$(H_2O)_2$

Оп 33725

1990

Vos R.J., Hendriks R.,
et al,

теорет.
расчет.

J. Comput Chem,
1990, 11, N 1, 1-18

SCF, MP2, and CEPA-1

Calculations of the $OH \cdots H$ Hydrogen Complexes $(H_2O)_2$ and (H_2O-H_2CO).

$(H_2O)_2$

Dm 33770 1990

1 Б1271. Субмиллиметровый вращательно-туннельный ($K_a = 0—1$) спектр димера воды. The ($K_a = 0 \rightarrow 1$) submillimeter rotation-tunneling spectrum of the water dimer / Zwart E., Ter Meulen J. J., Meerts W. L. // Chem. Phys. Lett.— 1990.— **166**, № 5—6.— С. 500—502. — Англ.

На субмиллиметровом спектрометре в области частот 350—500 ГГц с разрешением около 600 кГц и точностью 100 кГц измерен вращательно-туннельный спектр димера воды, $(H_2O)_2$, в основном колебат. состоянии. Кластеры воды генерировались с использованием сверхзвукового молек. пучка. С учетом микроволновых данных для туннельных состояний ($K_a = 0$) и ($K_a = 1$) в спектре идентифицировано 14 переходов подполосы $K_a = 0—1$. Полученные данные позволят более точно определить вращат. постоянную A и параметры туннельного расщепления состояний ($K_a = 0$) и ($K_a = 1$).

С. Н. Мурзин

М.П.

Х. 1991, N1

$(H_2O)_2$ Om·36345 1991

Bondarenko G.V., Gorbaty Yu.E.,

$(K_p, \Delta H, D_0)$ Mol. Phys. 1991, 74, N3,
639 - 647

$(H_2O)_2$

1991

структура
расчет

115: 99773g **Characterization of the bifurcated structure of the water dimer.** Marsden, Collin J.; Smith, Brian J.; Pople, John A.; Schaefer, Henry F., III; Radom, Leo (Sch. Chem., Univ. Melbourne, Parkville, 3052 Australia). *J. Chem. Phys.* 1991, 95(3), 1825-8 (Eng). The bifurcated structure of the water dimer was considered at the self-consistent-field (SCF) level of theory using finite basis sets that allow a close approach to the Hartree-Fock limit. As one approaches the Hartree-Fock limit, the bifurcated structure is predicted to be a true transition state, with one imaginary vibrational frequency, $\omega_{12}(B_2)$ ~200i cm^{-1}.

C.A. 1991, 115, N10

$(H_2O)_2$

1991

16 Б1091. Многочастичная симметризованная теория возмущений для межмолекулярного взаимодействия. Димеры H_2O **и** HF. Many-body symmetry-adapted perturbation theory of intermolecular interactions. H_2O and HF dimers / Rybak Stanislaw, Jeziorski Bogumil, Szalewicz Krzysztof // J. Chem. Phys.— 1991.— 95, № 9.— С. 6576—6601.— Англ.

Разработан многочастичный вариант симметризованной теории возмущений для прямого расчета межмолек. потенциалов как суммы электростатич. обменного, индукц. и дисперсионного вкладов. Проведены пробные расчеты димеров $(H_2O)_2$ и $(HF)_2$. Исследована зависимость энергии взаимодействия от геометрии и от использованного базиса. Получены значения энергии ассоциации —4,7±0,2 и —4,2±0,2 ккал/моль для $(H_2O)_2$ и $(HF)_2$ соотв. (эксперим. значения —5,4±0,7 и —4,9±0,1 ккал/моль соотв.). Библ. 88. А. А. Сафонов

М·П·

Ⓗ ☒

X. 1992, N16.

$(H_2O)_2$(2) Оп. 35985 1991

Slanina Z.,

Croat. Chem. Acta. 1991,
64, N 1, 37-42

A Note on the Flexible
BJH and MCYL Potentials:

A Fair Agreement with the Available Observed Thermodynamic Data on $(H_2O)_2(g)$ and $(D_2O)_2(g)$.

$(H_2O)_2$ От. 35565 1991

Slanina Z., Crifo J.-F.,

(Kp) Thermochim. Acta, 1991,
181, 109–118.

$(H_2O)_2$

1991

116: 30129e Flexible BJH- and MCYL-type potentials for the water dimer $(H_2O)_2(g)$: a successful reproduction of the observed monomer/dimer vibrational frequency shifts. Slanina, Zdenek (Max-Planck-Inst. Chem., W-6500 Mainz, Germany). *Z. Phys. Chem. (Munich)* **1991**, 171(1), 131-6 (Eng). Harmonic vibrational anal. of the water dimer is reported for 4 BJH-, 4 MCYL-, and 3 original CF-type flexible water-water potentials. For the 1st 2 mentioned potential groups, calcd. monomer/dimer frequency shifts reasonably well correspond to the available obsd. terms. An important role of anharmonic terms in the intramol. potential part is pointed out.

Колебат.-
аналит. расч

С.А. 1992, 116, N4

$(H_2O)_2$

1991

114: 215067k A vibrational analysis of the $(X_2O)_2(g)$ (X = hydrogen, deuterium, tritium) isotopomeric species. Slanina, Z. (Otto-Hahn-Inst., Max-Planck-Inst. Chem., Mainz, Fed. Rep. Ger.). *J. Radioanal. Nucl. Chem.* 1991, 149(1), 141-7 (Eng). Harmonic vibrational anal. is carried out for the water dimer (^1H or natural isotopic mixt.) and its ^2D and ^3T isotopomers in the gas phase, using the recently designed flexible potential energy functions. The results represent the most complete and reliable theor. evaluation of the vibrational frequencies, directly applicable to various observation interpretations. The complete data set can also be useful for a more general isotopomeric reasoning.

ν_i, расчет

(+2)

$(D_2O)_2$, $(T_2O)_2$

C. A. 1991, 114, N22

$(H_2O)_2$

1991

17 Б3059. Сравнительное исследование термодинамики газофазных димеров воды с использованием гибких потенциалов типа BIH и MCYL. A comparative study of the water-dimer gas-phase thermodynamics in the BIH- and MCYL-type flexible potentials / Slanina Z. // Chem. Phys.— 1991.— **150, № 3**.— С. 321—329.— Англ.

С использованием 8 модификаций гибких ПТ типа BIH и MCYL (т. е. ПТ, содержащих наряду с межмолек. частью также и внутримолек. часть) рассчитаны станд. термодинамич. х-ки образования газофазных димеров легкой и тяжелой воды при т-рах 370—577 К. Кроме того при т-рах 423—773 К рассчитан изотопный эффект, обусловленный замещением дейтерием, для второго вириального коэф. водяного пара. Значения изотопич. разности второго вириального коэф. водяного пара и значения станд. энтальпии, энтропии и свободной энергии Гиббса образования газофазных димеров воды, рассчитанные с использованием нек-рых модификаций гибких ПТ в общем удовлетворительно согласуются с имеющимися эксперим. данными.

В. Ф. Байбуз

(ΔG)

(H)

Х. 1991, N17

$(D_2O)_2$

$(H_2O)_2$ 1991

115: 57635q A comparative study of the BJH- and MCYL-type potentials applied to the gaseous water dimer. Slanina, Zdenek (Max-Planck-Inst. Chem., Mainz, Fed. Rep. Ger.). *Z. Naturforsch., A: Phys. Sci.* 1991, 46(5), 426-32 (Eng). Various refined potentials describing the intra- and inter-mol. force fields of water mols. are used to calc. the properties of the gas-phase water dimer. The intra-mol. parts have been taken from spectroscopic or quantum-chem. sources. The min. energy structure was found iteratively using the first derivs. of the potential; the force-const. matrix was constructed by numerical differentiation. A quite close agreement between the Bopp-Jancso-Heinzinger (BJH) and the Matsuoka-Clementi-Yoshimine-Lie (MCYL) potentials is found. The treatment is applied to seven obsd. water-dimer isotopomeric isomerizations.

силовые постоянные

C.A. 1991, 115, N 6

$(H_2O)_2$

1991

22 Б1047. $(H_2O)_2$ (г.): сдвиги колебательных частот при переходе от мономера к димеру в гибких потенциалах Боппа—Янксо—Хайнцингера и Мацуоки—Клементи—Иошимине—Ли. $(H_2O)_2$(g): Monomer/dimer vibrational frequency shifts in Bopp-Jancsó-Heinzinger- and Matsuoka-Clementi-Yoshimine-Lie-type flexible potentials / Slanina Zdeněk / J. Chem. Phys.— 1991.— 94, № 1.— С. 814—815.— Англ.

Восемь разновидностей ПТ Боппа—Янксо—Хайнцингера и Мацуоки—Клементи—Иошимине—Ли использованы для определения гармонич. частот меж- и внутримолек. колебаний димера $(H_2O)_2$(г.), имеющего равновесную геометрич. конфигурацию симметрии C_s. Показано, что для удовлетворит. описания сдвигов частот норм. внутримолек. кол. при переходе от мономера к димеру молек. силовое поле должно содержать кубичные и квартичные ангармонич. члены. Результаты, полученные при использовании указанных выше двух семейств ПТ, неожиданно хорошо согласуются друг с другом. Наиболее существенное отличие наблюдается для частоты торсионного колебания.

В. Б. Павлов-Веревкин

И·Л·

Х. 1991, N22

$(H_2O)_2$

1991

Б-10 Д81. **$(H_2O)_2(g)$: расчет сдвигов колебательных частот мономер/димер с использованием потенциалов типа Боппа—Янчо—Хейзингера и Мацуока—Клементи — Иошимина — Ли, учитывающих гибкость.** $(H_2O)(g)$: Monomer/dimer vibrational frequency shifts in Bopp—Jancsó—Heinzinger- and Matsuoka—Clementi—Yoshimine—Li-type flexible potentials / Slanina Zdeněk // J. Chem. Phys.— 1991.— 94, № 1.— С. 814—815.— Англ.

Рассчитаны частоты внутри- и межмолекулярных колебаний кластеров $(H_2O)_2$ с использованием известных из литературы 8 различных потенциалов, учитывающих деф. кол. молекул (гибкость). Определены сдвиги частот колебаний молекулы воды при образовании димера. Найденные значения сдвигов сравниваются с известными из экспериментов. Сделан вывод, что ангармонич. вклады к силовым постоянным кластера играют важную роль в происхождении этих сдвигов. Особо сравниваются результаты расчетов с применением двух принципиально различных потенциалов, предложенных авторами, перечисленными в названии. В. А. Морозов

М.П.

сф. 1991, N10

$H_2O \cdot H_2O$

1992

Coitine E.L., Ventura O.N., et al.,

структура и стабильн.

THEOCHEM 1992, 86, 315-28

(см. $NH_3 \cdot NH_3$ ● ; III)

$(H_2O)_2$

1992

118: 27743m Ab initio studies of the water dimer using large basis sets: the structure and thermodynamic energies. Kim, Kwang S.; Mhin, Byung Jin; Choi, U. Sung; Lee, Kuntack (Cent. Biofunctional Mol., Pohang Inst. Sci. Technol., Pohang, 790-600 S. Korea). *J. Chem. Phys.* **1992**, 97(9), 6649-62 (Eng). Ab initio calcns. with various large basis sets have been performed on the water dimer in order to study the structure, energetics, spectra, and elec. properties. As a ref. system, the calcns. of the water monomer were also performed. The second order Moller-Plesset perturbation theory (MP2) using a large basis set (O:13*s*, 8*p*,4*d*,2*f*/H:8*s*,4*p*,2*d*) well reproduces various water monomer exptl. data except for the somewhat underestd. abs. energy and hyperpolarizability. The monomer energy calcd. with the fourth-order Moller-Plesset perturbation theory (MP4) with the above basis set is −76.407 hartrees, which is only 0.073 hartree above the exptl. energy. To compare the theor. and exptl. dimer structures and thermal energies accurately, we summarized the quantum statistical thermodn. quantities with corrections for anharmonic vibrations, rotation, rotation-vibration coupling, and internal rotation. With the correction for the

теорет. расчет структуры, μ, νi, H-H, S, ΔG

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C. A. 1993, 118, N 4

$(H_2O)_2$ (H-H, S, ΔG)

anharmonic binding potential rotation, the predicted interoxygen distance of the dimer is 2.958 Å, which is so far the closest to the exptl. value 2.976 Å. The predicted dimer dipole moment is 2.612 D, which is the first agreement with expt. (2.60–2.64 D). The predicted frequency shift of the dimer with respect to the monomer is in good agreement with expt. With the MP2 calcn. using the large basis set, the basis set superposition error correction (BSSEC) of the dimer is only 0.33 kcal/mol, which is by far the smallest among the MP2 results reported. Without BSSEC, the predicted binding energy, enthalpy, free energy, and entropy are all in good agreement with expt. within the error bounds, whereas with BSSEC, some of them seem to be slightly off the exptl. error bounds. Nevertheless, the results with BSSEC can be more reliable than those without BSSEC.

$(H_2O)_2$ От. 36911 1992

Millot C., Stone A.J.,

ab initio
поверхн

Mol. Phys., 1992, 77, N3, 439 – 462

Towards an accurate intermolecular potential for water.

$(H_2O)_2$

1992

116: 181594d **Ab initio characterization of possible dissociation pathways for multiphoton ionization of the water dimer in supersonic free jets.** Sosa, Ramon M.; Irving, Kenneth; Ventura, Oscar N. (Inst. Fis., Fac. Ing., Montevideo, Urug. 11300). *THEOCHEM* 1992, 86, 453-63 (Eng). UHF and second-order Moeller-Plesset ab initio calcns. using several split-valence basis sets complemented with polarization and diffuse functions were done on H_2O^+ and $H_2O \cdot H_2O^+$. We studied the performance of the level of calcn. and the basis sets used in predicting the structure and energy ordering of the ground and excited states of the water radical cation. Very good agreement was found for the three states (ground $^2B_1$ and excited $^2A_1$ and $^2B_2$); deviations were less than 0.3 eV in all cases. The calcd. optimized structures were in close agreement with expt.

теор. расчет нижних энерг. состояний

C.A. 1992, 116, N18

We also made calcns. on the two lowest-lying A' and A" states of the water dimer radical cation at the optimized geometry of neutral $(H_2O)_2$ and at its own intermol. optimized structure within each basis set. The results predict a charge transfer complex for the A' state of the water dimer radical cation and that if no proton transfer is allowed both states require more or less the same excitation energy. This suggests the possibility of two potential energy hypersurfaces being close enough for a large coupling to take place. Comparison with previous theor. studies shows that inclusion of dynamic correlation through perturbation theory is sufficient to obtain as good an agreement with expt. as that obtained with the best CI calcns. done so far.

$(H_2O)_2$

1992

117: 138004v Ab initio studies on the structures and hydroxyl vibrations of small hydrogen-bonded systems. Van Duijneveldt, Frans B.; De Groot-den Hartogh, Marieke; Van Duijneveldt-Van de Rijdt, Jeanne G. C. M. (Theor. Chem. Group, Univ. Utrecht, 3584 CH Utrecht, Neth.). *Croat. Chem. Acta* 1992, 65(1), 1-9 (Eng). Ab-initio SCF + MP2 calcns. with the ESPB basis are reported for the systems $(H_2O)_2$, $(CH_3OH)_2$, H_2O-H_2CO, and $(H_2O)_3$. Anal. of the methodol. and comparison with expt. (where available) showed that the binding energies are reliable to about 1 kJ/mol, and the O...O distances accurate to 0.01 Å, provided the full counterpoise procedure was used to avoid the so-called basis set superposition error (BSSE). If, on the other hand, the BSSE was ignored, then unrealistically short O...O distances were obtained. Distinctly bent OH..O geometries were found for some of the complexes, suggesting that the distance of the closest approach was detd. by the H..O contacts and not by the O...O contacts involved. Nonadditivity in $(H_2O)_3$ shortened the O...O distance by 0.06 Å, and enhanced its OH vibrational frequency shift by some 50%.

теор. расчет структуры и энергетика

(+3) XI

C.A. 1992, 117, N 14

$(H_2O)_2$

1992

структурн. параметры и энергия связи, теор. расчет

С.А. 1992, 117, N26

117: 258617u Convergence to the basis-set limit in ab initio calculations at the correlated level on the water dimer. Van Duijneveldt-Van de Rijdt, J. G. C. M.; Van Duijneveldt, F. B. (Theor. Chem. Group, Univ. Utrecht, 3584 CH Utrecht, Neth.). *J. Chem. Phys.* 1992, 97(7), 5019-30 (Eng). The equil. structure and binding energy of the H_2O dimer were detd. in ab-initio quantum-mech. calcns. at the correlated level, using 2nd-order Moeller-Plesset theory (MP2) and coupled-electron pair theory (CEPA-1). Basis-set-superposition error was avoided by applying the counterpoise procedure throughout. Basis-set convergence was monitored by studying not only the total interaction energy, but also the first- and higher-order Hartree-Fock interaction energies, the partitioned intramol. and intermol. components of the MP2 interaction energy, and the monomer dipole moments. This was done at a near equil. geometry for more than 20 progressively improved basis sets. The largest set was used in MP2 and CEPA-1 geometry optimizations in C_s symmetry, keeping all intramol. coordinates fixed, except for the donor OH length. The equil. geometry is R_{OO} = 2.949(6) Å, θ_a = 55.2(2.0)°, θ_d = 57.6(2.0)°. The donor OH bond is lengthened by 0.0060(6) Å, but this has virtually no effect upon the final R_{OO}. The equil. binding energy is $\Delta E = -4.73(10)$ kcal/mol. The CEPA dipole moment is 2.60(10) D. The error bars on these results reflect the uncertainty due to the remaining incompleteness in the one-electron basis, as well as in the treatment of the electron correlation. Taking into account the vibrational effects present in exptl. data, the calcd.

results lie within the error bars of the exptl. data available. However, the present error bars are 2 to 7 times tighter, and s of the exptl. values lie outside the present ranges. The discrepancy is for ΔE, which is difficult to det. exptl. This i of importance for the modeling of H_2O properties, where e potentials, with ΔE ranging from -5.0 to -5.5 kcal/m customarily employed.

$(H_2O)_2$

1992

Yeo Geoffrey A.,
Ford Thomas A.
Struct. Chem. 1992,
<u>3</u>(2), 75-93.

структура
и стабиль-
ность,
теор.
расчёт

(см. $(NH_3)_2$; <u>III</u>)

$(H_2O)_2$

1993

11Д193. Димер воды. Расчеты корреляционной энергии. The water dimer. Correlation energy calculations / Chakravorty Subhas J., Davidson Ernest R. // J. Phys. Chem.. — 1993. — **97**, № 24. — С. 6373—6383. — Англ.

The binding energy of the water dimer at the experimental geometry has been calculated employing the Hartree—Fock (HF) method, Møller—Plesset theories MP2, MP3, and MP4, and the coupled cluster method with bouble excitations. Binding energies within quasi-degenerate variation perturbation theory, linearized coupled cluster method, and the average pair correction model are also calculated. The basis set developed and employed in the study yields — 76.0674 au for the HF energy of the water monomer at the experimental geometry. The MP2 interaction energy has been partitioned into pair energies to give a better understanding of the hydrogen bond. The present study is unable to yield

М.Л.

Ф. 1993, N 11-12

results close to — 5.4 kcal/mol, the experimental estimate for the interaction energy. Instead, values ranging from —4.2 to —4.7 kcal/mol have been obtained. Correlation energy density functional models yield interaction energies in the range of —5.2 to —5.8 kcal/mol. However, when the Hartree—Fock exchange term is replaced with exchange energy density functional models, values from —2.8 to —4.5 kcal/mol are obtained.

$(H_2O)_2$ 1993

Panas I.,

структура, Chem. Phys. Lett. 1993,
теор. расчет 226 (1-2), 173-9.

(см. $(HF)_{2 \div 4}$; III)

$(H_2O)_2$

1993

118: 154861y **Efficient elimination of basis-set-superposition errors by the local correlation method: accurate ab initio studies of the water dimer.** Saebo, Svein; Tong, Wen; Pulay, Peter (Dep. Chem., Mississippi State Univ., Mississippi State, MS 39762 USA). *J. Chem. Phys.* 1993, 98(3), 2170–5 (Eng). The main purpose of the calcns. was to investigate the magnitude of, and how to eliminate the basis set superposition errors at different levels of theory. At the Hartree–Fock level the superposition errors are insignificant with the largest basis sets, and the counterpoise method works well with all the basis sets used in this study. At the correlated level superposition errors are still significant even for very large basis sets, and the std. counterpoise technique leads to overcorrection. The most important result of the present study is that the local correlation methods give essentially the correct result for the correlation contribution to the assocn. energy even with modest basis sets. The assocn. energy at the MP4(SDQ) level is predicted to be 4.8 kcal/mol. The correlation contribution to the assocn. energy is 1.2 kcal/mol which can be decompd. into an attractive intermol. contribution of 1.8 kcal/mol and a repulsive intramol. contribution of 0.6 kcal/mol. Ionic terms contribute about 30% to the dispersion force at the equil. distance. If the effect of triple substitutions is taken into account the assocn. energy is estd. to be around 5.1 kcal/mol.

(теор. расч)

C.A. 1993, 118, N16

$(H_2O)_2$

1993

8Д133. О стабильности димера $(H_2O)_2$ в основном и низколежащих возбужденных состояниях / Зверева Н. А., Булдаков М. А., Ипполитов И. И., Терпугова А. Ф. // Изв. вузов. Физ.. — 1993. — **36**, № 3. — С. 11—15. — Рус.

Проведено исследование нижних S_1 и T_1 электронных состояний димера $(H_2O)_2$, влияния образования водородной связи на сдвиг максимума полосы поглощения, устойчивости комплекса в основном и возбужденном состояниях. Установлено, что существует только один глобальный минимум для системы с линейной водородной связью неплоской структуры димера воды; циклическая и разветвленная формы являются переходными состояниями и при возбуждении не образуют устойчивых комплексов. Для структуры, имеющей минимум в основном состоянии, существуют нераспадные состояния S_1 и T_1 с энергиями связи 2,0 и 4,4 ккал/моль соответственно. Образование водородной связи приводит к сдвигу максимума полосы поглощения в голубую область по сравнению с мономером. При возбуждении димера воды водородная связь ослабляется.

М.П.

Ф. 1993, N8

$(H_2O)_2$

1993

120: 62875u **Stability of the water dimer $(H_2O)_2$ in ground and low-lying excited states.** Zvereva, N. A.; Buldakov, M. A.; Ippolitov, I. I.; Terpugova, A. F. (Tomsk. Gos. Univ., Tomsk, Russia). *Izv. Vyssh. Uchebn. Zaved., Fiz.* 1993, 36(3), 11-15 (Russ). The low-lying singlet and triplet electronic states, H bond formation, the blue shift of the absorption max. (in respect to the monomer), and the stability in ground and excited states were studied. There is only one global min. for the non-planar dimer with linear H bond; the other isomers represent transition structures and are not stable if excited. The stable structure has bonding energies of 2.0 and 4.4 kcal/mol in S_1 and T_1 states, resp. The hydrogen bond weakens when the dimer is excited.

стабильность
в основн. и
нижних
возбужд сост.

С.А. 1994, <u>120</u>, N 6

1994

F: (H2O)2
P: 3
5Б149. Расчет межмолекулярных связанных состояний для димера воды. Calculation of the intermolecular bound states for water dimer / Althorpe S. C., Clary D. C. // J. Chem. Phys. - 1994. - 101, N 5. - С. 3603. - Англ.

РЖХ 1997

Гауссиан-2 (МП2) получены более низкие значения: -18 и -30 кДж/моль соотв. Сродство к протону (с образованием CH[2]SOH{+}) получено равным 787 кДж/моль (298K).

$H_2O_2 - H_2O$
димер

1994

120: 307889g Structure, vibrational frequencies and thermodynamic properties of hydrogen peroxide-water dimers. An ab initio molecular orbital study. Mo, O.; Yanez, M.; Rozas, I.; Elguero, J. (Departamento de Quimica, C-9, Universidad Autonoma de Madrid, Cantoblanco, Madrid, Spain 28049). *Chem. Phys. Lett.* 1994, 219(1-2), 45-52 (Eng). High levels of ab-initio MO theory were used to study the structures, binding energies, vibrational frequencies, and equil. consts. of hydrogen peroxide-water dimers. The geometries of the different possible conformers were optimized at the HF/6-311++G(2d, 2p) level of theory. Five different stationary points on the potential-energy surface were characterized at this level, but only two were min. The geometries and vibrational frequencies of these two min. were refined at the MP2/[6-311+G(d, p)] level. The stretching vibrations of the proton donors showed a sizable red shift. The global min. corresponded to a five-membered ring, where both monomers behave simultaneously as proton donors and proton acceptors. In the second min., which lies about 2.2 kcal/mol higher, the hydrogen peroxide monomer behaves as a proton acceptor, while water behaves as a proton donor. The binding energies of these two species were obtained at the QCISD(T)/[6-311+G(2d, 2p)] level, by using the MP2 optimized geometries; the corresponding equil. dimerization consts. were evaluated. A topol. anal. was made of the electronic charge densities of the dimers.

М. П.,
термод
св-ва,
ab initio
расчет

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(Н)

С. А. 1994, 120, N 24

на об.

$H_2O_2 - H_2O$
димер

(межмол.
вз-ва)
ab initio расч)

$(H_2O)_2$

1994

структура, Di, Kp, ab initio -расчет

C.A. 1994, 120, N18

120: 227627c Structure, vibrational frequencies, and thermodynamic properties of hydrogen peroxide dimers: an ab initio molecular orbital study. Mo, O.; Yanez, M.; Rozas, I.; Elguero, J. (Dep. Quim., Univ. Auton. Madrid, Madrid, Spain 28049). *J. Chem. Phys.* 1994, 100(4), 2871-7 (Eng). High levels of ab-initio-MO theory were used to study the structures, binding energies, vibrational frequencies, and equil. consts. of hydrogen peroxide dimers. The geometries of the different initial structures considered were optimized at the HF/6-311+ + G(2d,2p) level of theory. Five different stationary points were characterized at this level, but only two of them were min. The geometries of these two min. were refined at the MP2/6-311 + G(d,p) level. Their vibrational frequencies, calcd. at the same level of theory, showed a sizeable red shift of the stretching vibrations of the proton donors. The global min. corresponded to a six-membered ring having C_i symmetry; whereas, the second min. is a five-membered ring, which lies about 1.1 kcal mol^{-1} above the global one. The formation of the latter implies a considerable enhancement of the dipole moment. The binding energies of these two species were obtained at the QCISD(T)/6-311 + G(2d,p) level by using the MP2 optimized geometries. The equil. dimerization consts. for hydrogen peroxide are considerably smaller than those for water, due to significant entropy effects. A topol. anal. of the electronic charge densities of the dimers showed that both cyclic min. present weaker hydrogen bonds than noncyclic dimers.

$(H_2O)_2$ (2)

1994

Спектр газа и в матрице, Vi

120: 203201k **The dimerization shift of the OH-stretching fundamentals of the water dimer.** Ventura, Oscar N.; Irving, Kenneth; Latajka, Zdzislaw. (Catedra de Quimica Cuantica, Facultad de Quimica, Avda. Gral. Flores 2124, C.C. 1157, Montevideo, Urug. 11800). *Chem. Phys. Lett.* 1994, 217(4), 436–42 (Eng). The interpretation of the gas-phase and matrix-isolation vibrational spectra of the water dimer and monomer had led to contradictory conclusions as to the effect of dimerization on the OH-stretching fundamentals. Ab initio MPn/6-311+G(2d, 2p) and MPn/+VP^{s}(2d)^{s} calcns. (with n = 2–4) have been performed on the water dimer to det. accurately that dimerization shift. In order to assess the quality of the computational results, frequency shifts were calcd. at the same level also for several other binary complexes involving hydrogen

C.A. 1994, 120, N16

bonds, and for which there are not large discrepancies between the gas-phase and solid-matrix data. Full geometry optimization of the complexes was performed. Anal. (SCF, MP2) or numerically (MP3, MP4) detd. frequencies at the optimized geometries were employed to obtain the frequency shifts in question. In all cases a satisfactory agreement between the theor. and solid-matrix data was found. SCF calcns. underestimate and MP2 calcns. overestimate the shifts in all cases. However, in only one of the complexes studied, the $N_2{\cdot}HF$ dimer, were the MP2 results far off the exptl. ones. Both in this case and for the water dimer it was necessary to use a higher order of perturbation theory (MP3, MP4) to calc. the correlation correction, in order to obtain satisfactory convergence of the frequency shifts. In conclusion, the authors' theor. calcns. indicate that the gas-phase exptl. data on the dimerization shift of the OH fundamentals of the water dimer need to be reinterpreted. As a side result, the authors suggest a reassignment of the ν_3 vibrational transition of the water monomer, performed in the recent expts. of water trapped in a Ne solid matrix.

H_2O-H_2O ОМ 37638 1994

120: 280774b **Ab initio equilibrium constants for H_2O-H_2O and H_2O-CO_2.** Zhang, Nancy Renyou; Shillady, Donald D. (Dep. Chem., Virginia Commonw. Univ., Richmond, VA 23284-2006 USA). *J. Chem. Phys.* 1994, 100(7), 5230-6 (Eng). Ab initio 6-31G** electronic structure calcns. have been used to det. the min. energy geometries and vibrational frequencies of mol. clusters of water and carbon dioxide. Application of statistical thermodn. leads to theor. equil. consts. for gas phase dimerization of water and the formation of an adduct of carbon monoxide with water. The low energy vibrations of the clusters lead to much larger contributions to the vibrational partitioning of the energy than do the fundamental vibrations of the monomeric species. A new "Harmonic-Morse" formula is derived to est. anharmonicity from optimized harmonic frequencies and two addnl. values on the potential surface for each vibration. These ab initio calcns. of equil. consts. are very close to recent measurements and fall within the range of values obtained by other methods. This no-parameter treatment gives excellent agreement for the equil. of H_2O-CO_2 near the supercrit. fluid range of CO_2 and suggests that a "Theory of Significant Clusters" may be extended to a model of supercrit. fluids which includes the effects of anharmonicity.

K_p, ab initio расчет

☒ ⑪

C.A. 1994, 120, N22

H_2O-H_2O

1994

19 Б1145. Расчет неэмпирическим методом равновесных постоянных для $H_2O—H_2O$ и $H_2O—CO_2$. Ab initio equilibrium constants for $H_2O—H_2O$ and $H_2O—CO_2$ / Zhang Nancy Renyou, Shillady Donald D. // J. Chem. Phys. .—1994 .— **100** ,№ 7 .—С. 5230—5236 .—Англ.

Неэмпирическим методом ССП с использованием базисного набора 6—31 ГФ** проведены расчеты электронного и геометрич. строения и частот колебаний в димере воды и аддукте молекулы воды с CO_2 Применение методов статистич. термодинамики позволило оценить равновесные постоянные для этих систем: Предложена новая ф-ла для оценки ангармонизма в исследованных системах. Полученные результаты очень хорошо согласуются с эксперим. данными.

И. Н. Сенченя

Электрон. структура, геометрия, частоты колебаний

☒ (+1)

Х. 1994, №19.

$(H_2O)_2$

1995

23 Б188. Колебательная частота донорной ОН-группы в связанных Н-связью димерах воды, метанола и силанола: неэмпирические расчеты с учетом ангармоничности. The vibrational frequency of the donor OH group in the H-bonded dimers of water, methanol and silanol: Ab initio calculations including anharmonicities / Bleiber Andreas, Sauer Joachim // Chem. Phys. Lett. .— 1995 .— **238** , № 4 - 6 .— С. 243—252 .— Англ.

Неэмпирическим методом ССП МО ЛКАО в валентно-трехэспонентном базисе с включением поляризац. функций, с учетом поправки на суперпозицию базиса, и электронной корреляции в рамках МП2 и МП4 исследовано электронное строение связанных Н-связью димеров воды (I), метанола и силанола. Обнаружено, что приближение МП2 приводит к завышению частот вал. кол. ОН для мономеров и изменений частот при димеризации. Использование приближения МП4 приводит для I к согласию с эксперим. данными с точностью ±10 $см^{-1}$. С учетом этого результата оценки для димеров метанола и силанола привели к сдвигам частот соответственно в —126 и —175 $см^{-1}$. Библ. 35. Н. Л.

М.Л.

Х. 1995, N23

$(H_2O)_2$

1995

123: 297031s **Reactivity and Thermochemical Properties of the Water Dimer Radical Cation in the Gas Phase.** de Visser, Sam P.; de Koning, Leo J.; Nibbering, Nico M. M. (Institute of Mass Spectrometry, University of Amsterdam, 1018 WS Amsterdam, Neth.). *J. Phys. Chem.* 1995, 99(42), 15444–7 (Eng). The reactivity of the water dimer radical cation toward a series of substrates has been studied in the gas phase using a Fourier transform ion cyclotron resonance (FT–ICR) mass spectrometer. The water dimer radical cation, $H_4O_2^{\cdot +}$, has been prepd. at low pressure in the FT–ICR cell through an exchange reaction of the xenon dimer radical cation with water. Under the applied low pressure conditions the water dimer radical cation is shown to react as an electron acceptor, a proton donor, and a reagent which can exchange an OH• moiety. Independent bracketing of both electron transfer and proton transfer processes leads to an energy difference of 1029–1037 kJ mol^{-1} between the water dimer radical cation and two nonassocd. water mols. This corresponds to an adiabatic ionization energy of 10.81–10.90 eV for the water dimer, $(H_2O)_2$, significantly lower than the 11.21 and 11.1 eV values, obtained from photoionization and photoelectron spectroscopy studies, resp. The presently obtained results, however, seem to be consistent with results of ab initio calcns.

(У)

C. A. 1995, 123, N 22

$(H_2O)_2$

1995

F: (H2O)2
P: 3

05.Д.0087. Структурные и динамические свойства димера и тетрамера воды. Молекулярно-динамическое исследование. Structural and dynamical properties of water dimer and tetramer: Molecular dynamics study / Guvenc Z. B., Anderson M. A., Choi B. H. // Z. Phys. D. - 1995. - 35, N 1. - С. 51-55. - Англ.

A detailed evaluation of the structural and dynamical properties of isolated water dimers and tetramers using the Lemberg, Stillinger and Rahman potential energy surface and microcanonical molecular dynamics simulations are reported. The lowest-energy configurations of these clusters were obtained by simulated thermal quenching. Relative root-mean-square bond length fluctuations were used to characterize phase transitions. Solid-like, pre-melting, liquid-like, and dissociated states were identified. Global-local minimum transitions and the minimum energy path to dissociation of the dimer were also characterized.

Х. 1996, N5

$(H_2O)_2$

1996

124: 127479x Hydrogen Bond Energy of the Water Dimer. Feyereisen, Martin W.; Feller, David; Dixon, David A. (Cray Research Inc., Eagan, MN 55121 USA). *J. Phys. Chem.* **1996**, 100(8), 2993–7 (Eng). Large scale ab initio MO calcns. on the binding energy of the water dimer have been performed. These calcns. extend the previous correlation consistent basis set work to include larger basis sets (up to 574 functions), and core/valence correlation effects have now been included. The present work confirms the earlier est. of −4.9 kcal/mol as the MP2(FC) basis set limit. Core/valence correlation effects are found to increase the binding energy by −0.05 kcal/mol. The best est. of the electronic binding energy of the water dimer is −5.0 ± 0.1 kcal/mol. Correcting this value for zero−point and temp. effects yields the value ΔH(375) = −3.2 ± 0.1 kcal/mol. This value is within the error limits of the best exptl. est. of −3.6 ± 0.5 kcal/mol with the calcns. favoring the lower end of the exptl. energy range. It should be useful to adopt the present est. in empirical and semiempirical model potentials.

(энергии связи)

C. A. 1996, <u>124</u>, N 10

1996

F: (H2O)2
P: 3

14Б153. Структура кластеров воды. Учет многочастичных сил, релаксации [геометрии] мономеров и энергии нулевых колебаний. Structure of water clusters. The contribution of many-body forces, monomer relaxation, and vibrational zero-point energy / Gregory Jonathon K., Clary David C. [Journal of Physical chemistry] // J. Phys. Chem. - 1996. - 100, N 46. - C. 18014-18022. - Англ.

Место хранения ГПНТБ Приведены результаты расчетов структуры кластеров (H[2]O)[n] от димера до гексамера. Сопоставлены равновесные геометрич. параметры, полученные неэмпирич. квантово-хим. методом МП2/DZP и с модельными потенциальными поверхностями (см./C. Millot, A. J. Stone.//Mol. Phys. - 1992. - 77. - C. 439;/A. J. Stone.//Chem. Phys. Lett. - 1989. - 155. - C. 102), модифицированными таким образом, чтобы учесть

РЖХ 1997

многочастичные вклады в энергию взаимодействия. Квантовым диффузионным методом Монте-Карло определены ангармонич. частоты колебаний, что позволило для энергий диссоциации дать оценки не только для D[e], но и для D[0]. Показано, что колебательно-усредненные вращательные постоянные кластеров хорошо согласуются с эксперим. данными. Многочастичные вклады в энергию взаимодействия несколько уменьшают стабильность циклич. структур. Энергии нулевых колебаний существенно различны для различных изомеров. Наиболее стабильными структурами для тримера и тетрамера являются циклические структуры, причем не последнюю роль в балансе энергий играют многочастичные вклады. Для гексамера наиболее стабильной является нециклич. клеточная конфигурация в существенной степени вследствие низкой энергии нулевых колебаний.

$(H_2O)_2$

1997

127: 9641h Effect of Anharmonicities on the Thermodynamic Properties of the Water Dimer. Munoz-Caro, Camelia; Nino, Alfonso (E.U. Informatica de Ciudad Real, Universidad de Castilla-La Mancha, Ciudad Real, Spain 13071). *J. Phys. Chem. A* **1997**, 101(22), 4128-4135 (Eng), American Chemical Society. A study of the effect of anharmonicities and large amplitude vibrations on the thermodn. properties of the water dimer is presented. Different vibrational models were constructed by using ab initio data obtained at the MP2(Full)/6-311++G-(2d,2p) level. This is the first complete anal. of the rotation of the hydrogen donor monomer around the O-O axis. The potential barrier was found to be 221 cm^{-1}. A variational calcn. of the torsional energy levels yields a fundamental frequency of 105 cm^{-1}. The O-O stretching mode is described with the Morse function. The fundamental frequency and the dimerization energy are calcd. to be 153 cm^{-1} and 5.15 kcal/mol, resp., in agreement with the exptl. results. For the dimerization reaction were calcd. ΔS, ΔH, and the equil. const., K_p. The results show that inclusion of anharmonicity into the vibration modes favors the lower exptl. limit for ΔS and the upper limit for ΔH. In addn., the anharmonic corrections reduce the difference between calcd. and exptl. K_p. This difference decreases with temp. A high-temp. limit of 3.47×10^{-5} atm^{-1} was found for K_p.

V_0, ∂, ΔS, ΔH, K_p, торзион. ☒ димеризац.

C.A. 1997, 127, N 1

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ТО вн
связи

$(H_2O)_2$

1997

These results ar ... literature.

128: 299940q **The water dimer: post-Hartree-Fock and density-functional calculations on the potential energy surface.** Ventura, Oscar N.; Kieninger, Martina; Suhai, Sandor; Diercksen, Geerd H. F. (Catedra de Quimica Cuantica, Facultad de Quimica, Montevideo, Urug.). *Mol. Eng.* **1997**, 7(3-4), 317-348 (Eng), Kluwer Academic Publishers. Conventional ab initio and d.-functional methods with extended basis sets were employed in the study of a path on the water-dimer potential energy surface. The results show that d.-functional methods do depend strongly on the type of exchange-correlation potential employed, as well as on the quality of the basis sets, similarly to conventional ab initio methods, and on the d. of the grid. Gradient-cor. methods behave, as expected, better than uncorrected ones, the Becke-Lee-Yang-Parr (BLYP) potential being the one that gives the best results. However, too large chem.- and hydrogen-bond lengths and abs. energies, as well as too small relative total and correlation energies demonstrate that even BLYP calcns. with a relative large basis set are not good as MP2 calcns. of the same size. Adiabatically connected functionals (ACM), represented in this work by B3PW91, provide an improvement on the whole surface.

расчет
потенц.
поверхн.

С.А. 1998, 128, N24

$(H_2O)_2$

1998

129: 19858q Calculation of electronic affinity and vertical detachment energy of the water dimer complex using the density functional theory. Bouteiller, Y.; Desfrancois, C.; Schermann, J. P.; Latajka, Z.; Silvi, B. (Institut Galilee, Laboratoire de Physique des Lasers, Universite Paris–Nord, 93430 Villetaneuse, Fr.). *J. Chem. Phys.* **1998**, 108(19), 7967–7972 (Eng), American Institute of Physics. Though the electron attachment on the water dimer has been obsd., ab initio calcns. performed at the Hartree–Fock and post Hartree–Fock levels do not succeed in predicting a bound $(H_2O)_2^-$ anion. It is shown that the hybrid d. functional approach (B3LYP) yields results in reasonable agreement with expt., provided a systematic optimization of the basis sets in the variational sense. Neglecting the zero point energy (ZPE) correction, the adiabatic electron affinity (EA) is calcd. to be 21.2 meV (30 ± 2 exptl.) whereas the vertical detachment energy (VDE) is overestimated by about 10 meV (55.7 against 45). The ZPE correction has been estd. from the frequencies calcd. at the harmonic level. It improves noticeably the EA and the VDE which cor. values are 35.6 and 41.9 meV, resp. The sign and magnitude of the EA and VDE isotopic shifts between the hydrogenated and deuterated species are correctly predicted. The anal. of the electron d. difference and of the spin d. shows that the electron attachment occurs for one half between the two H_2O mols., the remaining being located outside in the dipole moment direction.

(Ae, расчет)

C.A. 1998, 129, N2

$(H_2O)_2$

1998

структура, энергия связи, ab initio расчет

129: 140937t **Ab initio MO−VB study of water dimer.** Famulari, A.; Raimondi, M.; Sironi, M.; Gianinetti, E. (Dipartimento di Chimica Fisica ed Elettrochimica and Centro CNR − CSRSRC, Universita degli Studi di Milano, 20133 Milan, Italy). *Chem. Phys.* **1998**, 232(3), 289−298 (Eng), Elsevier Science B.V.. The equil. structure and binding energy of the water dimer system were detd. by employing a general ab initio VB approach. Starting from the SCF−MI (SCF for mol. interactions) wave function, nonorthogonal virtual orbitals optimal for intermol. correlation terms have been detd. BSSE (basis set superposition error) is excluded in an a−priori fashion and geometry relaxation effects are

CA·1998, 129, N11

naturally taken into account. The equil. geometry corresponds to R_{O-O} = 3.00 Å, β = 134.5°, and α = 2.5°, in agreement with the exptl. values. The donor OH bond results elongated by 0.002 Å. The estd. equil. binding energy of the water dimer is −4.69 kcal/mol. Taking zero−point vibrational effects into account, the binding enthalpy is −3.1 kcal/mol, to be compared with the exptl. est. of −3.59 ± 0.5 kcal/mol, detd. from measurements of thermal cond. of the vapor.

F: (H2O)2
P: 3

1999

131:248406 Interaction optimized basis sets for correlated ab initio calculations on the water dimer. van Duijneveldt-van de Rijdt, J. G. C. M van Duijneveldt, F. B. Debye Institute, Theoretical Chemistry Group, Utre University Neth. J. Chem. Phys., 111(9), 3812-3819 (English) 1999

A compact basis set is constructed for the water dimer by focusing directly on an optimal description of the counterpoise-cor. interaction e (.DELTA.E) rather than on the total energy of the fragments. The optimiz criterion is that the basis set should be of uniform accuracy, i.e., the truncation error in .DELTA.E due to basis set incompleteness should be th for all symmetry types at all sites. Aiming at a truncation error of 10 .mu.hartree per symmetry at the SCF+MP2

(SCF+Moller-Plesset second-order) core level the resulting interaction optimized basis set comprises 249 functions. The compn. of this IO249 set is O/5s3p4d3f2g1h, H(donor)/2s4p H(else)/2s3p, bond function set/3s3p2d1f. An all-electron variant, IO275 described as well. A recipe to obtain interaction optimized sets for oth systems is given. The set IO249 yields a .DELTA.E(fc) value at the Felle Frisch geometry of -4.87 kcal/mol. Of the many orbital-based calcns. tha been reported for this system only Schutz' 1046-function calcn. [J. Chem. 107, 4597 (1997)] was more accurate. The small size of the interaction optimized sets opens the possibility for high-accuracy SCF+MP2 work on la systems than have been accessible before. It also brings higher-level correlated treatments within reach. An Appendix summarizes two additivit which allow the .DELTA.E for a larger basis set to be estd. to very high accuracy from the results of smaller basis sets.

$(H_2O)_2^+$

1999

130: 115339n **Ground State of the $(H_2O)_2^+$ Radical Cation: DFT versus Post–Hartree–Fock Methods.** Sodupe, Mariona; Bertran, Juan; Rodriguez–Santiago, Luis; Baerends, E. J. (Departament de Quimica, Universitat Autonoma de Barcelona, Bellaterra, Spain 08193). *J. Phys. Chem. A* 1999, 103(1), 166–170 (Eng), American Chemical Society. Correlated calcns. show the proton–transferred $OH-H_3O^+$ isomer to be the ground–state structure of the $(H_2O)_2^+$ dimer ion, with the C_{2h} hemibond structure being ca. 8 kcal/mol less stable. Modern d. functionals however favor the hemibond structure, overestimating the strength of the three–electron bond by ca. 17 kcal/mol. The wrong prediction of the relative stability of the two isomers is attributed to overestimation by the exchange functionals of the self–interaction part of the exchange energy in the hemibond ion due to its delocalized electron hole. It is cautioned that this erroneous behavior of the d. functionals for exchange, if unrecognized, may lead to wrong predictions for ground–state structures of systems with a three–electron bond.

осн. сост., теор. расчет

С. А. 1999, 130, N 9

1999

F: (H2O)2
P: 3

131:303575 Rearrangements of water dimer and hexamer. Wales, David J. University Chemical Laboratories Cambridge CB2 1EW, UK Theory At. Mol. Clusters, 86-110. Edited by: Jellinek, Julius. Springer: Berli Germany. (English) 1999

Rearrangement mechanisms of the water dimer and the cage form of the water hexamer are examd. theor. with particular ref. to tunneling splittings and spectroscopy. The three lowest barrier rearrangements of the water dimer are characterized by ab initio methods and compared with the results of previous constrained calcns. The acceptor-tunneling pathẇ does not proceed via a direct rotation around the C2 axis of the acceptor but rather via relatively asynchronous rotation of the donor about the hydrogen bond and an assocd. "wag" of the acceptor. Rearrangements betwe different cage isomers of the water hexamer are studied for two empirical potentials. The exptl. obsd. triplet splittings may be the result of fli and bifurcation rearrangements of the two single-donor, single-acceptor monomers. Two-dimensional quantum calcns. of the nuclear dynamics sugges that delocalization over more than one cage isomer may occur, esp. in excited states.

1999

F: (H2O)2-
P: 3
131:356258 Ab initio treatment of (H2O)2- and (H2O)6-. Weigend, Florian; Ahlrichs, Reinhart Institut fur Physikalische Chemie,

Universitat Karlsru Karlsruhe 76128, Germany
Phys. Chem. Chem. Phys., 1(19), 4537-4540
(English) 1999

MP2 level investigations of $(H_2O)_6^-$ are reported which were carried out assign its vertical electron detachment (VDE) spectrum. Extended basis s including a floating center are employed which yield an accuracy of a few eV for the VDE of $(H_2O)_2^-$ and $(H_2O)_3^-$ used as test cases. Results for (H differ considerably from previous treatments and lead to a new assignment VDE spectrum. It also turns out that $(H_2O)_6^-$ is probably adiabatically u since total energies are marginally higher than for the ground state of t neutral species in the most stable geometries.

2000

F: (H2O)2
P: 3

133:125518 Parallel implementation of a pseudo-spectral calculation of molecular energy levels: Application to the water dimer (H2O)2. Eggert, P.; Viel, A.; Leforestier, C. Institut fur Physikalische und Theoretische Chemie, Freie Universitat Berlin Berlin D-14195, Germany Comput. Phys. Commun., 128(1-2), 315-325 (English) 2000. Parallel implementation of an iterative detn. of energy levels of large mol. systems is presented. The basic step consists in acting the Hamiltonian operator H on a wavefunction u , and is achieved by means of a Pseudo Spectral Split Hamiltonian scheme (Leforestier et al., J. Chem. Phys. 106 (1997) 8527). The potential term evaluation V.u, which corresponds by far to the most time consuming part in the sequential code, has been distributed over all the processors. Application to the vibrational-rotational spectrum of water dimer shows a very good parallel efficiency up to 64 processors.

2000

F: (H2O)2

P: 3

133:64265 Computational determination of equilibrium geometry and dissoci energy of the water dimer. Klopper, W.; van Duijneveldt-van de Rijdt, J. C. M.; van Duijneveldt, F. B. Debye Institute, Utrecht University Utrecht TB, Neth. Phys. Chem. Chem. Phys., 2(10), 2227-2234 (English) 2000 The equil. geometry and dissocn. energy of the water dimer have been det as accurately as tech. possible. Various quantum chem. methods and high- basis sets have been applied, i.e., at the level of a nearly complete bas both the intermol. sepn. and the deformation of the donor and acceptor mo have been optimized at the level of CCSD(T) theory (coupled-cluster theor singles and doubles excitations plus a perturbation correction for connec triples). It is found at the

CCSD(T) level that the monomer deformation dimer amts. to 86% of the deformation computed at the MP2 level (second-o Moeller-Plesset perturbation theory) and that the core/valence electron correlation effects at the CCSD(T) level amt. to 80% of the same effects MP2 level. The equil. O.cntdot..cntdot..cntdot.O distance is detd. as Re 291.2 .+-. 0.5 pm and the equil. dissocn. energy as De = 21.0 .+-. 0.2 kJ with respect to dissocn. into two isolated water mols. at equil. Account zero-point vibrational energy, the theor. prediction for the dissocn. ene becomes D0 = 13.8 .+-. 0.4 kJ mol-1, a result which is open to direct exp verification.

$(H_2O)_2$

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(см. $(HF)_2$; ● III)