

**POTENTIAL ENERGY SURFACES AND DYNAMICS FOR
HIGH ENERGY SPECIES (AFOSR F49620-95-1-0077)
FINAL REPORT**
MARK S. GORDON

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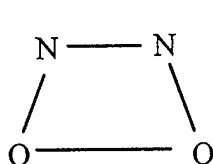
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13. ABSTRACT (Maximum 200 words) The stability of the asymmetric dimer of NO (a-N2-02: 3) with respect to spin forbidden radiationless decay has been investigated. The spin-allowed decay channel $\text{N2O2}(1A') \rightarrow \text{N2O}(X1+) + \text{O}(1D)$ is endoergic. However, the spin forbidden spin decay channel $\text{a-N2O2}(1A) \rightarrow \text{N2O9X1+} + \text{O}(EP)$ is exoergic. Large-scale multi-reference CI wave functions, approximately 300,000 - 1,400,000 configuration state functions, based on double zeta plus polarization and triple zeta plus polarization bases sets were used to study this process. The minimum energy crossing point of the ground singlet state and the lowest excited triplet state was determined, as was the interstate spin-orbit coupling. This electronic structure data was used in the context of a simple one-dimensional model to show that a N2O2 is rapidly predissociated to $\text{N2O}(X1+) + \text{O}(3P)$. This means a-N2O2 is not a good HEDM candidate, despite the high energy content of this compound.			
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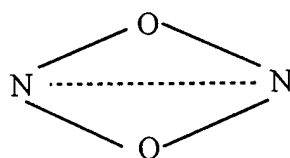
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N₂O₂ AND RELATED SPECIES

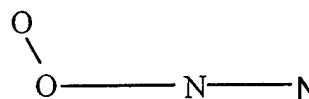
The stability of the asymmetric dimer of NO (a-N₂O₂: **3**) with respect to spin forbidden radiationless decay has been investigated¹. The spin-allowed decay channel a-N₂O₂(¹A') → N₂O(X¹+) + O(¹D) is endoergic. However, the spin forbidden decay channel a-N₂O₂(¹A') → N₂O(X¹+) + O(³P) is exoergic. Large-scale multi-reference CI wave functions, approximately 300,000 - 1,400,000 configuration state functions, based on double zeta plus polarization and triple zeta plus polarization bases sets were used to study this process. The minimum energy crossing point of the ground singlet state and the lowest excited triplet state was determined, as was the interstate spin-orbit coupling. This electronic structure data was used in the context of a simple one-dimensional model to show that a-N₂O₂ is rapidly predissociated to N₂O(X¹+) + O(³P). This means a-N₂O₂ is not a good HEDM candidate, despite the high energy content of this compound.



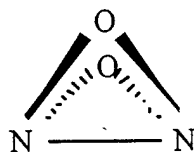
1 C_{2v}



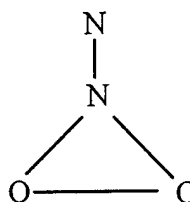
2 D_{2h}



3 C_s



4 C_{2v}



5 C_{2v}

Several other high energy isomers of N₂O₂ (**1**, **2**, **4**, **5**) have been identified². Two of these (**2**, **4**) may be thought of as bicyclic analogs of isoelectronic bicyclobutane. These two bicyclic isomers are predicted to be 49 and 82 kcal/mol above 2 NO, at the multi-reference (MR) second order perturbation (MP2) level of theory, using the extended 6-311+G(2d) basis set. Because of the significant configurational mixing in these species, single-configuration based methods (e.g., perturbation theory methods or the G2 method) are found to be unreliable for prediction of relative energies. The planar ring **1** is 53 kcal/mol above 2 NO at the same level of theory. While structure **5**

is also a high energy species¹, this species is predicted to be unstable to non-adiabatic dissociation, in a manner similar to structure 3.2c

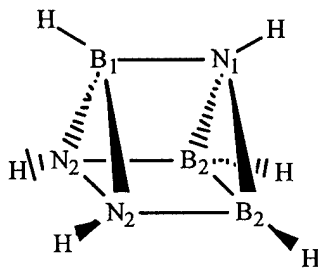
The remaining isomers are quite high in energy, ranging from 49 to 52 kcal/mol above 2 NO at the highest level of theory: second order multi-reference perturbation theory (CASPT2) with the 6-311+G(2d) basis set. In order to further assess their viability as HEDM candidates, the minimum energy paths (MEP) connecting each of these species with 2 NO, via the intervening transition state has been explored³. The adiabatic barrier heights separating these isomers from products are 40 (isomer 2), 20 (1), and 18 (4), kcal/mol, respectively. So, all three species are potential HEDM candidates, especially isomer 1.

One also must consider the crossings of the MEP with higher lying repulsive states (usually triplet states), since such crossings may lower the operational barriers, depending on where they occur. For isomer 1, the repulsive triplet crosses the singlet surface at about 10 kcal/mol below the singlet transition state. Depending on the strength of the non-adiabatic (i.e., spin-orbit) coupling between the two electronic states, this crossing could effectively reduce the barrier to dissociation by 10 kcal/mol, to about 30 kcal/mol. This is still a healthy barrier height. Such triplet crossings have no effect on the barriers for the other isomers, so 2 and 4 may still be viable candidates.

A new cyclic isomer of FN₃, a species which is isoelectronic with N₂O₂, has been found on the singlet potential energy surface⁴. This cyclic isomer is 15 kcal/mol higher in energy than the well known acyclic structure, at the MR-MP2/6-31G(d) level of theory. The barrier to dissociation to N₂ + NF (1) is 17 kcal/mol. Since the lowest triplet state crosses the ground singlet state *behind* this barrier, this species is stable with respect to non-adiabatic coupling to a dissociative triplet state.

HIGHLY STRAINED RINGS

In the process of investigating the general effect of replacing some or all of the carbon atoms in benzene with hetero atoms, we have discovered several very high energy, nonplanar isomers of these compounds⁵. The most promising of these compounds have the formula X₃N₃H₆ with the heavy atoms arranged in a prismane structure (shown below for X = B):



Using second order perturbation theory and modest basis sets, the BN prismane is found to be more than 160 kcal/mol higher in energy than the planar benzene analog. Extensive searches are under

way to determine pathways for the decomposition and isomerization of this high energy compound. Although we have performed extensive explorations of the ground state potential energy surface, we have not yet found a direct route from the BN prismane through a concerted transition state to the planar borazene isomer. So, it appears that this isomerization must be a multi-step process. This appears to be consistent with the analogous all carbon system, for which the isomerization also appears to occur in multiple steps. We have found minimum energy paths leading from BN prismane to several interesting species. The most promising of these may be the decomposition to two three-membered rings (BNN and NBB), since this decomposition is nearly isoenergetic. So, synthesis of these rings may be a possible route to the prismane species. Colleagues at Rockwell Science are attempting these syntheses. Subsequent calculations will address the effects of substituents on the potential of this and related compounds (e.g., X = Al) as HEDM species.

We have previously reported the existence of bond stretch isomerism in any silabicyclobutanes in which the bridgehead atoms are silicons⁶. We have now mapped out the MEP connecting the two isomers in the tetrasil case at the GVB/6-31G(d,p) level of theory, calculated the projected vibrational frequencies along the path and predicted the free energy path for the reaction⁷. We have found that the size of the groups attached at the bridgehead positions determine whether the short bond or the long bond isomer is lower in energy. When the bridgehead substituent is hydrogen, the highest levels of theory predict that the short bond structure does not even correspond to a minimum on the potential energy surface. On the other hand, the short bond structure is the lower energy isomer when bulky t-butyl groups are placed in the bridgehead positions. The next step is to make use of variational transition state theory to investigate the dynamics and kinetics for the bond stretch isomerization reaction. An interesting feature of this investigation will be to ask how vibrational excitation affects the rate constants and tunneling probabilities. A preliminary calculation of the specific impulse (I_{sp}) for silabicyclobutane, used as an additive to liquid hydrogen, suggests that this compound is a promising additive⁷ (see discussion in main body of proposal). The relative stabilities of the long- and short-bond isomers clearly depend on the substituents placed on both the peripheral and bridgehead silicons, and the compound is easier to synthesize and stabilize when the hydrogen substituents are replaced with bulkier groups. It is therefore necessary to determine the structures, thermodynamic properties, and I_{sp} 's for a variety of substituted compounds, to assess their utility as HEDM species.

When the two peripheral silicons in tetrasilabicyclobutane are replaced by carbon atoms, there are again two (long and short) bond stretch isomers. For these species, two connecting transition structures are found. Unlike the tetrasil analog, in this case both isomers remain minima on the potential energy surface at the highest levels of theory. Since this species may be easier to synthesize without bulky substituents, it is also a likely HEDM additive.

HYPERVALENT ANIONS

Pseudorotation in SiH_5^- has been investigated by following the minimum energy path (MEP) from the tetragonal transition state to the trigonal bipyramidal minimum, using MP2/6-31G(d,p) energies⁸. The reaction path hamiltonian was then determined. Using this RPH, we have predicted the rate of the pseudorotational motion at several temperatures using variational transition state theory (VTST) and the small curvature tunneling approximation. We are now in the process of fitting the PES to an analytic form, in preparation for investigating trajectories on this surface. A series of substituted pentacoordinated Si anions is being investigated in an analogous manner⁹. For SiH_4F^- , if correlated wavefunctions and/or extended basis sets are used, the equatorial isomer becomes a transition state. So the simple Berry notion of pseudorotation is an over-simplification for complex species. Similar results are found for polysubstituted pentacoordinated anions. PH_4F is isoelectronic with SiH_4F^- and exhibits a pseudorotation surface which is similar to that of the anion¹⁰. For this molecule, the MEP and several associated paths have been followed to demonstrate that as one proceeds from the highest transition state (square pyramid) down to the lower energy transition state (equatorial), the imaginary frequency disappears before the new imaginary frequency (corresponding to the MEP leading from equatorial to axial) appears. This is expected to have a major impact on pseudorotational dynamics.

The stationary points on the potential energy surfaces of NH_4^- and PH_4^- have now been identified at the MP2/6-311++G(d,p) level of theory, with single point energies being obtained with QC1/6-311++G(2df,2pd)¹¹. The transition states connecting the minima with each other and with $\text{XH}_2^- + \text{H}_2$ and with $\text{XH}_3 + \text{H}^-$ ($\text{X}=\text{N}, \text{P}$) have been identified, and the minimum energy paths mapped out. For both species, the highest energy isomer is the tetrahedral structure. Interestingly, there appears to be no transition state linking the T_d isomer with any other isomer or with dissociation products. In order to determine how this anion might dissociate to $\text{XH}_3 + \text{H}^-$, our new direct dynamics code, in which we can study *ab initio* trajectories "on-the-fly" was used to get a handle on the dissociation energetics. Based on these calculations, it appears that dissociation of tetrahedral NH_4^- and PH_4^- requires 35.5 and 5 kcal/mol, respectively.

WEAKLY BOUND SPECIES

There is currently considerable interest in doping solid hydrogen with a small amount (<5%) of light metal atoms, since many of the lighter metals react more exothermally with oxygen than does hydrogen. The key is to determine if these metals can form weakly bound (e.g., Van der Waals) species, so that oxidation does not have to overcome the binding energy of stronger M-H bonds. This means that if a Van der Waals species exists, it must be separated from any lower energy hydride by a substantial barrier, and there must not be an intersystem crossing that effectively lowers or even destroys the barrier.

The most interesting metals M, based on the heats of formation of their corresponding oxides, appear to be Li, Be, B, C, Na, Mg, Al, Si. So, we have carried out a preliminary study of the potential energy surfaces that connect the separated species $M + H_2$, potential Van der Waals species, and the much more stable hydrides, in order to determine barrier heights on the adiabatic surfaces and to identify state crossings that might lead to unwanted nonadiabatic couplings. These calculations were carried out using QCISD(T) with large basis sets¹². Based on these calculations, the most promising metals appear to be B and Al. As a result, we have proceeded to explore the Al- H_2 and B- H_2 potential energy surfaces in much more detail. This effort has already resulted in two additional papers on Al- H_2 and analogous efforts on B- H_2 are in progress.

In the first Al- H_2 paper¹³, the energies and derivative couplings were computed in the vicinity of the $1^2A' - 2^2A'$ seam of conical intersections for AlH₂. It was shown that the reaction path for the decomposition of excited vibrational levels of AlH₂(X^2A_1) to Al + H_2 passes quite close to the minimum energy crossing point (MECP), the minimum energy point on the seam of conical intersections. Near the MECP the seam of conical intersection exhibits an unusual trifurcation with a C_{2v} portion dividing into a branch that preserves C_{2v} symmetry and two symmetry equivalent branches that have only C_s symmetry. In the second AlH₂ paper¹⁴, portions of the C_{2v} , C_v and C_s potential energy surfaces were studied. The most stable Van der Waals complex with $2B_2$ symmetry is found to be kinetically stable, with the lowest energy crossing point with the $2A_1$ state estimated to occur at about 30 kcal/mol above the Al + H_2 dissociation limit. This result, plus the observation that the two states exhibit very little interaction when the symmetry is reduced to C_s , suggest that the probability for the adiabatic reaction Al--- H_2 ($2B_2$) → AlH₂ ($2A_1$) through an avoided crossing is very low. It should be strongly noted that much of the work on these weakly bound species benefitted greatly from continuing collaborations with Professor David Yarkony.

There are many remaining questions regarding this system, as well as for the closely related BH₂ system. These include the nature of Al interactions with H_2 clusters of increasing size, the ability of two Al atoms embedded in a H_2 matrix to find each other and form a stable diatomic, and the detailed nature of the reactions of such Al_n(H_2)_m clusters with oxygen. All of these questions will be addressed in future studies.

An off-shoot of the Al--- H_2 studies resulted from discussion at the HEDM contractors' meetings with Professor Michael Duncan, regarding the experimental uncertainty of the nature and energetics of Al---N₂ interactions¹⁵. Al-(N₂)_x Van der Waals complexes have recently been produced in molecular beam experiments and studied with threshold laser photoionization. We performed *ab initio* calculations at a very high level of accuracy, in order to determine the ionization potential and binding energy of Al---N₂. The calculated difference between the binding energies of the neutral and cationic species is very close to the experimental value determined by Duncan; however, the calculated binding energy is about 200-250 cm⁻¹ lower than the experimental value estimated by

McMahon. Given the quality of the calculations and the uncertainty in the experiments, it may be that the theoretical value is more reliable.

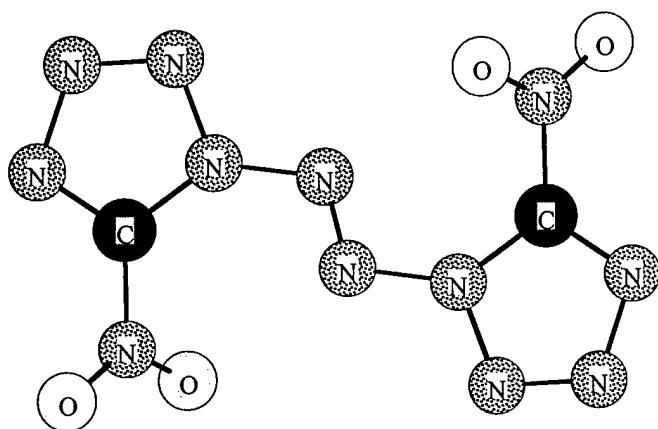
CUBANES

Cubane and derivatives of cubane have been the focus of continuing interest as potential fuels, because of their high heats of formation. During the past year, we have initiated a series of calculations on several heterocubanes¹⁶. Whereas cubane itself is one of the highest energy isomers with the chemical formula C_8H_8 , its persila analog is the most stable Si_8H_8 isomer. Consequently, this species, with alkyl groups replacing the hydrogens, has been synthesized and is stable to air and to thermal decompositions. In view of the interest in such species, we have performed a series of calculations which show that (a) Si_8H_8 is indeed quite stable to unimolecular decomposition or isomerization, (b) is stable to attack by H_2 , and (c) has a very high heat of formation. Unfortunately, due to its weight, this species is unlikely to be a useful HEDM candidate, unless the alkyl groups can be replaced by silyl groups. It would then have potential as a fuel additive.

The cubane analog in which all carbons are replaced by nitrogens has generated considerable interest, again due to its very high predicted heat of formation. To our knowledge, however, the potential energy surface that leads to the stable decomposition products $4 N_2$ has not been adequately explored, so the barriers separating the cubane from molecular nitrogens is unknown. Also, since such highly energetic species frequently have low-lying excited states, there is also a possibility that non-adiabatic interactions, resulting from surface crossings, like those described above for N_2O_2 , could reduce the kinetic stability of the azacubane. We have therefore initiated a study of the low-lying potential energy surfaces of this species. It is already clear from the calculations on the ground state singlet that the upper limit for the barrier separating cubic N_8 from $4 N_2$ is 20 kcal/mol. So, at best, N_8 is just at the edge of usefulness as a HEDM species. We have also had a brief look at $(CO)_4$, an isoelectronic analog of N_8 and cubane. While this species is even more energetic than azacubane, the barrier separating it from $4 CO$ is tiny, less than 0.1 kcal/mol, so it is clearly not useful in this context.

NEW HEDM CANDIDATES

In the 1996 HEDM Synthesis/Theory workshop, Rob Schmitt (SRI) proposed several (not yet synthesized) nitrogen-containing compounds as potential HEDM species, and requested that theorists provide some information about them. One such compound is shown below.



The geometry and vibrational frequencies of this compound have been determined at the SCF/6-31G(d) level of theory. Its heat of formation was predicted to be 456.8 kcal/mol, using a combination of isodesmic reactions and the G2 (MP2,SVP) model. This amounts to just under 1.8 kcal/g and to an I_{sp} of 329 sec, assuming decomposition to N_2 and CO_2 . This may be compared to I_{sp} 's of 240 for hydrazine and 300 for LOX/RP1. So, this proposed compound may be a viable monopropellant. The next steps in the study of this species will be to investigate its stability with respect to hydrolysis, oxidation, and attack by acid or base.

MODEL DEVELOPMENT

Calculations of accurate potential energy surfaces (PES's) for molecular isomerizations and dissociations are highly compute-intensive, frequently requiring the use of very large basis sets and multi-reference wave functions. Multi-reference wave functions are especially critical when more than one electronic state is involved in the calculation. Therefore, a major effort in our group has been to increase the efficiency of the calculations by developing electronic structure codes that may be used on parallel computers. Our philosophy has been to make the codes as general and (therefore) as portable as possible, so that they may be used in virtually any parallel environment. The platform used for the parallel developments is GAMESS¹⁷ [General Atomic and Molecular Electronic Structure System]. The currently distributed version (at no charge to users) includes parallel capability for all Hartree-Fock (RHF, UHF, ROHF), two-configuration (TCSCF or GVB) wavefunctions, multi-configurational wavefunctions, second order perturbation theory (MP2), and their associated analytic gradients¹⁷. For these levels of theory, the scalability of the calculations with increasing numbers of nodes is close to ideal (100%) for up to 16 nodes, as long as the size of the application is increased as the number of nodes is increased. Very little efficiency is lost through 32 nodes, and significant speedups are obtained even with 256 nodes. The calculations can be

performed on a variety of platforms, ranging from a small number of workstations of various types to massively parallel computers (e.g., IBM SP2's at Maui and Wright-Patterson, Cray T3E's at CEWES and SDSC).

The parallel capability has already had a major positive impact on our HEDM efforts, since the structure predictions and potential energy surfaces for the inorganic prismanes, the substituted silabicyclobutanes and cubanes, and the large nitrogen-containing species suggest by Schmitt and co-workers would have been virtually impossible without the ability to perform these calculations in parallel. New algorithms for calculating analytic Hessians¹⁸ and MCSCF wavefunctions¹⁹ in parallel have been developed, and much improved versions of these codes are under construction.

The study of PESs for chemical reactions often involves more than one electronic state. When this occurs, it is necessary to determine the spin-orbit coupling among these states. We have devised a general scheme for directly calculating the one-electron matrix elements and then using these results to parametrize the two-electron contributions, all using the GAMESS MCSCF and CI programs. The predictive ability of this method for diatomics and small polyatomic molecules is quite good²⁰⁻²². The next step is to develop general algorithms to permit the calculation of the full spin-orbit matrix elements.

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PRESENTATIONS AT MEETINGS

1. G. Chaban, "Potential Energy Surfaces for High Energy FN_3 and N_2O_2 Isomers", Midwest Theoretical Chemistry Conference, Evanston, IL, May 1995.
2. "Potential Energy Surfaces and Dynamics for Potential HEDM Compounds", AFOSR HEDM Contractor's Meeting, Woods Hole, MA, June 1995.
3. N. Matsunaga, "Potential Energy Surfaces for High Energy Prismanes", AFOSR HEDM Contractors' Meeting, Woods Hole, MA, June 1995.
4. G. Chaban, "Potential Energy Surfaces for Weak M- H_2 Complexes", AFOSR HEDM Contractors' Meeting, Woods Hole, MA, June 1995.
5. "Features and Applications of Parallel GAMESS", Maui Workshop on Parallel Computing, Maui Supercomputer Center, Kihei, Maui, HI, December 1995 (INVITED)
6. M.S. Gordon, "Potential Energy Surfaces and Dynamics for High Energy Species, AFOSR HEDM Contractors' Meeting, Boulder, CO, June 1996.
7. G. Chaban, "Potential Energy Surfaces for Weak M- H_2 Complexes", AFOSR HEDM Contractors' Meeting, Boulder, CO, June 1996.
8. "Metal - H_2 Van Der Waals Species", American Conference on Theoretical Chemistry, Park City, Utah, July 1996, presented by Galina Chaban.
9. "The Potential Energy Surfaces for Octasilacubanes", American Conference on Theoretical Chemistry, Park City, Utah, July 1996, presented by Michael Schmidt.
10. M.S. Gordon, "Van der Waals Complexes Between Main Group Metals and H_2 Clusters, National American Chemical Society Meeting, Orlando, FL, August 1996 (INVITED).
178. "Current Status of Parallel GAMESS", Cornell Theory Center Workshop, October 1996 (INVITED).
11. "New Directions for Parallel Electronic Structure Theory", National ACS meeting, San Francisco, April 1997, INVITED.
12. "The Effective Fragment Method for Solvation", National ACS Meeting, San Francisco, April 1997, presented by J. Jensen.

13. "An Approach to Parallel MP2 and CI Gradients", National ACS Meeting, San Francisco, April 1997, presented by G. Fletcher (INVITED)
14. "Quantum Chemistry Tools for Chemical Synthesis", AFOSR HEDM Meeting, Washington, DC, June 1997
15. "High Energy Isomers of N₂O₂", AFOSR HEDM Meeting, Washington, DC, June 1997, presented by G. Chaban.
16. "The Effect of Solvation on Chemical Processes", Ninth International Congress on Quantum Chemistry, Atlanta, GA, June 1997 (INVITED)
17. "Parallel SCF and MP2 Algorithms", Ninth International Congress on Quantum Chemistry, Atlanta, GA, June 1997, presented by G. Fletcher.
18. "Applications of the Effective Fragment Solvation Model: Water Clusters and Dynamic Reaction Coordinates", Ninth International Congress on Quantum Chemistry, Atlanta, GA, June 1997, presented by G. Merrill.

AWARDS AND HONORS

1. Editorial Advisory Board, Journal of Physical Chemistry
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3. Vice Chair, Theoretical Chemistry Subdivision, American Chemical Society, 1994-95
4. Chair-Elect, Theoretical Chemistry Subdivision, American Chemical Society, 1995-96
5. Chair, Theoretical Chemistry Subdivision, American Chemical Society, 1996-97
6. Secretary-Treasurer, Physical Chemistry Division, American Chemical Society, 1996-2001