ies of neutral triatomic hydrogen, H_3. This technique yields the branching
o into H_2+H and H+H+H channels, the ro-vibrational distribution of the H_2
gments, as well as the momentum vector correlation in the event of three-
body breakup. The correlation experiments reveal complex phase-space
ages of the nonadiabatic coupling, which opens the bound excited state to the
sociative continuum. This correlation has been studied for excited s-, p-, and
manifolds for various vibrational and rotational levels in H_3 and in the heavy
isotopic isotope, D_3. A second experiment [I. Mistrik *et al.*, Phys. Rev. A 68
2711 (2001)] investigates the competition between predissociation and
ionization of triatomic hydrogen at the ionization threshold. These experi-
ments capture intermediates active in dissociative recombination. We will
discuss our results in the spirit of dissociative recombination of slow electrons
with H_3^+.

Research supported by the Deutsche Forschungsgemeinschaft under SFB 276
TP3.

M.

COMBINATION OF H_3^+ AND D_3^+ WITH ELECTRONS: LOW LIMIT OF THE COMBINATION RATE COEFFICIENT. ***Juraj Glosik***, *Radek Plasil, Vitoria Zakouzka, Pavel Kudrna, Milan Tichy, and Andriy Pysanenko, Mathematics and Physics Faculty, KEVF, Charles University, Prague, Czech republic, V Holesovickach 2, 180 00, Prague, Czech Republic, Fax: +420-2-6885095, Juraj.Glosik@mff.cuni.cz*

In the decay of plasma in the mixture of He, Ar and H_2 (or D_2) we deter-
mined the overall rate constant (α) of the recombination of H_3^+ and D_3^+ ions
with electrons. We observed pronounced dependence of α on partial pressure of
hydrogen (deuterium). The dependence of α on the H_2 (or D_2) indicates that
observed recombination proceeds most probably via formation of long lived
Rydberg states that are stabilised against the reverse autoionisation by collision
with neutral molecule. From our study it follows that binary dissociative
recombination of H_3^+ ions with electrons is very slow process (at 270 K) - with
a coefficient $\alpha < 3\times10^{-9}$ cm^3s^{-1}.

This work was supported in part by Grant Agency GACR No. 202/99/D061,
202/01/1689, by Charles University under project No. 146/2000/B FYZ MFF. The
studies were carried out with support of EU in frame of the ETR network
HPRN-CT-2000-00142).

I.

STRUCTURAL STUDY OF $(ALN)_N$, $(GAN)_N$, AND $(INN)_N$ (N= 3 - 6): FROM N-N DOMINATED MOLECULES TO METAL-N DOMINATED SOLID-LIKE CLUSTERS. *Kumar **Kandalam**[1], Ruth Franco[2], Aurora Costales[2], Miguel A. Blanco[2], Ravindra Pandey[1]. (1) Department of Physics, Michigan Technological University, 1400 Townsend Drive, Houghton, MI 49931, Fax: 906-487-2933, @mtu.edu, (2) Departmento de Química Física y Analítica, Universidad de Oviedo*

Group-III nitride materials are widely known for their applications in
opto-electronic industry (LEDs, CCDs) and hence are widely studied at their
bulk-phase. The thermodynamically stable structure for these materials was
found to be wurtzite, with tetrahedral coordination. As the research at molecular
level is still lacking, a first principles calculation, based on the generalized
gradient approximation (GGA) to the density functional theory, was initiated. Our
research is on understanding the structural properties of small nitride clusters and
to study the emergence of bulk-like properties with increase in the cluster
size. Preliminary results for M_3N_3 and M_4N_4 (M=Al, Ga, In) clusters, show a
distinct structural difference between the most stable isomers of Al, and those
of Ga and In. For Al_nN_n (n=3, 4) clusters, the metal-nitrogen bond is found to
dominate the structural properties. For Ga_nN_n, and In_nN_n (n=3, 4), the nitrogen-
nitrogen bond is preferred over other bonds. Calculations are in progress for
M_5N_5 and M_6N_6 (M=Al, Ga, In), whose results will also be presented.

AB INITIO AND DFT STUDIES OF SULFUR TRIOXIDE-WATER COMPLEXES. ***M. Standard**, and Douglas H. Pulsifer, Department of Chemistry, Illinois State University, Normal, IL 61790-4160, standard@ilstu.edu*

One of the principal components of acid rain is sulfuric acid, which is formed
from the reaction of sulfur trioxide and water. In this work, sulfur trioxide-water
complexes have been investigated using ab initio and DFT methods. Levels of
theory employed include HF, MP2, and B3LYP. Full geometry optimizations and
vibrational frequency calculations have been carried out, utilizing basis sets up
to 6-311++G(2df,2pd) for the smaller complexes and up to 6-311++G(d,p) for
the larger complexes. Results from gas phase MP2 and DFT studies of sulfur
trioxide interacting with from one to four water molecules are presented and
compared with previous experimental and computational studies. In addition,
results are reported from HF and DFT investigations of sulfur trioxide interacting
with one to four water molecules in which additional solvation effects are
modeled using a continuum solvent approach. Significant differences in the
structural characteristics of the sulfur trioxide-water complexes are observed
when continuum solvent results are compared with gas phase results.

207. 2.0033649

COMPUTATION OF GEOMETRICAL AND ELECTROSTATIC PARAMETERS FOR A CLUSTER MODEL OF SILICA. ***Marsha Collins**[1], Eugene Demchuck[2], and Thomas A. Holme[1]. (1) Department of Chemistry, University of Wisconsin - Milwaukee, 3210 North Cramer Ave., Milwaukee, WI 53211, marshac@uwm.edu, (2) Exposure Assessment Branch, CDC/NIOSH - Morgantown, WV*

Respiration of crystalline silica has long been recognized as a causative agent
for silicosis, a form of pulmonary fibrosis. However, the exact etiology remains
to be learned. As part of a larger study, silica is being considered from a
computational perspective. Calculations of $Si(OH)_4$, $Si_2O(OH)_6$, $Si_3O_2(OH)_8$,
$Si_4O_3(OH)_{10}$, $Si_5O_4(OH)_{12}$, and $Si_8O_7(OH)_{18}$ were performed with HF/6-
311+G(d,p), MP2/6-31G(d), and B3LYP/6-31G(d) methods. This poster will
present structural and electronic parameters from these calculations.

208.

FIRST PRINCIPLES CALCULATIONS OF VIBRATIONS IN VAN DER WAALS CLUSTERS. ***Laurence E. Fried**, Chemistry and Materials Science Department, Lawrence Livermore National Laboratory, L-282, P. O. Box 808, Livermore, CA 94551, Fax: 925-424-3281, lfried@llnl.gov, and Kurt R. Glaesemann, Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory*

The nuclear motion of molecules and clusters is a quantum mechanical
phenomenon. We present calculations of interacting rare gas atoms. In our
calculations, both electrons and nuclei are treated in a rigorously first principles
manner. Electronic interactions are treated via Moller-Plesset perturbation
theory. The quantum vibrations are handled via a numerically efficient Monte
Carlo path integral scheme. We employ a multi-stage parallel algorithm that
scales efficiently up to thousands of processors. We will discuss a novel
"renormalized thermodynamic" estimator for the total energy that can substan-
tially improve numerical efficiency. Calculations of the quantum vibrations of He
clusters at the MP2 level will be presented. The effects of electron correlation on
the vibrational dynamics of rare gas atoms will be discussed.

209.

IR OPTICAL STUDIES OF MODEL TROPOSPHERIC ORGANIC AEROSOLS. *Allison M. Potscavage, Elena M. Lucchetta, and **Richard F. Niedziela**, Department of Chemistry, DePaul University, 1036 West Belden Avenue, Chicago, IL 60614, Fax: 773-325-7421, rniedzie@condor.depaul.edu*

Particulate matter in the troposphere is thought to have a profound effect on
our environment, impacting everything from human health to global warming.
The extent of this impact is not well known at this time due to insufficient
knowledge about the chemical, physical, and optical properties these small
particles, especially those composed of organic materials. This poster will
present the results of experiments designed to quantify the optical properties, in
terms of complex refractive indices, of several organic materials with biogenic
origins found in aerosols. Additional experiments designed to probe the
hygroscopicity of organic aerosols, and hence evaluate their role in cloud
formation, will also be discussed. All of the experiments were carried out in a
recently constructed aerosol flow cell that is designed to study processes
involving organic aerosols under tropospheric conditions.

210.

KNUDSEN CELL AND FT-IR STUDIES OF NO2 ON SOOT AND HNO3 ON OXIDE AND CARBONATE PARTICLES. ***Hind A. Al-Abadleh**, and Vicki H. Grassian, Department of Chemistry, The University of Iowa, Iowa City, IA 52242, Fax: 319-353-1115, hind-al-abadleh@uiowa.edu*

Carbonaceous and mineral aerosols are abundant in the troposphere and may
provide reactive surfaces for heterogeneous reactions of pollutant gases.

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Item Author:
Item Place:
Item Publisher:
Item Edition:
ISSN/ISBN: 0065-7727
Cited In:
Cited Title:
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