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Research performed over the three-year period February 16, 1998 – February 15, 2001 supported by the U.S. Army Research Office (Grant number: DAAG55-98-1-0089) is described. This research program is concerned with the development of methods and simulations to study the reaction dynamics of polyatomic molecules and molecular crystals of interest as energetic materials. The work during this grant focused on the following: (1) The development and demonstration of methods for treating unimolecular reactions in IVR-limited regime, with applications to molecules and reactions pathways relevant to the decomposition of energetic materials. (2) Studies of the decomposition of energetic molecules in liquids. (3) The development and testing of condensed-phase (solids and liquids) models for energetic materials. (4) The development of semiclassical methods that can be used to incorporate quantum effects in multidimensional MD simulations. (5) Studies of the products of decomposition reactions of energetic materials with metals.

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THEORETICAL STUDIES OF ELEMENTARY REACTIONS

IN ENERGETIC MATERIALS

FINAL TECHNICAL REPORT

REPORT PERIOD:
February 16, 1998 – February 15, 2001

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GRANT NUMBER:
DAAG55-98-1-0089

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Index

Abstract

Research performed over the three-year period February 16, 1998 – February 15, 2001 supported by the U.S. Army Research Office (Grant number: DAAG55-98-1-0089) is described. This research program is concerned with the development of methods and simulations to study the reaction dynamics of polyatomic molecules and molecular crystals of interest as energetic materials. The work during this grant focused on the following:

(1) The development and demonstration of methods for treating unimolecular reactions in IVR-limited regime, with applications to molecules and reactions pathways relevant to the decomposition of energetic materials.

(2) Studies of the decomposition of energetic molecules in liquids.

(3) The development and testing of condensed-phase (solids and liquids) models for energetic materials.

(4) The development of semiclassical methods that can be used to incorporate quantum effects in multidimensional MD simulations.

(5) Studies of the products of decomposition reactions of energetic materials with metals.

SCIENTIFIC PROGRESS AND ACCOMPLISHMENTS:

Our research during this report period has focused on the following areas:

- The development and demonstration of methods for treating unimolecular reactions in IVR-limited regime, with applications to molecules and reactions pathways relevant to the decomposition of energetic materials. This theoretical development provides a means of computing rates from the low-energy statistical regime (where TST is valid) up to the high-energy, IVR-limited regime (where MD calculations are feasible). It was demonstrated for bond-fission reactions in RDX and dimethylnitramine.

- Studies of the decomposition of RDX in liquid Xe as a function of pressure. The results provide a possible explanation for why the ring-fission reaction in the decomposition of RDX has not been observed for condensed phases.

- The development and testing of condensed-phase (solids and liquids) models for energetic materials. This work, carried out in collaboration with Dr. Betsy Rice at ARL, has led to a model that accurately predicts static and dynamic properties of a wide range of energetic molecular solids.

- The development of semiclassical methods that can be used to incorporate quantum effects in multidimensional MD simulations. Atomic-level modeling of energetic materials is rapidly becoming practical. The purpose of this work is to develop methods for accounting for quantum effects such as tunneling and constrained zero-point energy.

- Studies of the products of decomposition reactions of energetic materials with metals. This work represents a minor part of this project. It was done in collaboration with Dr. Cary Chabalowski at ARL. It was undertaken because we had, in the course of our other work, developed methods that are particularly applicable to problems related to gun tube erosion, and thus we extended our studies to include this work.

Diffusion Theory Method for Predicting Unimolecular Reactions Rates in the Statistical and Dynamical Regimes in the Gaseous and Condensed Phases

The basic assumption of statistical theories of unimolecular reactions such as RRK and RRKM is that IVR is rapid compared to the rate of reaction, and that the rate constant $k(E)$ corresponds to a microcanonical ensemble. This is certainly the case when the dynamics are chaotic. The dynamics of large molecules tend to display quasiperiodic behavior at energies well in excess of reaction threshold. Nevertheless, there is sufficient mode mixing that "statistical" reaction rates are commonly observed. That is, at energies near the reaction threshold the rates of reaction tend to be slower than the rates of IVR, and the rate constant can be predicted by statistical theories such as RRKM and VTST. However, at high energies, the rate of reaction can become much faster than the rate of IVR, and reaction rate must be calculated by a method that takes into account the nonstatistical dynamics. This is illustrated in the figure below. In region of the reaction threshold energy the energy dependence of the rate generally obeys the RRK equation; that is, a plot of ln k vs. ln(1-E*/E) is linear as shown by the solid line in the figure. This

behavior extended well above the threshold; however, at energies well in excess of that the true rate begins to deviate from this linear behavior, as illustrated by the dashed curve.

log(1-E*/E)
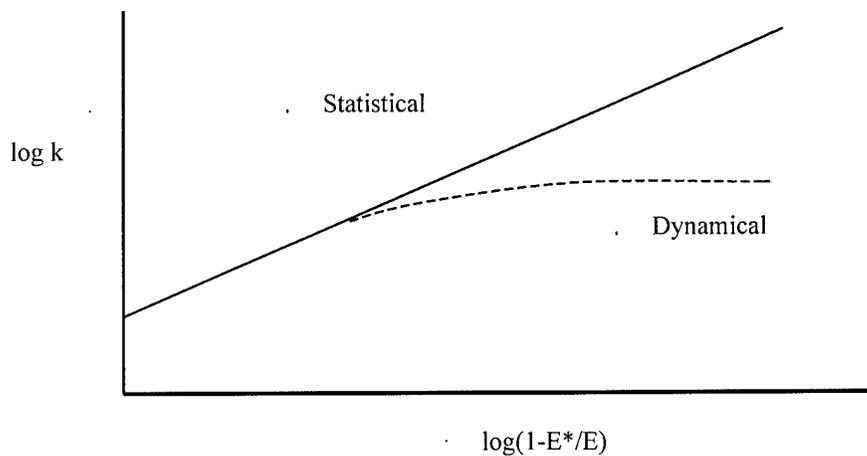
We have illustrated the behavior shown this figure for realistic models of various kinds of molecules (including RDX and dimethylnitramine) by comparing MCVTST and classical trajectory simulation results. At higher energies, the statistical rate is always greater than the true rate, which is controlled by the IVR rate. The behavior at high energies is the result of weak coupling between the vibrational "bath" and reaction coordinate modes (or, more precisely, vibrational states) of the molecule. This is the intramolecular equivalent to the low-pressure behavior in gas-phase unimolecular dissociation reactions where the rate of intermolecular energy transfer to the molecules limits the reaction rate. This is similar to the situation in crystals where the energy flow is from the phonon to molecular modes. Thus, our plan to extend these ideas to solids corresponds to the traditional applications.

In the standard classical trajectory approach, an ensemble of initial phase space points are selected by a Monte Carlo procedure and propagated in time by numerically integrating Hamilton's equations of motion. The reaction rate constant can be obtained from the computed lifetimes of the molecules. Even when initial conditions are randomly selected according to a microcanonical distribution, the computed rate constant can be lower than that predicted by a statistical theory, particularly at high energies. In fact, nonstatistical behavior can be most clearly distinguished by comparing classical trajectory rates to those computed by using a classical transition-state theory, particularly if the calculations use the same potential energy surface (PES). Comparisons are usually made between trajectory and experimental results or those predicted by RRKM or RRK. Since these statistical theories are based on harmonic vibrations, the causes of any disagreements are not clear. The RRK equation $k(E)=v(1-E*/E)^{s-1}$ is often used as a convenient analytical function for fitting the energy dependence of unimolecular rates. The value of s, the number of effective degrees of freedom, then indicates the extent of the statistical dynamics if the harmonic approximation is valid (which it can be for experiments since the average energy per mode is small). Theoretically $s = 3N-6$, but the

values obtained by fitting trajectory results are often significantly smaller. The RRK theory usually fits the energy dependencies of rates in the reaction threshold region; however, trajectory results are usually for much higher energies, and there the fits are not so good. The fits are often good for small molecules, where all the bonds are identical, but large molecules composed of different types of bonds show greater nonstatistical behavior and thus the fits are usually not good.

What this means in practice is that one needs to use different methods for different energy regimes for computing the decay rates of large molecules. The rates near threshold can be computed using a statistical theory and those at high energies by classical trajectory simulations. We have shown that the rates in the intermediate region can be computed by using a dynamically parameterized diffusion theory, which we refer to as *intramolecular dynamics diffusion theory* (IDDT).

We have used MCVTST to calculate the unimolecular dissociation rate coefficients for RDX over the energy range 170-450 kcal/mol, thus spanning the range from the IRMPD experiments to that of our trajectory results (200-450 kcal/mol). The MCVTST-computed branching ratio at 170 kcal/mol is in excellent agreement with the experimental value. Comparisons of the trajectory and MCVTST results show that there are significant dynamical effects at the higher energies when the reaction is IVR-limited. That is, at high energies the trajectory rates are smaller than the statistical rates.

The practical difficulties in calculating rates by MD at the lower end of the energy range where there are still significant dynamical effects, led us to explore the use diffusion theory (IDDT). We demonstrated the accuracy of the IDDT method for predicting the dynamical rates of chemical reactions for simple bond fission in DMNA (dimethylnitramine) $(CH_3)_2N-NO_2 \rightarrow (CH_3)_2N\cdot + \cdot NO_2$, $H_3Si-SiH_3 \rightarrow 2\ SiH_3$, and for the N-N bond and ring fission reactions in RDX. We find that IDDT accurately predicts the dynamical rates. The rates calculated by using IDDT are quite close to the results obtained from classical trajectory simulations; in fact, they are in quantitative agreement.

This work has been published in two papers: J. Chem. Phys. **110**, 5514 (1999) and *ibid.* **110**, 5521 (1999).

We next carried out studies to extend IDDT to reactions in condensed phases. In the first study, we used the generalized Kramers' model to compute rates by numerically solving the general energy diffusion equation. We demonstrated the method with applications to a simple model and to dimethylnitramine in liquid xenon. This work has been published: Phys. Chem. Chem. Phys. 1, 1293 (1999).

Finally, we have developed a method for computing thermal and microcanonical unimolecular reaction rates by solving the general energy diffusion equation. The solution provides the rates in the diffusion limit for fast reactions and the statistical (TST) rates for slow reactions. The rates between the two limits can be easily obtained by solving a one-dimensional Schrödinger-like equation transformed from the diffusion equation. We applied the method to the unimolecular dissociation of RDX, and compared the results with those from classical trajectory and Monte Carlo variational transition-state theory calculations. The method provides a practical means of computing accurate microcanonical rates at considerable savings in computer time compared to

trajectory simulations. This work has been published: J. Phys. Chem. A **103**, 10308 (1999).

RDX Decomposition in Liquid Xenon

We have used molecular dynamics simulations to study the decomposition of RDX in liquid xenon. This work has been published: J. Phys. Chem. B, **103**, 10599 (1999). The Abstract follows:

The unimolecular dissociation of RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine) in liquid xenon is investigated to determine condensed-phase effects on the N-N bond fission and ring-opening reactions. The dependence of the rate constants on pressure at a fixed temperature is studied using molecular dynamics simulations, and the results is consistent with the experimental finding that the ring-opening channel is suppressed in a condensed phase environment. The effects of intramolecular vibrational energy redistribution (IVR) and intermolecular energy transfer on reaction rates are also studied by putting a "hot" RDX molecule in liquid xenon. The reaction rates are calculated using a statistical approach and direct simulations. The statistical rate for the bond fission is 45% larger than the corresponding dynamical one, indicating that the rate of IVR is not faster than that of reaction.

Studies of Energetic Materials Crystalline Solids.

Working in collaboration with Dr. B. M. Rice at ARL, we have continued our studies of the fundamental behavior of molecular crystals. We have completed three major studies this grant period.

As discussed in our last report, we have expanded our studies to assess the transferability of our interaction potential to non-nitramines. That work has been published: J. Phys. Chem. **A103**, 989 (1999). The Abstract follows:

We have analyzed the transferability of a previously proposed intermolecular potential for nitramine crystals to reproduce the experimentally determined crystal structures (within the approximation of rigid molecules) of 51 nitro compounds. These compounds include different types of acyclic, monocyclic and polycyclic molecules. It is shown that this potential model accurately reproduces the experimentally determined crystallographic structures and lattice energies for the majority of these crystals. The best agreement with experimental structural and energetic data is obtained when the electrostatic charges have been determined using *ab initio* methods that include electron correlation effects, namely MP2 and B3LYP. The use of the electrostatic charges calculated at the Hartree-Fock level results in large differences between the predicted and the experimental values of the lattice energies. This difference can be significantly decreased by scaling the electrostatic charges with a general factor without introducing significant variations of the predicted crystallographic parameters. Further testing of the proposed intermolecular potential has

been done by performing isothermal-isobaric molecular dynamics (MD) simulations over the temperature range 100-450 K, at atmospheric pressure, for the monoclinic phase of the 2,4,6-trinitrotoluene (TNT) crystal and for the polymorphic phase I of the pentaerythritol tetranitrate (PETN I) crystal. In each case, the results show that throughout the MD simulations the average structures of the crystals maintain the same space group symmetry as the one determined experimentally and there is a good agreement between the calculated crystallographic parameters and the experimental values. The thermal expansion coefficients calculated using the present model indicate an overall anisotropic behavior for both TNT and PETN I, with a thermal isotropy for PETN I along cell directions a and b.

In another study we performed calculations to assess the quality of our potentials. In particular we have examined the hydrostatic compression of some energetic materials to determine if the structural changes observed experimentally are described accurately with the present set of potentials. That work has been published: J. Phys. Chem. B **103**, 6783 (1999). The Abstract follows:

A previously developed intermolecular potential for nitramines and several other classes of nitro-compound crystals has been used to investigate the behavior of the energetic materials hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX), 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX), 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIW) and pentaerythritol tetranitrate (PETN) under hydrostatic compression. Isothermal-isobaric molecular simulations (assuming the rigid molecule approximation) and molecular packing calculations were used to perform the analyses. In the case of the RDX, HMX and HNIW crystals the results indicate that the proposed potential model is able to reproduce accurately the changes in the structural crystallographic parameters as functions of pressure for the entire range of pressures that has been investigated experimentally. In addition, the calculated bulk moduli of RDX and HMX were found to be in good agreement with the corresponding experimental results. In the case of the PETN crystal, the crystallographic parameters have been reproduced with an acceptable accuracy at pressures up to about 5 GPa. The larger deviations from the experimental results at greater pressures indicate the limitations of the rigid-molecule model when applied to floppy molecules. The similarity of the results determined in molecular packing calculations relative to those from molecular dynamics simulations suggest that the former method can be used as an efficient tool for rapid tests of the crystal structure modification under pressure.

In a third study, we performed simulations of solid nitromethane. A manuscript has been written and is being submitted for publication. The Abstract follows:

A classical potential to simulate the dynamics of a nitromethane crystal as a function of temperature and pressure is described. The intramolecular part of the potential was taken as superposition of bond stretching, bond bending and torsional angles terms. These terms were parameterized based on the geometric and spectroscopic (vibrational frequencies and eigenvectors) data obtained using *ab initio* molecular orbital

calculations performed at the B3LYP/6-31G* level on an isolated molecule. The intermolecular potential used is of the Buckingham 6-exp form plus charge-charge Coulombic interactions and has been previously developed by us (Ref.1) to simulate crystals containing nitramine molecules and several other classes of nitro-compounds. The analyses performed using constant pressure and temperature molecular dynamics simulations and molecular packing calculations indicate that the proposed potential model is able to reproduce accurately the changes of the structural crystallographic parameters as functions of temperature or pressure for the entire range of values investigated. In addition, the calculated bulk modulus of nitromethane was found in excellent agreement with the corresponding experimental results. Moreover, it was determined that the present potential predicts correctly an experimentally-observed 45° change in methyl group orientation in the high pressure regime relative to the low-temperature configuration. The analysis of the linear expansion coefficients and linear compression data indicate anisotropic behavior for the unit cell edges.

This work is currently being extended to simulations of liquid nitromethane.

Studies of Energetic Materials on Metal Surfaces

Two studies were initiated in this report period to investigate fundamental aspects of energetic materials reactions at metal surfaces.

A collaboration with Dr. Cary Chabalowski at the ARL focuses on determining the interactions of the decomposition products of energetic materials with iron. *Ab initio* calculations with DFT is being used to study CO adsorption on Fe surfaces. A slab model is used to simulate the surface with periodic boundary conditions in all three directions. Full relaxation of atoms in the solid as well as of the adsorbed molecules is considered in order to generate accurate adsorption configurations. We have performed the following types of investigations:

a) Prediction of equilibrium crystallographic properties of bulk iron: the lattice dimensions, elastic constants, bulk modulus.

b) Prediction of the density of states and band structure of bulk iron.

c) Analysis of the relaxation of the Fe(100) surface as a function of the number of layers in the slab model.

d) Investigation of the adsorption properties of CO at different sites on Fe(100). Particularly we consider the adsorption at: (a) on-top site; (b) 2-folded site (bridging between two Fe atoms) and (c) 4-folded site.

Based on these calculations we have determined:

a) The adsorption energies of CO on Fe(100).

b) The adsorption configurations of CO on Fe(100), their vibrational characteristics, and the corresponding surface relaxations.

These studies will provide:

c) The analysis of the total and local density of states and distribution of electrostatic potential will give insight into the mechanism of chemisorption of CO on Fe(100).

d) An accurate potential that describes of interactions between CO and Fe(100).

e) Finally, the dynamical effects for CO dissociative chemisorption will be studied based on *ab initio* molecular dynamics calculations as a function of temperature. These studies can readily be extended to other Fe surfaces such as (111) and (110). A manuscript is being prepared for publication of this work.

In another study, we are carrying out a classical trajectory study of the desorption of NO produced by the photodissociation of methyl nitrite on Ag(111). These studies are being done in collaboration with Prof. J. M. White, U. Texas, Austin. Professor White's group has performed a series of experiments to investigate the photodissociation of various nitrites on metals surfaces. Our calculations are focusing on the step following the fission of the O-N bond. We begin the simulations with a monolayer of molecules, with one of them dissociated – that is, NO + OCH_3. We are computing the behavior of the NO as it is ejected from the surface for the experimental energy and spatial distributions. A manuscript is being prepared for publication of this work.

PUBLICATIONS, REPORTS, AND THESES

Manuscripts submitted and published:

Yin Guo, Thomas D. Sewell, and Donald L. Thompson,
"Semiclassical Calculations of Tunneling Splitting in Tropolone,"
J. Phys. Chem. A, **102**, 5040-5048 (1998).

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Phys. Chem. Chem. Phys. 1, 1293-1297 (1999).
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Yin Guo, Donald L. Thompson, and William H. Miller,
"Thermal and Microcanonical Rates of Unimolecular Reactions from an Energy Diffusion Theory Approach,"
J. Phys. Chem. A **103**, 10308-10311 (1999). (Kent Wilson Special Issue).

Dan C. Sorescu, Betsy M. Rice, and Donald L. Thompson,
"Theoretical Studies of Solid Nitromethane,"
J. Phys. Chem. B **104**, 8406-8419 (2000).

BOOK CHAPTERS AND REVIEW ARTICLES

Yin Guo and Donald L. Thompson,
"Multi-Dimensional Semiclassical Tunneling,"
in **Methods in Multidimensional Molecular Dynamics**, edited by
D. L. Thompson (World Scientific Pub., New Jersey, 1998), pp.713-737.

Donald L. Thompson,
"Practical Methods for Calculating Rates of Unimolecular Reactions,"
International Reviews in Physical Chemistry, **17**, 547-569 (1998).

OTHER PUBLICATIONS AND REPORTS

Paras M. Agrawal, Dan C. Sorescu, Betsy M. Rice, and Donald L. Thompson,
"A Model for predicting the Solubility of RDX in Supercritical CO_2: Isothermal-Isobaric Monte Carlo Simulations"
Technical Report, ARL-TR-1947, May 1999.

B. M. Rice, J. Hare, G. Krasko, W. Mattson, S. V. Pai, S. F. Trevino, D. C. Sorescu and D. L. Thompson,
"Theoretical Chemistry: An Emerging Practical Tool in Army Research",
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B. M. Rice, J. Hare, S. V. Pai, W. Mattson, G. Krasko, S. F. Trevino, D. C. Sorescu, and D. L. Thompson, "Theoretical Chemistry: Applications in Energetic Materials Research," Proceedings of the International Workshop on New Models and Predictive Methods for Shock Wave/Dynamic Processes in Energetic Materials and Related Solids, July, 1999.

B. M. Rice, J. Hare, G. Krasko, W. Mattson, S. V. Pai, S.F. Trevino, D. C. Sorescu and D. L. Thompson, "Theoretical Chemistry: An Emerging Practical Tool in Army Research", Proceedings of the 1998 Army Science Conference, June, 1998.

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