbatively treated connected triple excitations [CCSD(T)]. The potential energy hypersurface is very flat and is sensitive to the level of theory. At the highest level of theory the global min. is the structure with C_2 symmetry, but the transition state with C_s symmetry is only 0.4 kcal/mol higher in energy. Some low energy excursions into C_1 symmetry are carefully examd. The theor. dissocn. energy for the $H_3O^+-H_2O$ system is predicted to be 33.4 kcal/mol, and is in good agreement with exptl. measurements. The harmonic vibrational levels are reported.

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$2(H_3O^+-H_2O)$

c.A. 1994, 121, N18

$H_5O_2^+$

Konec - Graus -
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(7) $H_9O_4^+$

C.A. 1994,
120, n18 Δ

120: 230213x Vibration-rotation spectroscopy of the hydrated hydronium ions $H_5O_2^+$ and $H_9O_4^+$. Yeh, L. I.; Lee, Y. T.; Hougen, J. T. (Dep. Chem., Univ. California, Berkeley, CA 94720 USA). *J. Mol. Spectrosc.* 1994, 164(2), 473-88 (Eng). High-resoln. vibration-rotation spectra in the OH antisym. stretching region near 3700 cm^{-1} are reported for $H_5O_2^+$ and $H_9O_4^+$. The clusters are produced in a corona discharge ion source, cooled by supersonic expansion, mass-selected, and trapped in an radiofrequency octopole ion trap. Spectroscopic interrogation using a 2-color laser scheme leads to rovibrational excitation of the trapped ions followed by preferential multiphoton dissociation of the vibrationally excited ions and detection of the resultant fragment ions. More lines appear in the partially resolved vibration-rotation spectra of $H_5O_2^+$ than can be explained if the mol. is rigid, and presumably these addnl. lines arise from tunneling splittings caused by large-amplitude internal motions in this ion. Despite the low signal-to-noise ratio, all the obsd. spectral features can be grouped into roughly 12 R branches with a line spacing only 14% less than the B + C value calcd. from the ab initio structure. Theor. expected splitting patterns were calcd. using a formalism developed earlier for tunneling motions in N_2H_4 , since H_2N-NH_2 and $H_2O-H^+-OH_2$ are group-theor. similar if the central H^+ of the ion is located sym. between the 2 H_2O mois. The 12 branches represent the overlapping of 6 tunneling-split components for the in-phase and 6 for the out-of-phase OH antisym. stretching vibrations expected in this region, but the low signal-to-noise ratio in the present measurements prevented unambiguous comparison of theory and expt.

1994
4551

$O_2H_5^+$

1995

122: 274518w Ab Initio Calculations of Protium/Deuterium Fractionation Factors in $O_2H_5^+$ Clusters. Edison, Arthur S.; Markley, John L.; Weinhold, Frank (Department of Biochemistry, University of Wisconsin, Madison, WI 53706 USA). *J. Phys. Chem.* 1995, 99(20), 8013-16 (Eng). Fractionation factors have been calcd. for the H/D isotopic equil. reactions of $O_2H_5^+$ clusters. The calcns. used ab initio geometries and force consts. to evaluate the reduced isotopic partition functions for each isotopic species. We find good agreement with exptl. gas-phase measurements [Graul, S. T.; Brickhouse, M. D.; Squires, R. R. *J. Am. Chem. Soc.*, 1990, 112, 631-639] at higher levels of Hartree-Fock theory. By contrast, Moeller-Plesset second order perturbation theory (MP2) yielded somewhat poorer agreement with expt., presumably because the calcd. hydrogen bond distances are underestimated at this level.

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C.H. 1995, 122, N 22

1995

H_5O_2^+ , H_9O_4^+
сфрежис., сфабикн.
Терр. раога

Intern. J. Quant. Chem.
Sym. 29, p. 657.

$H_5O_2^+$

1995

структура,
стабильность,
 D_e , меолен.
расчет

124:17696h Potential energy surfaces and vibrational spectra of $H_5O_2^+$ and larger hydrated proton complexes. Ojamae, Lars; Shavitt, Isaiah; Singer, Sherwin J. (Dep. of Chemistry, The Ohio State Univ., Columbus, OH 43210 USA). *Int. J. Quantum Chem., Quantum Chem. Symp.* 1995, 29(Atomic, Molecular, and Condensed Matter Theory and Computational Methods, Proceedings of the International Symposium, 1995), 657-68 (Eng). Calcns. are presented of the structure, binding energetics, potential energy surfaces, and vibrational spectra of $H_5O_2^+$. The 15-dimensional potential energy surface for the 7 nuclei in the ionic complex was computed by pointwise ab initio Moeller-Plesset 2nd-order perturbation (MP2) calcns., using the correlation-consistent pVTZ basis set augmented with diffuse basis functions on O. The potential energy surface for the proton-transfer mechanism was studied, and the effects of surrounding H_2O mols. on the proton-transfer potential energy curve was studied. D. functional calcns. for the proton transfer potential surface are compared to the MP2 results. Geometry-optimized structures, binding energies, and harmonic vibrational spectra of $H_5O_2^+$ and $H_9O_4^+$ are presented. The energy-min. structure of $H_5O_2^+$ using the augmented pVTZ basis set is of C_2 symmetry, whereas for $H_9O_4^+$,

C. A. 1996, 124, ~2

using the TZ2P basis set, it is of C_3 symmetry. The H-bonded OH stretching harmonic frequency of $H_5O_2^+$ is low, 913 cm^{-1} , whereas for $H_9O_4^+$ it is 2927 cm^{-1} . The subspace spanned by the H-bonded OH distance and the O-O distance were used in 1- and 2-dimensional calculations of the anharmonic vibrational spectrum using collocation methods. The coupling of the OH stretch with the O-O vibration causes a red shift and the anharmonicity a blueshift of the OH frequency: the resulting fundamental frequency of the H-bonded OH vibration is 1275 cm^{-1} . Zero-point energies of the proton vibration and pathways for exchange of protons within $H_5O_2^+$ are discussed.

$H_5O_2^+$

1995

123: 18324b Comment on "The protonated water dimer: Extensive theoretical studies of $H_5O_2^+$ ". Pudzianowski, Andrew T. (Macromolec. Structure Div., Bristol-Myers Squibb Pharmaceut. Res. Inst., Princeton, NJ 08543-4000 USA). *J. Chem. Phys.* 1995, 102(19), 7761 (Eng). A polemic is given on the work of Y. Xie, et al., (ibid. 1994, 101, 4878) concerning correlated calcns. of the dissocn. energy of the protonated water dimer.

Do, meop. pac.

C. A. 1995, 123, N 2

$H_5O_2^+$

1997

127: 86388h CASSCF/CASPT2 Studies of the Lowest States of $H_5O_2^+$. Klein, Stephane; Kochanski, Elise; Strich, Alain; Sadlej, Andrzej J. (Laboratoire de Chimie Theorique et Laboratoire de Chimie Quantique Federation de Chimie, Universite Louis Pasteur, 67008 Strasbourg, Fr.). *J. Phys. Chem. A* 1997, 101(26), 4799-4806 (Eng), American Chemical Society. CASSCF and CASPT2 calcns. have been performed on the ground and two lowest singlet and triplet excited states of the protonated dihydrate. Two subsystems can be identified in the excited states: an excited water mol. and a ground state oxonium ion. The elec. properties have been computed (dipole moment and dipole polarizabilities). The dipole polarizabilities are very large in the excited states of the complex (up to 500 au for the largest component). This can be due to the presence of nearly degenerate higher excited states or to an easy proton/hydrogen transfer process. The excitation energies, around 8 eV for both states, show that the photodissocn. of $H_5O_2^+$ is probably possible in the atm. The stabilization energy of the excited states with respect to the isolated subsystems is about 5-6 kcal/mol, including the relaxation contribution.

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C.A. 1997, 127, N 6

H₅O₂⁺

1998

129: 8817z The protonated water dimer: Brueckner methods remove the spurious C₁ symmetry minimum. Valeev, Edward F.; Schaefer, Henry F., III (Department of Chemistry, Center for Computational Quantum Chemistry, The University of Georgia, Athens, GA 30602-2556 USA). *J. Chem. Phys.* 1998, 108(17), 7197-7201 (Eng). American Institute of Physics. The H₅O₂⁺ system has been studied using a variety of coupled cluster methods based on a Brueckner ref. determinant with levels of correlation up to double and perturbatively treated connected triple excitations [B-CCD(T)]. Basis sets as large as the triple- ζ plus double polarization basis augmented with f functions on oxygen and d functions on hydrogen [TZ2P(f,d)] were used. Harmonic vibrational frequencies were also predicted. In contrast with previous high-level ab initio studies, a stationary point of C₁ symmetry was not found. An absence of imaginary vibrational frequencies at all levels of theory for the stationary point of C₂ symmetry proves it to be the global min., lying only -0.4 kcal/mol lower in energy than the transition state of C_s symmetry.

теор. расчет
структур,
дискриминант.

C. A. 1998, 129, N 1

1999

F: H5O2+

P: 3

132:2

~~13033~~ Density-functional study of the hydrogen-bonded water cluster Kim, Yong-Hoon; Lee, In-Ho; Martin, Richard M. Department of Physics, University of Illinois Urbana, IL 61801, USA AIP Conf. Proc., Volume Date 1999, 501(Stochastic Dynamics and Pattern Formation in Biological and Complex Systems), 366-372 (English) 2000 We study the H5O2+ mol. as a basic unit of the proton transfer in hydrogen-bonded water networks

C.A. 2000, 132

in d.-functional theory (DFT) scheme using finite-difference pseudopotential method. The comparison of dissocn. ene obtained from the local-d. approxn. (LDA) and the generalized-gradient ap (GGA) with exptl. results and other accurate quantum chem. calcns. shows (1) the GGA in DFT is a reliable scheme for this system, and (2) we can o the effect of including higher correlation by using the GGA over the LDA. also address the tech. issue of implementing the GGA exchange-correlation potential in the real space.

F: H502+

P: 3

1999

132:200475 Electronic spectra of the symmetric
and asymmetric dihydronium cations. Muguet,

Francis F. Laboratoire de Mathematiques
Appliquees (L.M.A), E.N.S. Techniques Avancees

Paris 75739, Fr. Internet J. Chem., 2,
No pp. Given, Article 25 (English) 1999

H502+ is a chem. structure of fundamental
importance to understand proton transfer in H₂O. In
the ground electronic state, ab initio methods predict
very little energy difference between a C₂ sym.
geometry a C_s geometry where the proton is located in
an asym. fashion between the atoms. At the C₂ sym.

C.A. 2000, 132

geometry, electronic excitation spectra (energies oscillator strengths) were computed with MCSCF/RPA, HF/RPA and MS2/SOPPA methods. At the Cs asym. geometry, electronic excitation spectra were computed with HF/RPA and MP2/SOPPA methods. Comparison of the electronic excitation spectra, at these 2 geometries, shows quite remarkable difference and tends to demonstrate that the wavefunctions at the proton-sym. and asym. geometries are not similar, despite a small geometrical distortion between them.

 electronic spectra sym asym dihydronium
cation

F: H5O2+

P: 3

131:314377 Hydrogen bonding and the protonated water
dimer. Testa, A. C. Department of Chemistry, St.
John's University Jamaica, NY 11439, USA
Spectrosc. Lett., 32(5), 819-828 (English) 1999

A semiempirical AM1 study of hydrogen bonding and protonation in water has been carried out to illustrate the two different O-H vibrational frequencies present in the protonated water dimer, H₅O₂⁺. Using the MOPAC quantum mechanics program, it is shown that the optimized geometry for this species is C_{2h}, an O-H bond distance of 1.20 Å, and the fifteen normal frequencies have been determined. Results predict the two O-H vibrational frequencies at 553 and 330 with the former being the H-bond stretching mode. A grid calculation illustrating how the potential energy surface of water varies with the H-O-H angle and H bond distance is also presented.

H₅O⁺

Am. 40781

2001

Mikhail V. Vener et al.,

IR spectra

O...H...O

parameters

J. Chem. Phys.,

114, N1,

2001,
240-249.

The improved
the O...H...O



spectrum of
fragment of

$H_5O_2^+$: ~~Ab~~ initio classical
molecular dynamics and
quantum 4D model calculations.