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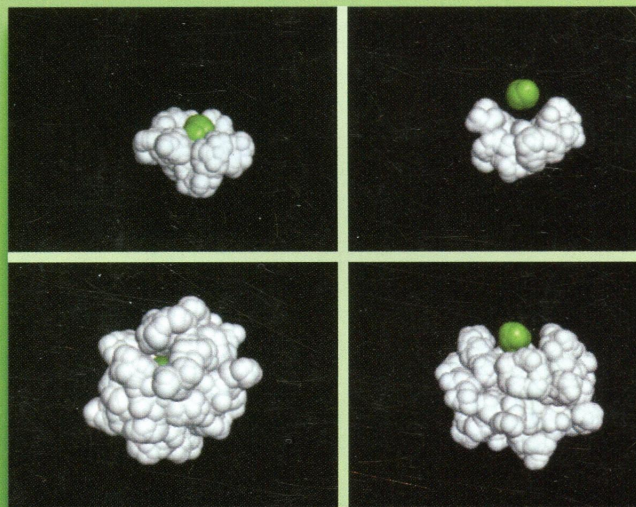
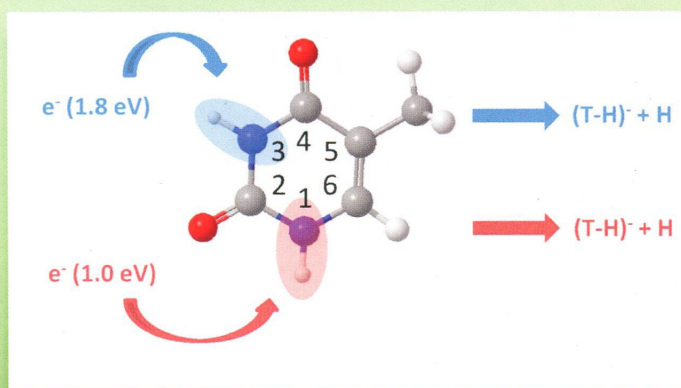
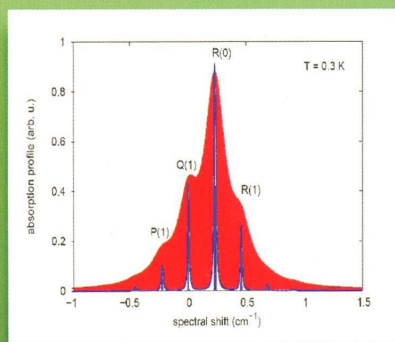
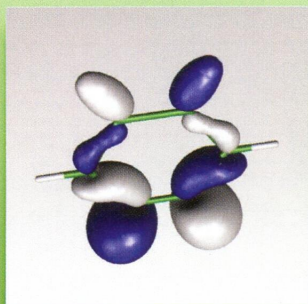
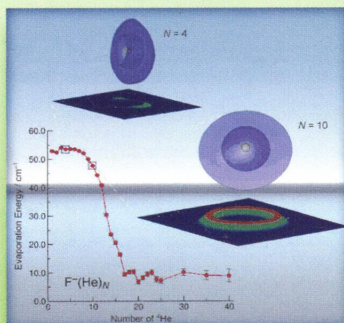
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Some Theoretical Findings Obtained by Franco Gianturco and His Collaborators in Various Fields of Physical Chemistry (see page 5A)

FRANCO GIANTURCO Festschrift



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ON THE COVER: Some theoretical findings obtained by Franco Gianturco and his collaborators in various fields of Physical Chemistry. (Left upper panel) Stochastic quantum Monte Carlo (MC) simulations of anionic fluoride in bosonic helium clusters: evaporative energies as a function of the number (N) of He atoms and spatial shapes of the latter ones showing that at $N = 10$ the anion is already solvated (reproduced with permission from Coccia, E.; Marinetti, F.; Bodo, E.; Gianturco, F. A. *Chemical Solutions in a Quantum Solvent: Anionic Electrolytes in ^4He Nanodroplets*. *ChemPhysChem* **2008**, *9*, 1323–1330, Copyright 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim). (Right upper panel) Interactions of low-energy electrons with thymine leading to bond- and site-selective loss of hydrogen, relevant for electron-induced damage of DNA (reprinted from Baccarelli, I.; Bald, I.; Gianturco, F. A.; Illenberger, E.; Kopyra, J. *Electron-induced damage of DNA and its components: Experiments and theoretical models*, *Phys. Rep.* **2011**, *508*, 1–44 with permission from Elsevier). (Central left panel) Shape of the real part of the scattering wave function for the σ^* resonance in collisions of electrons with *ortho*-benzynes as an example of electron-driven reactions in proto-planetary atmospheres (Carelli, F.; Sebastianelli, F.; Baccarelli, I.; Gianturco, F. A. *Electron-Driven Reactions in Proto-Planetary Atmospheres: Metastable Anions of Gaseous o-Benzynes*. *ApJ*. **2010**, *712*, 445, DOI: 10.1088/0004-637X/712/1/445. Copyright AAS. Reproduced with permission). (Left bottom panel) In the framework of a quantum chemistry-like treatment, simulated infrared absorption profile of iodine monochloride embedded in fermionic helium nanodroplets resembling the experimental behavior of carbonyl sulfide in the same environment (Villarreal, P.; de Lara-Castells, M. P.; Prosimi, R.; Delgado-Barrio, G.; López-Durán, D.; Gianturco, F. A.; Jellinek, J. *Spectral simulations of polar diatomic molecules immersed in He clusters: Application to the ICl (X) molecule*, *Phys. Scr.* **2007**, *76*, C96–C103, DOI: 10.1088/0031-8949/76/3/N15. Copyright The Royal Swedish Academy of Sciences. Reproduced with permission of IOP Publishing. All rights reserved). (Right bottom panel) Snapshots of path integral MC simulations at low temperature of calcium-bosonic helium clusters showing whether the calcium atom is solvated or remains in a dimple on the surface. The upper figures correspond to $N = 10$ helium atoms, while $N = 40$ is shown in the lower ones. Left and right panels differ in the potential model used to describe the Ca–He interaction, stronger to the left and weaker to the right (Reproduced with permission from Rodríguez-Cantano, R.; González-Lezana, T.; Villarreal, P.; López-Durán, D.; Gianturco, F. A.; Delgado-Barrio, G. *Path integral Monte Carlo calculations of calcium-doped ^4He Clusters*, *Int. J. Quantum Chem.* **2014**, DOI: 10.1002/qua.24622. Copyright 2014 Wiley Periodicals, Inc.). This special issue was organized by Guest Editors Gerardo Delgado-Barrio and Pablo Villarreal.

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Guest Editors: Gerardo Delgado-Barrio and Pablo Villarreal

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Upper Limits to the Reaction Rate Coefficients of C_n^- and C_nH^- ($n = 2, 4, 6$) with Molecular Hydrogen

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Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment

Tapta Kanchan Roy, Tucker Carrington Jr., and R. Benny Gerber*

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Correction to “Coupled 3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates: Application to the Adiabatic Singlet-State ($1^1A'$) $D^+ + H_2$ Reaction”

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