D - F

$(HF)_2$, <u>$(DF)_2$</u>, HFDF (м. в. спектр, структура) 1972

Dyke T.R., Howard B.J., XI 1970
Klemperer W.,
J. Chem. Phys., 1972, <u>56</u>, N5 2442–
–54 (англ.)

Radio frequency and microwave
3 spectrum of the hydrogen
fluoride dimer, a nonrigid
molecule.

10 CA, 1972, 76, N16, 92353n

$(HF)_2$, $(DF)_2$, HFDF ($r_{F \ldots F}$) XI 2970 1972

Dyke T. R., Howard B. J., Klemperer W.,

J. Chem. Phys., 1972, 56, N5, 2442-2454
(англ.)

Radiofrequency and microwave spectrum of the hydrogen fluoride dimer: a non rigid molecule.

РЖ Физ, 1972, 8Д503 Ю Ч Ф

1973

DF-DF

Колеб. релаксац.

151165q **Temperature dependence of deuterium fluoride vibrational relaxation.** Hinchen, J. J. (United Aircr. Res. Lab., East Hartford, Conn.). *J. Chem. Phys.* **1973**, 59(5), 2224–8 (Eng). Vibrational relaxation times for DF–DF and HF–HF were measured by laser fluorescence at 300–1000°K. The results coincide with shock tube data at <1000°K and show temp. dependence for DF relaxation similar to that for HF. Also, DF–HF relaxation times, detd. at ≤ 573°K, were between the values for DF and HF self-relaxation. Comparisons are made with current theories for vibrational relaxation.

C.A. 1973, N 26, 79

60503.7216
Ch, Ph, TC

$D_2 + F \to FD + D$
40592
$D + F_2 \to DF + F$
$F + DH \to FD + H$

1976
4213

Halavee U., Shapiro M.

A collinear analytic model for atom-diatom chemical reactions.

"J.Chem.Phys.", 1976, 64, N 7, 2826-2839
(англ.)

0805 [illegible]

591 592 597

ВИНИТИ

60715.1257 Ch, TC, MGU	попер. сечения 29864 (-Ро) T+HF', T+DF *	1976 ц-13938

Malcolme-Lawes David J. Excitation functions for the reactions of tritium atoms with HF and DF. "J. Chem. Soc. Faraday Trans.", 1976, Part 2, 72, N4, 878-882

(англ.)

0659 ПИК

629 632 G S I.

ВИНИТИ

HFDF

От. 21260

1984

Howard B. J., Dyke T. R.,
et al.

мв переходн.
спектроскоп.
постоян.

J. Chem. Phys., 1984, <u>81</u>,
N 12, Pt 1, 5417-5425.

$(DF)_2$ (от. 21260) 1984

Howard B.J., Dyke T.R.,
et al.

ν в переходн., спектроскоп. постоян.

J. chem. Phys., 1984, 81,
N 12, Pt 1, 5417–5425.

HFDF 1985

Hunt Rodney D.,
Andrews Lester,

ИК спектр.
в матрице

J. Chem. Phys.
1985, 82(10), 4442-
-4448.

(см. $(HF)_2$; III)

$(DF)_2$ 1985

Hunt Rodney D.,
Andrews Lester.

ИК спектр
в матрице

J. Chem. Phys.
1985, <u>82</u>(10), 4442-
-4448.

(см. $(HF)_2$; <u>III</u>)

$(DF)_2$

оттиск 20233

1984

Pine A. S.; Lafferty W. J., et al.

J. Chem. Phys., 1984, 81 (7), 2939-2950.

спектр
высокого
разрешен.
вращений.
постоян.,
колебаний.
предиссоц.

F·D_2

1984

100: 74273w Dependence of reaction attributes, including differential cross sections and resonance features, on changes in the potential energy surface for the atomic fluorine + diatomic deuterium reaction. Walker, Robert B.; Blais, Normand C.; Truhlar, Donald G. (Theor. Chem. Div., Los Alamos Natl. Lab., Los Alamos, NM 87545 USA). *J. Chem. Phys.* **1984**, 80(1), 246–54 (Eng). Comparisons were made of dynamical reaction attributes for the reaction F + D_2 → FD + D. Three potential energy surfaces were used: Muckerman surface no. 5 and 2 surfaces suggested more recently. These surfaces differ in barrier height and bending potential. The dynamical calcns. were based on the quasiclassical trajectory method and on the bend–cor. rotating linear model. New surface no. 2 does allow for significant reaction probability at 0.8 kcal/mol, as required to agree with mol. beam expts. The wider bending potential of new surface no. 2 does not, however, have a large effect on the angular distribution. Although it is known from previous work that the barrier in the entrance channel is important for the compd.–state resonance in this reaction, lowering the barrier from 1.06 kcal/mol in Muckerman surface no. 5 to 0.74 kcal/mol in the new surfaces does not make a qual. change in the resonance features of the results. The new surface no. 2 is more accurate than the widely studied Muckerman surface no. 5 and provides a better starting point for future work.

(потенц.
поверхн.)

C.A.1984, 100, N10

$(DF)_2$

1985

103: 131512m Microwave rotational spectra, hyperfine interactions, and structure of the hydrogen fluoride dimers. Gutowsky, H. S.; Chuang, Carl; Keen, John D.; Klots, T. D.; Emilsson, Tryggvi (Noyes Chem. Lab., Univ. Illinois, Urbana, IL 61801 USA). *J. Chem. Phys.* 1985, 83(5), 2070-7 (Eng). The hyperfine structure was resolved for the 2 $J = 0 \to 1$ transitions of $(DF)_2$, for the low frequency $J = 0 \to 1$ transition of $(HF)_2$, and for the $J = 0 \to 1$ transition of the mixed species HFDF. Also, the $J = 0 \to 1$ transition and hyperfine structure were obsd. for the other mixed species DFHF, not found previously. The relative intensities of the transitions for HFDF and DFHF, and their zero-point vibrational frequencies, correspond to an effective equilibration temp. between the 2 species of ~50 K in the gas expansion. Resoln. and assignment of the $(DF)_2$ and $(HF)_2$ hyperfine structure was aided by a method for suppressing the Doppler doubling in a Flygare spectrometer; it improved resoln. 2-fold to a full width at half. max. of 5 kHz at 11-14 GHz. The results bear on several features of the angular structure of this unusual system. At equil., the end H/DF in HFDF and DFHF is bent 60 ± 2° from the F···F axis, while the H/DF in the H bond is bent 7 ± 3° in the opposite direction. The

мв спектр, структура, м.п.

C.A. 1985, 103, N 16.

tunneling in $(DF)_2$ gives an av. angle between the DF's and the *a* axis (39.3 and 38.7° for the 2 transitions) which is 1.5° larger than the composite (37.5°) of the DF4s in DFHF and HFDF. For the $(HF)_2$ transition, the obsd. av. angle (40°) is also 1.5° larger than the composite (38.5°) of the HF angles in the mixed species. The H bonding in HFDF and $(DF)_2$ decreases the elec. field gradient at the D by ~15% from its value in free DF.

$(DF)_2$ (OM-31109) 1985

Hunt R.D., Andrews L.,

J. Chem. Phys. 1985, <u>82</u>, N 10, 4442–4448.

Photolysis of hydrogen and fluorine in solid argon. Matrix infrared spectra of $(HF)_2$, $(HF)(DF)$, and $(\mathcal{D}F)_2$.

(HF)(DF) ом. 31109 1985

Hunt R.D., Andrews L.,

J. Chem. Phys. 1985, 82, № 10,
4442–4448.

Photolysis of hydrogen and fluorine in solid argon.
Matrix infrared spectra

Of $(HF)_2$, $(HF)(DF)$, and $(DF)_2$.

D₂O ..., DF

1985

5 Л186. Колебательные сателлиты вращательного перехода $J=3\leftarrow2$ комплекса $D_2O\ldots DF$: форма функции потенциальной энергии для неплоского изгибного колебания. Vibrational satellites in the $J=3\leftarrow2$ rotational transitions of $D_2O\ldots DF$: confirmation of the form of the potential energy function for the out-of-plane bending mode. Kisiel Z., Legon A. C., Millen D. J. «J. Mol. Struct.», 1985, **131**, № 3—4, 201—213 (англ.)

На штарковском МВ-спектрометре вблизи 40 ГГц при т-ре 230 К и давл. 100—200 мТор исследован МВ-спектр комплекса $D_2O\ldots DF$. Идентифицированы линии вращательных переходов $3_{12}-2_{11}$, $3_{03}-2_{02}$, $3_{22}-2_{21}$, $3_{21}-2_{20}$ и $3_{13}-2_{13}$ в 9 состояниях с возбуждением 3 межмолекулярных колебаний комплекса с энергией ниже 340 см$^{-1}$. Определены значения вращательных постоянных B_v, $C\varepsilon$ и центробежных постоянных $D_J{}^v$ и $D_{JK}{}^v$. По колебательной зависимости вращательных постоянных найдена ф-ция потенц. энергии для неплоского изгибного колебания комплекса $V(Z)=a(z^4+bz^2)$, где $a=64{,}31$ см$^{-1}$ и $b=-2{,}80$. М. Р. Алиев

(М.П.)

ф. 1986, 18, N.5

$D_2O \dots DF$

ОМ · 22980 1985

10 Б1232. Колебательные спутники вращательных переходов $J=3-2$ $D_2O\dots DF$: подтверждение формы функции потенциальной энергии для неплоского деформационного колебания. Vibrational satellites in the $J=3\leftarrow2$ rotational transitions of $D_2O\dots DF$: confirmation of the form of the potential energy function for the out-of-plane bending mode. Kisiel Z., Legon A. C., Millen D. J. «J. Mol. Struct.», 1985, 131, № 3—4, 201—213 (англ.)

В дополнение к ранее выполненному отнесению вращат. переходов $J=2-1$ в колебат. состояниях (000) и (100) МВ-спектра гетеродимера $D_2O\dots DF$ (Bevan I. W. «Proc. R. Soc. London», 1980, 372A, 441) полностью идентифицированы вращат. переходы $J=3-2$ в колебат. состояниях (200), (010) и (110) и частично в состояниях (020), (101), (001) и (002). Подтверждено, что низкочастотная неплоская изгибная мода Н-связи димера может быть представлена одномерной функцией потенциальной энергии с двумя минимумами. Определены зависимости вращат. постоянных и постоянных квартичного центробежного искажения от колебат. квантовых чисел. С. Н. Мурзин

М.М., Dij

Х.1986, 19, N10

$D_2O \cdot DF$ Om·22980 1985

104: 26359q **Vibrational satellites in the $J = 3 \leftarrow 2$ rotational transitions of $D_2O...DF$: confirmation of the form of the potential energy function for the out-of-plane bending mode.** Kisiel, Z.; Legon, A. C.; Millen, D. J. (Inst. Phys., Pol. Acad. Sci., Warsaw, Pol.). *J. Mol. Struct.* 1985, 131(3-4), 201-13 (Eng). Complete assignments of the $J = 3 \leftarrow 2$ transitions in the states (2, 0, 0), (0, 1, 0) and (1, 1, 0) of $D_2O...DF$ were made in addn. to those previously assigned for the states (0, 0, 0) and (1, 0, 0). Partial assignments were also made for the states (0, 2, 0), (1, 0, 1), (0, 0, 1) and (0, 0, 2), where the notation used is ($v_{\beta(0)}$, $v_{\beta(i)}$, v_{σ}), the vibrational quantum nos. referring to the out-of-plane, the in-plane and the H-bond stretching modes, resp. Rotational consts. for the state (2, 0, 0) are in good agreement with those predicted and thus confirm the quant. form of the double-min. potential function for the mode $v_{\beta(0)}$. Rotational consts. for the combination states are well-behaved in the sense that they agree with those calcd. on the basis of additivity of contributions from the vibration-rotation consts. α_i.

Вращат. спектр, м.л.

C.A. 1986, 104, N4

$F+D_2$ Ст. 22-124 1985

Pollak E.,

ab initio
расчёт

Chem. Phys. Lett.,
1985, <u>119</u>, N1, 98-104.

$(DF)_2$ 1986

Michael Daniel W.,
Lisy James M.

м.п. J. Chem. Phys., 1986,
85, N 5, 2528-2537.

(см. $(HF)_3$; III)

$(HF)_2DF$
$HF(DF)_2$

1986

Michael Daniel W.,
Lisy James M.

Лр. п.

J. Chem. Phys. 1986,
85, N 5, 2528-2537.

(см. $(HF)_3$; III)

D_2F От 24183 1986

104: 215735v Direct experimental evidence for a metastable state of deuterium fluoride (D_2F), an analog of deuterium oxide D_3O). Raksit, Asit. B.; Jeon, Seung Joon; Porter, Richard F. (Baker Lab. Chem., Cornell Univ., Ithaca, NY 14853 USA). *J. Phys. Chem.* 1986, 90(11), 2298–300 (Eng). The D_2F radical was studied by a combination of neutralized ion beam and charge stripping techniques. Neutrals formed by D_2F^+/Na charge exchange were obsd. in metastable and dissoc. states. The lifetime of metastable D_2F is >0.4 μs. Metastability is not obsd. for HDF or H_2F. The dissoc. state of D_2F releases ~1.29 eV of kinetic energy in its fragmentation products (DF + D). The vertical electron affinity of H_2F^+ is 6.6 ± 0.1 eV. The possibility of observing an emission continuum from electronically excited H_2F formed by H_2F^+/K charge exchange is suggested. Similarities in the mass spectra of D_2F and the isoelectronic D_3O radical are indicated.

метастаб-
состоян.

(+2)

☒ 1) D_3O (метастаб. сост.) 2) H_2F^+ (Ae)

C.A. 1986, 104, N 24

$D_2 \cdot DF$ 1987

Hunt R.D., Andrews L.

J. Chem. Phys., 1987, 86,

и.п.

N7, 3781-3786.

(см. ● $H_2 \cdot HF$; III)

$\underline{H_2DF}$, HDHF, 1987

HDDF, D_2HF Hunt R.D., Andrews L.

J. Chem. Phys., 1987, 86,

и.п. N 7, 3781 – 3786.

(см. H_2·HF; III)

$D_2F_3^-$

1987

Hunt R.D., Andrews L.

спектр
в
матрице

J. Chem. Phys., 1987,
<u>87</u>, N 12, 6819–6823.

HDF_3^- | OM 29011 | 1987

Hunt R.D., Andrews L.,

спектр в матрице

J. Chem. Phys., 1987, <u>87</u>, N12, 6819-6823.

$(DF)_2$ (Оп. 26881) 1987

Lafferty W. J.,
Suenram R. D. et al.

и. п.

J. Mol. Spectrosc., 1987,
123, N2, 434-452.

(см. $(HF)_2$; III)

HFDF (от. 26881) 1987

DFHF

Lafferti W.J., Suenram R.D., Lovas F.J.,

Мв спектр

J. Mol. Spectrosc., 1987, 123, N 2, 434-452.

HFDF
DFHF

1987

Lafferty W.J.,
Suenram R.D., et al.

Мв,
м.п.

J. Mol. Spectrosc.
1987, <u>123</u> (2), 434-52.

(см. $(HF)_2$; <u>III</u>)

$(DF)_2$ (От. 26881) 1987

Lafferty W.J., Suenram R.D., Lovas F.J.,

м/в спектр J. Mol. Spectrosc., 1987, 123, N 2, 434–452.

(см. $(HF)_2$, III)

DOF 1988

Bürger H., Pawelke G., et al.

м.п. J. Mol. Spectrosc., 1988, 128, N1, 278-287.

●

(см. HOF; III)

1988

DOF Halonen L., Ma T.K.

м.п. J. Chem. Phys. 1988. 89, N8. C. 4885-4888.

(см. HOF; III)

D_2HF

От 31646

1988

7 Л133. ИК-спектр D_2HF. The infrared spectrum of D_2HF / Lovejoy Christopher M., Nelson David D., (Jr), Nesbitt David J. // J. Chem. Phys.— 1988.— 89, № 12.— С. 7180—7188.— Англ.

Исследован ИК-спектр поглощения в области 3940—3960 см$^{-1}$ комплексов D_2HF, образованных в процессе истечения со сверхзвуковой скоростью из щелевого сопла смеси охлажденных газов HF (1%), D_2 (30%) и He при давлении 1500 Тор. Наблюдена система линий, обусловленная валентными колебаниями HF в D_2HF, которая состоит из 2 перекрывающихся полос сравнимой интенсивности. Полоса П—П, отнесенная к пара-D_2HF, имеет *P*-, *Q*- и *R*-ветви, составленные из дублетных линий, с началом при 3948,0240(8) см$^{-1}$. Полоса Σ—Σ, отнесенная к орто-D_2HF, имеет только *P*- и *R*-ветви, с началом при 3949,5563(6) см$^{-1}$. Анализ спектра показывает, что П-состояния D_2HF

М.Л.

ф.1989, №7

являются более устойчивыми, чем Σ-состояния. Приведены оценки величин потенц. барьера для заторможенного вращения D_2 внутри комплекса, вращательных постоянных и постоянной вращательной дисторсии D_2HF. Определена скорость колебат. предиссоциации D_2HF, приблизительно в 25 раз превышающая таковую в случае комплексов H_2HF, что, предположительно, обусловлено процессом (*V*—*V*)-переноса, приводящим к колебат. возбуждению фрагмента D_2. Библ. 32. А. М. М.

D_2HF

ОМ 31646

1988

16 Б1152. Инфракрасный спектр D_2HF. The infrared spectrum of D_2HF / Lovejoy Ch. M., Nelson D. D., Nesbitt D. J. // J. Chem. Phys.— 1988.— 89, № 12.— С. 7180—7188.— Англ.

Методом лазерной ИК-спектроскопии высокой чувствительности измерен спектр поглощения молекул D_2HF в обл. вал. кол. HF в газ. фазе при сверхзвуковом истечении из щелевого сопла. В спектре наблюдаются полосы системы $\Pi \leftarrow \Pi$ молекулы пара-D_2HF и системы $\Sigma \leftarrow \Sigma$ орто-D_2HF, в отличие от спектра H_2HF, в к-ром наблюдались лишь $\Pi \leftarrow \Pi$-полосы. Анализ спектра показывает, что состояния Π молекулы D_2HF являются более сильно связанными по сравнению с состояниями Σ. На основании дублетного расщепления оценены барьеры внутр. вращения D_2 в молекуле комплекса. Скорость колебат. предиссоциации в D_2HF примерно в 25 раз превышает таковую в H_2HF, что предположительно может служить каналом для колебат. возбуждения фрагмента D_2. По резюме

М.П.

④ ☒

Х.1989, N16

D_2HF ОМ. 3164б 1988

(Ик спектр)

110: 84459g **The infrared spectrum of the molecular deuterium-hydrogen fluoride complex (D_2HF).** Lovejoy, Christopher M.; Nelson, David D., Jr.; Nesbitt, David J. (Natl. Bur. Stand., Univ. Colorado, Boulder, CO 80309-0440 USA). *J. Chem. Phys.* 1988, 89(12), 7180-8 (Eng). Ultrasensitive IR laser absorption spectroscopy in a slit supersonic expansion was used to obtain the spectrum of the HF stretching fundamental of D_2HF. Both a $\Pi \leftarrow \Pi$ band due to para-D_2HF and a $\Sigma \leftarrow \Sigma$ band due to ortho-D_2HF are obsd., in contrast to the H_2HF spectrum which consists of the $\Pi \leftarrow \Pi$ band alone. Anal. of the spectrum indicates that the D_2HF states are more strongly bound than the Σ states. Doublet splittings in the $\Pi \leftarrow \Pi$ band are analyzed to det. barriers to internal rotation of D_2 within the complex. The vibrational predissocn. rate of D_2HF is approx. 25 times faster than that of H_2HF, suggesting the opening of a channel which results in vibrational excitation of the D_2 fragment.

C.A.-1989, 110, N10

$(DF)_2$ (от. 30555) 1988

Nesbitt D.J.,

Di, ИК
спектр,
Do
(обзор)

Chem. Rev. 1988, <u>88</u>,
N 6, 843-870.

FD_2 OM· 31638 1988

Petsalakis I. D., Theodorakopoulos G., et al.,

теорет-
расчет

J. Chem. Phys., 1988, 89, N11, 6841-6849.

Theoretical investigation involving electronic and vibrational calculations of the $2^2A_1(3p) \to 1^2B_2(3p)$ and the $3^2A_1(4s) \to 1^2B_2(3p)$ transitions in FH_2 and FD_2.

ДOF 1988

Thiel W., Scuseria G.,
et al.

м.п. J. Chem. Phys. 1988.
<u>89</u>, N8. C. 4965–4975.

●

(см. F_2O; III)

F·D_2O 1988

Yates Brian F.,
Schaefer Henry F., III.
et al.

ИК,
ab initio

J. Am. Chem. Soc. 1988,
110 (19), 6327–32.

(см. F·H_2O; III)

$(DF)_2$ Bunker P.R., Gomez P.C., et al., 1989

An Ab Initio Semirigid Bender Calculation of the Rotation and Trans-Tunnelling Spectra of $(HF)_2$ and $(DF)_2$

Eleventh Colloquium On High Resolution Molecular Spectroscopy, Giessen, September 18-22, 1989, A1, D16.

$(DF)_2$ Ом·34092 1989

ab initio
расчёт

Bunker P.R., Carrington T., Jr., Gomez P.C. et al.

J. Chem. Phys. 1989, <u>91</u>, N 9, 5754–5759.

An ab initio semirigid bender calculation of the rotation and trans-tunneling spectra of $(HF)_2$ and $(DF)_2$.

HF·DF

1989

111: 86476e Vibrational predissociation in the H–F stretching mode of hydrogen fluoride-deuterium fluoride (HF–DF). Fraser, G. T.; Pine, A. S. (Mol. Spectrosc. Div., Natl. Inst. Stand. Technol., Gaithersburg, MD 20899 USA). *J. Chem. Phys.* 1989, 91(2), 633-6 (Eng). The high-resoln. IR spectrum of the K = 1–0 subband of the H–F stretching vibrational band of the hydrogen-bonded HF–DF complex was recorded using a mol.-beam elec. resonance optothermal color-center-laser spectrometer. The spectrum exhibits minor perturbations and vibrational predissocn. linewidths of 23 ± 2 MHz full width at half-max. for comparison to the 11 ± 1 MHz widths found for the corresponding mode of the homonuclear HF–HF dimer.

(ИК)

C.A.1989, <u>111</u>, N10

$(DFHF)_2$ 1989

Ruoff R. S., Klots T., et al.

12th Int. Symp. on Mol. Beams, Perugia, May 29 – June 2, 1989; Abstr. pap. Perugia, [1989]. C. 320-323.

(см. C_2H_5OH; III)

фуры
мв спектры
м.п.

$(HFDF)_2$ 1989

Ruoff R.S., Klots T., et al.
12th Int. Symp. on Mol.
Beams, Perugia, May 29–
June 2, 1989: Abstr. pap.
Perugia [1989]. C. 320–
–323. ● (См. C_2H_5OH; III)

фури
И в спектры
м.п.

FDF^- 1990

Bouteiller Y.,
Mijoule C.

расчёт
структуры
и силовых
постоянных

THEOCHEM 1990,
<u>67</u>(3-4), 189-96.

● (см. FHF^-; <u>III</u>)

H_2DF Clary D. C., 1990
Chakravarty Ch. et al.

Dyn. Poyatom. Van der Waals
м. п. Complexes: Proc. NATO Adv.
Res. Workshop, Castera-
Verduzan, Aug. 21-26, 1989.

New York; London, 1990. с.
355–369.
(См. ArHCl; III)

1990

D_2HF

H_2DF

расчет
вандер-
ваальс.
спектров

Clary D.C., Knowles P.J.,

J. Chem. Phys. 1990, <u>93</u>, N 9, 6384–6849.

(см. H_2HF, <u>III</u>)

MFDF 1990

Jensen Per, Bunker P.R.,
et al.

расчёт ν_1, ν_2

J. Chem. Phys. 1990,
93(9), 6266–80.

● (см. $(HF)_2$; III)

$(DF)_2$

1990

Jensen Per, Bunker P.R., et al.

J. Chem. Phys. 1990, <u>93</u>(9), 6266-80.

расчёт ν_1, ν_2

(см. $(HF)_2$; <u>III</u>)

$(DF)_2$ (OM · 34346) 1990

Quack M., Suhm M.A.,

потенц. Mol. Phys. 1990, <u>69</u>,
поверхн. N 4, 791-801.

Potential energy surface and energy levels of $(HF)_2$ and its Disotopomers.

HFDF (DM 34346) 1990
DFHF

Quack M., Suhm M.A.,
Mol. Phys. 1990, <u>69</u>,
N4, 791–801.

потенц.
поверхн.

Potential energy surface and energy levels of $(HF)_2$ and its D isotopomers

D_2HF

1992

116: 94328b Vibrational predissociation in the molecular deuterium-hydrogen fluoride complex (D_2HF). Clary, David C. (Dep. Chem., Univ. Cambridge, Cambridge, UK CB2 1EW). *J. Chem. Phys.* 1992, 96(1), 90–7 (Eng). Calcns. are presented of linewidths for the vibrational predissocn. of D_2HF induced by excitation of the HF stretching vibration in the weakly bound mol. A potential energy surface based on ab initio computations with the correct leading multipole terms was used. The vibrational predissocn. linewidths are obtained from accurate close-coupling computations of scattering resonances for the D_2 + HF collision. The calcd. linewidths are in excellent agreement with those obtained from IR absorption expts. and confirm that the mechanism for vibrational predissocn. is $D_2HF(v = 1) \rightarrow D_2\ (v = 1) + HF(v_2 = 0)$. The vibrational predissocn. linewidths assocd. with the Σ vibration in para-D_2 HF are about five times narrower than those for the Π vibration. This implies that it should be possible to observe the $D_2HF(v = 0,\Pi \rightarrow v = 1,\Sigma)$ transition in IR spectroscopy measurements. The rotational distributions of the D_2 + HF products of the vibrational predissocn. process are predicted and should be observable.

колебат. предиссоциац.

C.A. 1992, 116, N 10

D_2HF 1992

11 Д85. Колебательная предиссоциация в D_2HF. Vibrational predissociation in D_2HF / Clary D. C. // J. Chem. Phys.— 1992.— 96, № 1.— С. 90—97.— Англ.

Проведены расчеты ширин линий для колебательной предиссоциации D_2HF, индуцированной возбуждением валентного колебания HF в слабо связанной молекуле. Использована поверхность потенц. энергии, построенная на основе неэмпирич. расчетов. Ширины линий получены путем точных расчетов резонансов рассеяния для столкновения D_2+HF в приближении сильной связи. Рассчитанные ширины линий согласуются с данными ИК-спектроскопии и подтверждают, что механизмом колебательной предиссоциации является: $D_2HF(v=1)\rightarrow D_2(v_1=1)+HF(v_2=0)$.

М.Л.

Ф. 1992, N 11-12

D_2HF

1992

(колеб. предис-
социация)

117: 97849d **A time-dependent, golden-rule, wave-packet calculation for vibrational predissociation of molecular deuterium-hydrogen fluoride (D_2HF).** Zhang, Dong H.; Zhang, John Z. H.; Bacic, Zlatko (Dep. Chem., New York Univ., New York, NY 10003 USA). *J. Chem. Phys.* **1992,** 97(2), 927–34 (Eng). Calcns. of the total and partial decay widths are presented for the vibrational predissocn. of D_2HF. The calcn. is done for the total angular momentum $J = 0$ of the mol. and for the dissocn. process D_2HF ($v = 1$) → D2 ($v = 1$) + HF ($v = 0$), which is the dominant decaying channel. A time–dependent wave packet method, in the golden rule approxn., is employed in the numerical calcn. for the decay widths. Computed total and partial decay widths are in good agreement with those from a time–independent scattering calcn. The time–dependent golden rule wave packet method, which does not solve coupled channel scattering equations, offers an efficient alternative to the time–independent scattering method for computing the decay widths in vibrational predissocn. for relatively large mols.

C. A. 1992, <u>117</u>, N10

$(DF)_3$

1993

118: 262993b **High-resolution infrared spectroscopy of the deuterium fluoride trimer: a cyclic, ground-state structure, and deuterium fluoride stretch-induced intramolecular vibrational coupling.** Suhm, Martin A.; Farrell, John T., Jr.; Ashworth, Stephen H.; Nesbitt, David J. (Dep. Chem. Biochem., Univ. Colorado, Boulder, CO 80309-0440 USA). *J. Chem. Phys.* **1993**, 98(7), 5985-9 (Eng). The authors present high-resoln., IR laser absorption spectra of $(DF)_3$ in a slit supersonic jet expansion. In contrast to previous structureless near-IR spectra of $(HF)_3$, the $(DF)_3$ data reveal clear rotational structure characteristic of a cyclic, 6 membered ring, and therefore provide the first accurate exptl. evidence for the equil. geometry of any HF oligomer beyond the well studied dimer. Furthermore, the spectra display homogeneous rotational fine structure 2-3 orders of magnitude in excess of what could be anticipated from a single vibrational band. Anal. of this fine structure, elucidates a novel IVR mechanism which involves single hydrogen bond cleavage, and consequent opening of the $(DF)_3$ ring on the 10 ps time scale.

ИК спектр
высокого
разрешения

C.A. 1993, 118, N 26

D_2HF 1994

Nesbitt D.J.,
Lindeman T.G. et al.

Ик
спектр.

J. Chem. Phys. 1994,
100 (2), 775–85.

(см. N_2HF; III)

(DF)$_2$

1996

126: 38837m **Plucking a hydrogen bond: A near infrared study of all four intermolecular modes in (DF)$_2$.** Davis, Scott; Anderson, David T.; nesbitt, David J. (JILA, Univ. Colorado Natl. Inst. Standards Technol., Boulder, CO 80309−0440 USA). *J. Chem. Phys.* **1996**, 105(16), 6645−6664 (Eng), American Institute of Physics. The near IR combination band spectra of supersonically cooled (DF)$_2$ at 2900−3300 cm^{-1} were recorded with a high resoln. slit jet spectrometer. Twelve vibration−rotation−tunneling (VRT) bands are obsd., representing each of the 4 intermol. modes (van der Waals stretch ν_4, geared bend ν_5, out−of−plane torsion ν_6, and antigeared bend ν_3) built as combination bands on either the ν_1 (free) or ν_2 (bound) DF stretches. Anal. of the rotationally resolved spectra provide spectroscopic consts., intermol. frequencies, tunneling splittings, and predissocn. rates as a function of both intra− and intermol. excitation. The intermol. frequencies demonstrate a small but systematic dependence on intramol. mode, which is exploited to yield frequency predictions relevant to far−IR studies, as well as facilitate direct comparison with full 6−D quantum calcns. on trial potential surfaces. The tunneling splittings demonstrate a much stronger dependence upon intermol. mode, increasing by as much as an order of magnitude for geared bend excitation. Conversely, high resoln. line shape anal. reveals that vibrational predissocn. broadening is only modestly

(ИК, Di)

C.A. 1997, 126, N3

affected by intermol. excitation, and instead exhibits mode specific behavior controlled predominantly by intramol. excitation. Detailed H/D isotopic vibrational shifts are obtained by comparison with previous combination band studies of all 4 intermol. modes in $(HF)_2$. In contrast to the strong state mixing previously obsd. for $(HF)_2$, the van der Waals stretch and geared bend degrees of freedom are largely decoupled in $(DF)_2$, due to isotopically detuning of resonances between bend−stretch intermol. vibrations. Four−dimensional quantum calcns. of the $(HF)_2$ and $(DF)_2$ eigenfunctions indicate that the isotopic dependence of this bend−stretch resonance behavior is incorrectly predicted by current H bond potential surfaces.

$(DF)_2$

1996

22Б1314. Изотопическое замещение в водородной связи. Изучение внутримолекулярных колебаний в $(DF)_2$ в ближней инфракрасной области. Isotopic substitution of a hydrogen bond: A near infrared study of intramolecular vibrations in $(DF)_2$ / Davis S., Anderson D. T., Farrell J. T. (Jr), Nesbitt D. J. // J. Chem. Phys.— 1996.— **104**, № 21.— С. 8197–8209.— Англ.

В областях 2878–2901 и 2831–2839 см$^{-1}$ полос ν_1 и ν_2 спектра $(DF)_2$ измерены частоты 110 и 156 линий подполос $K=0\leftarrow0$, $K=1\leftarrow0$ и $K=0\leftarrow0$, $K=1\leftarrow1$ ветвей P, Q, R. Определены изменения молекулярных постоянных по мере удаления от основного колебат. состояния. Наблюдаются туннельные расщепления и предиссоциационные уширения.

М. А. Ковнер

М.П.

Х.1997, н22

HF · DF

$(HF)_n(DF)_n$

1997

127: 25123w FTIR spectroscopy of hydrogen fluoride clusters in synchronously pulsed supersonic jets. Isotopic isolation, substitution and 3-d condensation. Quack, Martin; Schmitt, Ulrich; Suhm, Martin A. (Laboratorium fuer Physikalische Chemie der ETH Zuerich (Zentrum), CH-8092 Zurich, Switz.). *Chem. Phys. Lett.* **1997**, 269(1,2), 29–38 (Eng), Elsevier. Synchronously pulsed supersonic jet FTIR spectra of HF/DF expansions in rare gases were studied over a wide range of cluster compns. Size-resolved $(DF)_n$ bands and spectra of $(HF)_n(DF)_m$ with various n and m are reported and assigned. At higher backing pressures, the spectra are dominated by crystal-like absorptions, which the authors tentatively assign to 3-d nanometer solids. The new exptl. results support the authors' previous size, structure and vibrational mode assignments and provide new insights into spectra and dynamics of HF clusters, including intramol. vibrational redistribution.

(FTIR)

C. A. 1997, <u>127</u>, N 2