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FINAL REPORT

"Electron Transfer, Proton Transfer and Photoaddition Reactions in Isolated Clusters"

by

E. R. Bernstein

Department of Chemistry
Colorado State University
Fort Collins, Colorado 80523

December 1992

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The work completed during this period has been carried out by many co-workers supported by the ONR and has been reported in published papers and more than 80 Technical Reports.

The people involved have been both graduate students and postdoctoral fellows.

Dion, C. (GS) Hineman, M. (PD)

Disselkamp, R. (PD) Shang, Q. Y. (PD)

Together in one report below are the abstracts of the published and to be published papers from this work. They include studies of the structure of nonrigid molecules, the formation of clusters and dimers, liquid cluster structure, chemical reaction studies, and studies of cluster dynamics.

Published papers, 1991 to present: see attached

Papers in press but not published: see attached

Papers to be submitted: see attached

Honors - E. R. Bernstein

American Physical Society Fellow 1992

Mass resolved excitation spectroscopy of radicals: Benzyl and phenylnitrene

H. S. Im^{a)} and E. R. Bernstein

Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

(Received 12 April 1991; accepted 22 July 1991)

Two-color mass resolved excitation spectra are obtained for the benzyl and "phenylnitrene" radicals. The spectrum previously assigned to the benzyl radical is generated by a species with mass 91 amu. This finding is consistent with the proposed $C_6H_5\dot{C}H_2$ benzyl radical structure. The origin of this $1^2A_2 \rightarrow 1^2A_1$ transition lies at $21\,997\text{ cm}^{-1}$. The ionization energy for the benzyl radical is $\sim 7.236\text{ eV}$. The phenylnitrene radical spectrum is associated with a species of 90 amu. The phenylnitrene designation is not appropriate for this mass number: the suggested cyanocyclopentadienyl radical species (C_5H_4CN) is consistent with this mass. This radical has an ionization threshold of $\sim 9.05\text{ eV}$. Lifetimes are reported for a number of the vibronic states of both radicals.

Supersonic Jet Studies of Ethoxybenzenes: Geometry of Their Minimum Energy Conformations

E. R. Bernstein,* Hoong-Sun Im, and Mark A. Young†

Department of Chemistry, Condensed Matter Sciences Laboratory, Colorado State University, Fort Collins, Colorado 80523

Henry V. Secor, Ronald L. Bassfield, and Jeffrey I. Seeman*

Phillip Morris Research Center, P.O. Box 26583, Richmond, Virginia 23261

Received February 13, 1991

Supersonic jet mass resolved excitation spectroscopy and MOPAC 5/AMI calculations are employed to demonstrate that the minimum energy conformation of ethoxybenzene and a number of its ortho-unsubstituted (i.e., sterically unhindered) derivatives is the planar form for which $\tau_1(C_{ortho}-C_{ipso}-O-C_2) = 0^\circ$ and $\tau_2(C_{ipso}-O-C_2-C_1) = 180^\circ$. For 1-ethoxy-3-methylbenzene, two spectroscopic origin transitions are observed, one each for the conformations in which the $C_6H_4-C_7H_3$ fragment is syn and anti to the C(3)-methyl substituent. For 1-ethoxy-4-ethylbenzene, a single origin transition is observed, as demonstrated by examination of two deuterated derivatives.

Vibrational dynamics of aniline (N_2)₁ clusters in their first excited singlet state

M. F. Hineman, S. K. Kim,^{a)} E. R. Bernstein,^{b)} and D. F. Kelley^{b)}

Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

(Received 27 June 1991; accepted 20 December 1991)

The first excited singlet state S^1 vibrational dynamics of aniline(N_2)₁ clusters are studied and compared to previous results on aniline(CH_4)₁ and aniline(Ar)₁. Intramolecular vibrational energy redistribution (IVR) and vibrational predissociation (VP) rates fall between the two extremes of the CH_4 (fast IVR, slow VP) and Ar (slow IVR, fast VP) cluster results as is predicted by a serial IVR/VP model using Fermi's golden rule to describe IVR processes and a restricted Rice-Ramsperger-Kassel-Marcus (RRKM) theory to describe unimolecular VP rates. The density of states is the most important factor determining the rates. Two product states, 0^0 and $10b^1$, of bare aniline and one intermediate state $\bar{0}^0$ in the overall IVR/VP process are observed and time resolved measurements are obtained for the 0_0^0 and $\bar{0}_0^0$ transitions. The results are modeled with the serial mechanism described above.

Solvation effects on the electronic structure of 4-*N*, *N*-dimethylaminobenzonitrile: Mixing of the local $\pi\pi^*$ and charge-transfer states

Quan-yuan Shang and Elliot R. Bernstein

Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523

(Received 30 January 1992; accepted 23 March 1992)

The effect of polar solvents acetonitrile and water on the electronic excited states of 4-*N*,*N*-dimethylaminobenzonitrile (DMABN) is studied through the optical spectroscopy of small clusters of DMABN/solvent. The clusters are created in a supersonic jet expansion. The results of mass resolved excitation spectroscopy (MRES), fluorescence excitation (FE), dispersed emission (DE), and photodepletion studies demonstrate that the solvent molecule can bind to DMABN at two distinct sites for the one-to-one cluster. Both DMABN (H_2O)₁ clusters generate small blue shifts for the S_1-S_0 cluster transition and evidence low-energy vibronic structure nearly identical to that found for the bare molecule. The DMABN (CH_3CN)₁ clusters behave quite differently. One cluster geometry induces a small blue shift of the S_1-S_0 electronic transition with little change in its vibronic structure and intensity pattern. We suggest this binding site involves the cyano end of the DMABN molecule. The second cluster geometry induces a large red shift ($\sim 1000\text{ cm}^{-1}$) and significant broadening ($> 10^3\text{ cm}^{-1}$) of the lowest-energy transition. This red shifted transition is associated with a charge-transfer transition within the DMABN molecule lowered in energy due to the acetonitrile coordination with the DMABN aromatic ring. The lowering of the charge-transfer state in DMABN (CH_3CN)_{*n*}, *n* = 1, ..., 5 clusters is supported by the following data: long wavelength emission from clusters with broad red shifted absorption; distinct lifetimes for emission at 350 nm (4.6 ns) and 400 nm (6.0 ns); broad red shifted absorption for one geometry of the DMABN (CH_3CN)₁ cluster. These results support the idea that the charge-transfer transition in DMABN is stabilized by short-range dipole-dipole interactions between DMABN and polar nonhydrogen bonding solvents.

Toluene-water clusters: Ion fragmentation and chemistry

Shijian Li and Elliot R. Bernstein

Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

(Received 22 January 1992; accepted 30 March 1992)

Toluene/water cluster ion fragmentation is studied for isolated cold clusters by means of one- and two-color mass resolved excitation spectroscopy, time resolved pump (S_1-S_0) probe ($I-S_1$) spectroscopy on the nanosecond time scale, and nozzle/laser delay timing experiments. These experiments lead to an identification of parent clusters for all fragment ion clusters observed. Fragmentation reactions depend on cluster size and on the energy deposited in the ion by the two photon $I-S_1-S_0$ excitation sequence. Fragments identified by these techniques include (H_2O)_{*x*}H⁺ (*x* = 3, ..., 6) and toluene⁺ (H_2O)_{*n-1*} for toluene(H_2O)_{*n*} clusters and (H_2O)_{*x*}D⁺, (H_2O)_{*x*}H⁺, and toluene-d₃⁺ (H_2O)_{*n-1*} for toluene-d₃(H_2O)_{*n*} clusters. For *n* < 3 the preferred cluster fragmentation pathway is loss of a single H₂O molecule, while for *n* > 4 the preferred cluster fragmentation pathway is generation of (H_2O)_{*n*}H⁺. Cluster ion fragmentation is prevalent in this system because of product stability (i.e., solvated protons and the benzyl radical) and because the $I-S_1$ transition leaves the cluster ion in a very highly excited vibrational state ($\Delta v \gg 0$ for the $I-S_1$ transition). The fragmentation of toluene⁺ (H_2O)₃ to generate (H_2O)₃H⁺ and a benzyl radical takes place by two distinct pathways with generation times $\tau_1 < 60\text{ ns}$ and $\tau_2 = 480\text{ ns}$. The toluene⁺ (H_2O)₂ fragmentation from toluene⁺ (H_2O)₃ has a generation time of $\tau < 60\text{ ns}$. The possible energetics, kinetics, and mechanisms for these fragmentations are discussed.

Excited-state proton transfer in 1-naphthol/ammonia clusters

M. F. Hineman, G. A. Brucker,^{a)} D. F. Kelley, and E. R. Bernstein
Colorado State University, Department of Chemistry, Fort Collins, Colorado 80523

(Received 31 January 1992; accepted 26 May 1992)

Excited-state proton transfer dynamics are reported for the 1-naphthol(NH_3)_n cluster system for $n=3$ and 4. Picosecond time- and mass-resolved pump ($S_1 \leftarrow S_0$)-probe ($I \leftarrow S_1$) experiments demonstrate the following results: (1) excited-state proton transfer occurs for $n=3$ and 4 clusters only; (2) for $n=5$ clusters the proton is transferred in the ground state and for $n=2$ clusters no proton transfer can be observed; (3) the proton transfer time in the $n=3$ cluster at the 0_0^0 transition is ca. 60 ps; (4) this time is reduced to ca. 40 ps and ca. 10 ps for 800 and 1400 cm^{-1} of vibrational energy in S_1 , respectively; (5) for the $n=4$ clusters these times are approximately 70, 70, and 30 ps, for 0, 800, and 1400 cm^{-1} of vibrational energy in S_1 , respectively; (6) both $n=3$ and 4 clusters exhibit a second low-amplitude decay component, which is about an order of magnitude slower than the initial decay; and (7) 1-naphthol- d_1 (ND_3)_n clusters have a greatly reduced rate constant for the excited-state proton transfer dynamics. These observations are well fit and explained by a simple statistical/barrier penetration model involving proton tunneling and the effect of van der Waals vibrations on the height and width of the barrier to proton transfer.

Toluene-ammonia clusters: Ion fragmentation and chemistry

Shijian Li and Elliot R. Bernstein
Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

(Received 22 January 1992; accepted 30 March 1992)

The toluene/ammonia cluster system is studied by mass resolved excitation spectroscopy: like the toluene/water system, an extensive ion chemistry is found to exist generating ammonia solvated protons and (solvated) benzyl radicals. Extensive cluster fragmentation (dissociation) is observed even at "threshold ionization energies." Nozzle delay and deuteration studies are applied to elucidate the ion chemistry and dissociation of this cluster system. Proton transfer/cluster fragmentation reactions in this system are driven by the stability of the benzyl radical and (NH_3)_m H^+ and solvation stabilization of the toluene ion. Cluster fragmentation by loss of a single ammonia molecule is not observed. Fragmentation is so extensive for this system that spectral features could not be identified with parent clusters

Potential energy surfaces of substituted anilines: Conformational energies, deuteration effects, internal rotation, and torsional motion

R. Disselkamp, H. S. Im,^{a)} and E. R. Bernstein
Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

(Received 13 April 1992; accepted 17 August 1992)

Mass resolved excitation spectra (MRES) are presented for a series of substituted anilines including 2- and 3-methylaniline, 2- and 3-ethylaniline, 2-aminobenzyl amine, and 2-aminobenzyl alcohol. The observed spectra show the following phenomena: nearly free internal rotation of the methyl substituent in the S_1 state; long vibrational progressions attributed to C-C, C-N, and C-O side chain torsional motion; an inequivalence of the two amino hydrogens for both ring and side chain amino groups as determined from the spectra of deuterated species; and the existence of two conformers for 2-aminobenzyl alcohol. Semiempirical and *ab initio* calculations are performed on these systems to aid in the analysis of the potential energy surfaces and in the interpretation of the experimental results.

Benzyl alcohol-water and benzyl alcohol-ammonia clusters: Ion fragmentation and chemistry

S. Li and E. R. Bernstein

Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

(Received 28 May 1992; accepted 13 August 1992)

Benzyl alcohol/ammonia, α,α -dimethylbenzyl alcohol/ammonia, and benzyl alcohol/water cluster ion fragmentation and chemistry are studied for isolated cold clusters by means of one and two-color mass resolved excitation spectroscopy, nozzle/laser timing delay, and deuteration experiments. Experiments lead to an identification of parent clusters for all fragment ion clusters observed. Three types of cluster ion fragmentation are observed for these systems: dissociation— $\text{solu}^+(\text{solv})_n \rightarrow \text{solu}^+(\text{solv})_k + m \text{ solv}$; acid-base chemistry— $\text{ArCH}_2\text{OH}^+(\text{B})_n \rightarrow \text{ArCH}_2\text{O}(\text{B})_k + \text{B}_m\text{H}^+$; and (benzyl) radical chemistry— $\text{ArCH}_2\text{OH}^+(\text{B})_n \rightarrow \text{Ar}\dot{\text{C}}\text{HOH}(\text{B})_k + \text{B}_m\text{H}^+$, $\text{ArCD}_2\text{OH}^+(\text{B})_n \rightarrow \text{ArCDHOH}^+(\text{B})_k + \text{B}_m\text{B}-d_2$ and $\text{ArCMe}_2\text{OH}^+(\text{B})_n \rightarrow \text{Ar}\dot{\text{C}}\text{MeOH}^+(\text{B})_k + \text{B}_m\text{Me}$. Fragmentation reactions depend on cluster size, structure, and (weakly) on the vibrational energy deposited in the ion. Specifically, for benzyl alcohol $^+(\text{NH}_3)_1$ only cluster radical chemistry and dissociation take place, while for higher order clusters, the acid-base reaction rate increases and this reaction becomes a major fragmentation pathway for benzyl alcohol $^+(\text{NH}_3)_4$. For the benzyl alcohol $(\text{H}_2\text{O})_n$ system, cluster radical chemistry is not observed with $n=1$, only a weak α -hydrogen transfer reaction is observed with $n=2$, and acid base chemistry is not observed for clusters of any size. Cluster dissociative fragmentation is also a function of cluster size; large water and ammonia clusters dissociate much more easily than do $n=1$ clusters. The possible mechanisms for these fragmentation patterns are discussed.

Minimum energy conformation of *ortho*-xylene in its ground and first excited electronic states

R. Disselkamp and E. R. Bernstein

Colorado State University, Chemistry Department, Fort Collins, Colorado 80523

Jeffrey I. Seeman and Henry V. Secor

Philip Morris Research Center, P. O. Box 26583, Richmond, Virginia 23261

(Received 21 April 1992; accepted 27 August 1992)

The geometry of *ortho*-xylene is studied through supersonic jet cooling and one color mass resolved excitation spectroscopy. By examining the $S_1 \leftarrow S_0$ transition origin region of various (d_0 - d_2) methyl deuterated *o*-xylene species, the conformation of the two methyl groups in S_0 and S_1 can be determined. A comparison between the predicted and experimentally observed number and intensity of origin features for the various partially deuterated *o*-xylenes shows that two highly symmetric methyl group structures are possible, each structure having C_{2v} point group symmetry—the antiplanar conformation (A1), in which $\tau_1(\text{C}_2-\text{C}_1-\text{C}_\alpha-\text{H}_\alpha) = 180^\circ$; $\tau_2(\text{C}_1-\text{C}_2-\text{C}_\alpha-\text{H}_\alpha) = 180^\circ$; and the *syn*, planar conformation (A2) in which $\tau_1 = \tau_2 = 0^\circ$. The experimentally determined structures are consistent with *ab initio* calculations and microwave studies which predict the anticonformation to be most stable. Spectroscopic data, in conjunction with further *ab initio* calculations, are used to investigate the ground and excited state potential energy surfaces. In addition, a repulsive, intramolecular, nonbonded interaction between the two methyl groups is identified through an empirical potential energy calculation to be the most important interaction defining the lowest energy structure.

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Chemical Reactions in Clusters

Elliot R. Bernstein

*Chemistry Department, Colorado State University, Fort Collins, Colorado 80523 (Received June 30, 1992
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Four different classes of cluster chemical reactions are reviewed and specific examples from our laboratory are given for each class. Solvent-induced electron-transfer reactions are illustrated by our studies of 4-(dimethylamino)benzonitrile/acetone clusters. The electron-transfer reaction depends on solvent polarity and on cluster structure. The reaction is induced by only one properly oriented CH_3CN solvent molecule. Proton-transfer reactions in neutral clusters are exemplified by the 1-naphthol/ammonia cluster system. Proton transfer occurs in the first excited singlet state of the 1-naphthol (NH_3)_n cluster of the proper geometry. Two time decays are measured for this event: one dealing with proton transfer and the other with "solvent reorganization or relaxation" following the transfer event. Isotope, energy, cluster size dependence, and model calculations demonstrate a proton tunneling mechanism is appropriate for this reaction. Cluster ion chemistry for toluene, toluene-*d*₇, benzyl alcohol, benzyl- α , α -*d*₂ alcohol, α , α -dimethylbenzyl alcohol/ammonia and water clusters is also discussed. These ionic reactions are characterized by benzyl-like radical formation, solvation of protons, and extensive cluster fragmentation following both ion formation and proton transfer. Finally, a preliminary study of radical reactions in clusters is presented for the benzyl radical clustered with ethylene, propylene, and acetylene.

Solvation effects on reactive intermediates: The benzyl radical and its clusters with Ar, N₂, CH₄, C₂H₆, and C₃H₈

R. Disselkamp and E. R. Bernstein
Chemistry Department, Colorado State University, Fort Collins, Colorado 80523

(Received 1 September 1992; accepted 2 December 1992)

Mass resolved excitation spectra are presented for the benzyl radical and its clusters with Ar, N₂, CH₄, C₂H₆, and C₃H₈. The cluster spectra exhibit small redshifts ($< 50 \text{ cm}^{-1}$) relative to the unclustered benzyl radical for the $D_1(1^2A_2) - D_0(1^2B_2)$ and $D_2(2^2B_2) - D_0(1^2B_2)$ electronic transition regions. A unique set of low energy van der Waals modes is observed for these clusters for each excited electronic state investigated. The cluster spectra also reveal significant vibronic coupling between the two excited electronic states of the benzyl radical, as evidenced by a single vibrational predissociation threshold for each cluster. *Ab initio* calculations are performed on the benzyl radical to examine excited electronic state structure, predict transition energies, estimate ionization energy, and determine partial atomic charges in the electronic states of interest. The resulting partial charges are used in empirical atom-atom potential energy calculations to aid in the understanding of cluster spectroscopic shifts, binding energies, and van der Waals modes.

Proton Transfer Dynamics and Cluster Ion Fragmentation in Phenol/Ammonia Clusters

Max F. Hineman, David F. Kelley and Elliot R. Bernstein

Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523

(To Be Submitted)

Excited-state proton transfer dynamics are reported for the phenol(NH₃)_n cluster system. Excited state proton transfer is shown to occur for this system by isotopic substitution of the hydroxyl proton and ammonia protons. The observed dynamics slow from 80 ps to 600 ps upon cluster deuteration. The effects of cluster vibrational energy and ammonia concentration in the expansion gas are also studied. The results of these experiments are compared with a previous study [Syage and Steadman, *J. Chem. Phys.* **95**, 2497 (1991)] which used a single excitation energy and varied ionization energy. Our experiments indicate that a significant amount of cluster ion fragmentation occurs for this system and caution must be exercised in assigning the decays observed in a given ion mass channel to a particular parent cluster. Due to the difficulties of associating a given decay curve with a cluster of particular mass, a previously proposed model of proton transfer in isolated clusters [Hineman *et al.*, *J. Chem. Phys.* **97**, 3341 (1992)] which details the effect of cluster vibrational energy on the proton transfer rate, cannot be applied to the phenol/ammonia system.

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