H502

$H_5O_2^+$ **Anway A.R.** 1969

(A.P.) J. Chem. Phys., 1969, 50, 5, 2012

(См. H_4O^+) III

$H_5O_2^+$

1970

50382d Vibrational spectroscopy of the $H_5O_2^+$ 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 $H_5O_2^+$ and $D_5O_2^+$ were identified in the cryst. compds. $HClO_4.2H_2O$ and $DClO_4.2D_2O$ 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 $H_5O_2^+$ (*Bu* class vibrations) with those of H_3O^+ are made. The bending vibration of end OH's (1680 cm^{-1}) is strongly coupled with the asym. vibration of the bridge. RCOQ

cul. n.

C·A·1970·73·10

1970

$H_5O_2^+$

21 Б200. Колебательная спектроскопия иона $H_5O_2^+$ (дигидратированного протона). Исследование в предположении обобщенного валентного силового поля. Chemouni 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 $HClO_4\cdot 2H_2O$ (**I**) и $DClO_4\cdot 2D_2O$ (**II**) при —180° в области 400—3600 *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 $H_5O_2^+ClO_4^-$, т. е. в тв. состоянии в крист. решетке **I**, **II** присутствует дигидратиро-

сил. пост.

V: 1970 · 21

ванный протон $H_5O_2^+$ (**III**) ($D_5O_2^+$ (**IV**)). В крист. состоянии **I**, **II** имеют пространственную группу *Pnma* (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 H 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 OH-групп $\nu_{12}(B_u) = 1680$ *см*$^{-1}$ иона **III** сильно взаимодействует с асимм. вал. кол. H-мостика $\nu_{11}(B_u) = 1770$ *см*$^{-1}$ (1420 *см*$^{-1}$ для **IV**). А. Александров

XI 1078 1970

HF_2^-, $H_5O_2^+$ (потенц. поверхност)

Kollman P.A., Allen L.C.

J. Amer. Chem. Soc., 1970, 92, N21, 6101-7

Ю (см. HF_2) III

$H_2OHOH_2)^+$ XI - 1079 1970

91476f SCF MO LCGO [linear combinations of gaussian orbitals] studies on hydrogen bonding. The system $(H_2O\text{-}HOH_2)^+$. 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

Кв. мех. расчет

C.A. 1970. 73. 18

45-02

XI-1079

1970

$(H_2OHOH_2)^+$

10 Д133. Исследование водородной связи методом самосогласованных МО в виде линейных комбинаций гауссовых орбиталей. Система $(H_2OHOH_2)^+$. Kraemer Wolfgang P., Diercksen Geerd H. F. SCF MO LCGO studies on hydrogen bonding. The system $(H_2OHOH_2)^+$. «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 O и по 6 — *s*-типа для H, сжатых до 5 и 4 соответственно для O и 3 для H, с дополнительным включением 2 поляризационных ф-ций *d*-типа для каждого атома O и *p*-типа для H) исследовано электронное строение двух геометрич. конфигураций системы $(H_2OHOH_2)^+$. Орбитальные экспоненты поляризационных ф-ций предварительно оптимизировались для H_2O. Миним. энергией

ξ_i

D_0

(расчет)

Ф. 1970. 10Д

обладает конфигурация с линейной симметричной H-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 H-связь центрального протона обладает очень слабо выраженным минимумом, ввиду чего возможно его отклонение от положения равновесия примерно на 0,3Å без заметного изменения энергии.

В. Л. Лебедев

II XI 410 1970

H_2O (Ар) (OH^-, H_3O^+, $H_5O_2^+$, $H_7O_3^+$; $H_9O_4^+$,
r_e, м.п., - $H_3O_2^-$, $H_5O_3^-$, $H_7O_4^-$)

Paz M. de, Ehrenson S., Friedman L.,
J. Chem. Phys, 1970, 52, №7, 3362-3368 (англ
Study of the H+ and OH- hydrated ions by the CNDO/2 method.

Ю (см. OH^-; II)
10 т

РЖФиз, 1970, 8Д165

1970

$H_5O_2^+$

V_i

XI-409

116283b 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-H-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

$H_5O_2^+$

XV -3203

1972

(νi)

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. $HCl.2H_2O$ 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. A. 1972. 77. 12

$H_5O_2^+$

потенц. поверх.

ν_i

Ф. 1974 №3

1973

[XI-3-41]

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 $[H_2OHOH_2]^+$. 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 ф-ций 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

ЖЛ-3741

1973

$H_2OHOH_2^+$

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 $H_2OHOH_2^+$ 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.

потенц.
поверхн.
кв. мех. расчет.

С.А. 1973, №26, 79

$H_5O_2^+$

XI – 3989

1973

м.н. расчет

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 calcns. 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.

С.А. 1974. 80 №2

$[H_5O_2]^+$

1973

1 Д128. **Влияние корреляционных эффектов на энергетические кривые переноса протона. Катион $[H_5O_2]^+$.** Meyer Wilfired, 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
$H_5O_2^+$ Оп

1974
4-6426

Bates J.B., Toth L.M.

Vibrational spectra of $H_5O_2^+$ ion in crystalline $YH_5O_2(C_2O_4)_2 \cdot H_2O$.

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

(англ.) 0199

162 165 . 1 0 1 ВИНИТИ

$\underline{XI}$-4~~2~~19 1974.

H_3O^+, $\underline{(H_2O)_2H^+}$, CH_3^+, CH_3OH_2,
$(CH_3OH)_2H^+$ (A.P.)

Heinen H.J., Roellgen F.W.,
Beckey H.D.,
Z. Naturforsch., Teil A, 1974, $\underline{29}$(5),
773-81.
Appearance potentials of field ions

Ю Ⓕ

C.A. 1974. $\underline{81}$ №12. 70013c (см. H_3O^+, $\overline{\underline{III}}$)

$H_5O_2^+$ 1975

(Ji)

Picotin G.

„Adv. Mol. Relax Processes"

1975, 7, N3, 177-188 (англ)

(см $HSbCl_6$; III)

70218.3710
Ch,TC

водор. св836
54997 GR
$H_5O_2^+$

1976
* ч-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, B102, N 5-6, 169-174
(англ., рез. нем.)

0812 ПМК

773 775 804

ВИНИТИ

$H_5O_2^+$ обзор [оттиск 5905] 1977.
(см. сборник в шкафу сборников)
Sunner J.

ион-мол.
р-ции,
ионизация

Reactions of gas-phase ions studied by the charge transfer technique.
Lund, 1977. (Sweden)

$H_5O_2^+$ оттиск 6641 1978

Janoschek R., et al.

стр. 1238–1245

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

$(H_5O_2)^+$

$(H_3O_2)^-$

r_{O-O}

водородн.
связь
потенц.
кривые

оттиск 8447 | 1979

Peinel G.

Chem. Phys. Lett.
1979, <u>65</u> (2), 324-26

$(H_2O\ldots H-OH_2)^+$

оттиск 10098 1980

Desmeules P.J.; et a.

молекул. геометрия, энергия образов. комплекса

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

$H_5O_2^+$

1983

99: 202777p Calculation of infrared spectra of $H_5O_2^+$ and $H_3O_2^-$ groups. Yukhnevich, G. V.; Kokhanova, E. G. (USSR). *Zh. Prikl. Spektrosk.* 1983, 39(4), 617–21 (Russ). The frequencies of the harmonic vibrations of $H_5O_2^+$ 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 $H_5O_2^+$ ion absorption and scattering spectra should have bands near 400 cm⁻¹ and 700 cm⁻¹, resp.

ν_i, ИК спектр

☒ (H) $H_3O_2^-$

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 см$^{-1}$. Резюме

ν_i ;

Ⓗ ☒

х. 1984, 19, N6

$H_5O_2^+$

От. 18991

1984

Голубев Н.С.

строение

Хим. физ., 1984, 3,
N 5, 772-774.

$H_5O_2^+$

1984

$H_3O^+ \cdots H_2O$

102: 101009q **Theoretical determination of the potential surface for the system $H_3O^+ \bullet\bullet\bullet H_2O$ [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
расчет
потенц.
поверхн.

C.A. 1985, <u>102</u>, N12

$H_5O_2^+$ 1984

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

Di, сим.
носит.

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

(см. 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 calcns. using as basis set functions (11*s*,7*p*) and (4*s*) 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 ≃ 178°). The various structures of $H_5O_2^+$ exhibited in solid medium are in the range of the predicted structures.

C.A.1984, 100, N 14

$H_3O^+ + H_2O = H_5O_2^+$ 1984

ион., стр.,
ΔH, ΔS, ΔG;

16 Б1116. Неэмпирический расчет термохимических данных для газофазного кластерообразования $H_3O^+ + H_2O = H_5O_2^+$. Ab initio calculation of the thermochemical data on the $H_3O^+ + H_2O = H_5O_2^+$ 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 $H_3O^+ + H_2O = H_5O_2^+$. 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-

Х.1984, 19, N16

фектов менее значителен. Ниалучшие значения термохим. данных, полученные для исследованной р-ции, равны: $\Delta H^\circ = -35{,}5$ ккал/моль, $\Delta S^\circ = -28{,}8$ э. е. и $\Delta G = -26{,}9$ ккал/моль ($T = 298{,}15$ K). И. Н. Сенченя

$O_2H_5^+$

Отт. 22492

1985

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

теорет. расчет структуры

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

$H_5O_2^+$

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 А

Х. 1986, 19, N4

$H_5O_2^+$

ОМ. 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. Yukhneviech 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.)

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. O...H...O в ионах $H_5O_2^+$ и $H_3O_2^-$. Из полученных величин силовых коэф. и электрооптич. параметров вычислены частоты и интенсивности ИК-полос поглощения этих ионов. Результаты расчета согласуются с эксперим. данными. Отмечено, что наблюдаемое снижение частоты валентного колебания OH-связи при образовании H-связи связано со снижением величины валентной силовой постоянной F_{11}, положительный коэф. взаимодействия F_{12} не дает заметного вклада в частоту.

М. Р. Алиев

расчет колебат. спектров

(+1) ☒

ф. 1985, 18, N10

$H_5O_2^+$ ОМ · 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) О...Н...О мостиковых связей в ионах $H_5O_2^+$ (**I**) и $H_3O_2^-$ (**II**), контуры к-рых свидетельствовали о почти идеальной симметрии ионов и сильном положит. динамич. взаимодействий связей О..Н. На основе аппроксимации ПП рядом Тейлора 4-й степени вычислены силовые константы связей, оценены силовые константы и коэф. эл. ангармоничности углов, соседних к Н-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. (~1000 см$^{-1}$) расположены в последовательности $\nu_{\gamma *} > \nu_{Q\,as} > \nu_{\gamma}$. Н. Л. Арюткина

расчет
колебат-
спектра

☒

(Н)

Х.1985,19,N18

$H_5O_2^+$ (От. 21360) 1985

теор. расчет
сил. пост.;
ν_i;

103: 44955q **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. (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 consts. 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.

Ⓣ ☒ $H_3O_2^-$

C.A. 1985, 103, N6

$H_5O_2^+$ 1986

Burshtein K. Ya.,
Isaev A.N.

потенц.
поверхн.,
теор.
расчёт

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

(см. $H_3O_2^-$; III)

$H_5O_2^+$

$H_7O_3^+$

1986

11 Д73. Неэмпирическое исследование колебательных спектров гидратов ионов $H^+(H_2O)_2$ и $H^+(H_2O)_3$. An ab-initio study of the vibrational spectra of the ion hydrates $H^+(H_2O)_2$ and $H^+(H_2O)_3$. 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 $(H_2O)_2$ (**III**). Показано, что наиболее выгодными являются структуры $H^+(H_2O)_2$ для **I** и $H_3O^+(H_2O)_2$ 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 O—H—O в сравнении с **III** проявляется в увеличении колебательных частот.

В. Л. Лебедев

(М.Л.)

Н

ф. 1986, 18, N 11 (см $H_5O_2^+$; III)

$H_5O_2^+$ 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 hydrates clusters and those of the neutral $(H_2O)_2$ cluster are discussed.

(колеб. спектр, ν_i)

⑫ ☒ $H_7O_3^+$, ● $(H_2O)_2$

C.A. 1986, 105, N10

$(H_2O)_2H^+$
$(H_2O)_3H^+$

28167

1987

Shiromaru H.,
Shinohara H.,
et al.

Chem. Phys. Lett., 1987,
141, N 1-2, 7-11.

(см. $(H_2O)_2^+$; III)

$H_3O^+ \cdot H_2O$ отт. 29182 1988

Briznyuk A.A., Voityuk A.A.

теор. расчёт

J. Mol. Struct. Theochem., 1988, <u>164</u>, N3-4, 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 ($H_3PW_{12}O_{40}.6H_2O$). 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, теор. расчет

C.A. 1988, <u>109</u>, N26

$H_5O_2^+$ 1988

Тараканова Е. Г.

м. п.

Ж. прикл. спектроскопии. 1988. 49, № 4. С. 636–642.

(См. $H_3O_2^-$; III)

$H_5O_2^+$
(р-р)

1989

(ИК)

111: 66864b IR spectrum of diaquahydrogen ($H_5O_2^+$) ion in acid solutions. Maiorov, V. D.; Librovich, 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 ~2350 cm^{-1} that was not attributed to $H_5O_2^+$ before.

C.A.1989, 111, N8

$H_5O_2^+$

Ом 32154

1989

Колебат. постоян.

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 $HClO_4.2H_2O$, 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 $HFe(SO_4)_2.4H_2O$ and $HIn(SO_4)_2.4H_2O$, 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 $H_5O_2^+$.

$H_5O_2^+$

1990

114: 215012p **Study of the geometrical configuration, internal rotation and the proton transfer process for diaquahaydrogen(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.

геометрия,
расчёт

С.А.1991, 114, N 22

$H_5O_2^+$

(Оп-35978)

1991

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 thermodn. insight to the formation reaction.

– структура, расчёт

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 ВИНИТИ 03.01.91, № 49—В91

Рассчитан спектр иона $H_5O_2^+$ с учетом динамического и электрооптич. ангармонизма колебаний. Полученные 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-поглощения. Показано, что основной причиной возникновения непрерывного поглощения в спектре иона $H_5O_2^+$ является электрооптич. ангармонизм колебаний симметричной водородной связи. Автореферат

М·Л-

Ф. 1991, N4

$H_5O_2^+$

1991

(Di)

116: 94334a **Nature of the high-intensity bands of combination vibrations of $(A...H...A)^{\pm}$ complexes.** Yukhnevich, 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 $(A...H...A)^{\pm}$ 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 calcns. of the frequencies and intensities of the bands of fundamental vibrations, combination vibrations with the total quantum no. [illegible], and overtones up to the 5th order were performed for $H_5O_2^+$, $D_5O_2^+$, $(MeOH)_2H^+$, $H_3O_2^-$, $D_3O_2^-$, and $(MeO)_2H^-$ complexes.

(75) ☒ $D_5O_2^+$, $H_3O_2^-$, $D_3O_2^-$, $(CH_3O)_2H^-$, $(CH_3OH)_2H^+$

C.A. 1992, <u>116</u>, N 10

$H_5O_2^+$

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 calcns. (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.

(теор. расчет)

C.A. 1993, 118, N8

$H_3O^+ - H_2O$

$H_5O_2^+ - H_2O$

$H_7O_3^+ - H_2O$

$H_9O_4^+ - H_2O$

1993

120: 62827e **Stepwise solvation enthalpies of protonated water clusters: collision-induced dissociation as an alternative to equilibrium studies.** Dalleska, 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 dissocn. (CID) to lose one water mol. At higher energies, addnl. water mols. are lost successively, indicating that evapn. is the primary pathway for dissocn. 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 dissocn. lifetimes are properly accounted for, the following bond dissocn. energies (in eV) are detd.: $D_0[H_3O^+-H_2O]$ = 1.35 ± 0.06, $D_0[H_5O_2^+-H_2O]$ = 0.86 ± 0.06, $D_0[H_7O_3^+-H_2O]$ = 0.71 ± 0.06, $D_0[H_9O_4^+-H_2O]$ = 0.52 ± 0.06, and $D_0[H_{11}O_5^+-H_2O]$ = 0.51 ± 0.08. These results are in very good agreement with enthalpies of solvation detd. by equil. methods.

D_0, теор.

(расчет)

C.A. 1994, 120, N 6

$H_5O_2^+$ 1993

Sun Zemin, Li Jinshan
et al.

см. пост., Di

Gaodeng Xuexiao Hua-
xue Xuebao 1993, $\underline{14}$(11),
1560-4.

(см: H_3O^+; $\underline{\widehat{III}}$)

$H_5O_2^+$

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.

неэмпи-
расчет, Di

$D(H_3O^+-H_2O)$

C.A. 1994, 121, N18

$H_5O_2^+$

Колеб.-вращ. спектр

(+) $H_9O_4^+$

C.A. 1994, 120, N18 △

1994

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 dissocn. of the vibrationally excited ions and detection of the resultant fragment ions. More lines appear in the partially resolved vibration-rotation spectrum 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 $H_2N\text{-}NH_2$ and $H_2O\text{-}H^+\text{-}OH_2$ are group-theor. similar if the central H^+ of the ion is located sym. between the 2 H_2O mols. 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.

$O_2H_5^+$

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.

ab initio
расчет
структуры,
сил. пост.

C.A. 1995, 122, N 22

$H_5O_2^+$, $H_9O_4^+$ 1975

структ., стабильн. Intern. J. Quant. Chem.
Теор. расчет Symp. 9, p. 657.

$H_5O_2^+$

1995

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 $H_9O_4^+$,

структура, стаб-ильность, Di, теорет. расчет

C. A. 1996, <u>124</u>, N2

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 calcns. 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.

D_0, теор. рас.

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.

низшие
электрон.
сост.,
теор. расчет

C. A. 1997, <u>127</u>, N 6

$H_5O_2^-$ 1998

129: 8817z The protonated water dimer: Brueckner methods remove the spurious C_1 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 $H_5O_2^+$ 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 C_1 symmetry was not found. An absence of imaginary vibrational frequencies at all levels of theory for the stationary point of C_2 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 структуры, Di, стабильн.

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: H5O2+
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

H5O2+ is a chem. structure of fundamental importance to understand proton transfer in H2O. In the ground electronic state, ab in methods predict very little energy difference between a C2 sym. geometry a Cs 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 differe and tends to demonstrate that the wavefunctions at the proton-sym. and as geometries are not similar, despite a small geometrical distortion betwee them.

electronic spectra sym asym dihydronium cation

F: H5O2+
P: 3

1999

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 h been carried out to illustrate the two different O-H vibrational frequenc present in the protonated water dimer, H5O2+. Using the MOPAC quantum me program, it is shown that the optimized geometry for this species is C2h, an O-H bond distance of 1.20 A, and the fifteen normal frequencies have b detd. Results predict the two O-H vibrational frequencies at 553 and 330 with the former being the H-bond stretching mode. A grid calcn. illustra how the potential energy surface of water varies with the H-O-H angle and H bond distance is also presented.

$H_5O_2^+$ Om. 40781 2001

Mikhail V. Vener et al.,

IR спектр
O…H…O
фрагментов

J. Chem. Phys., 2001,
114, N1, 240 – 249.

The infrared spectrum of
the O…H…O fragment of

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