Theoretical Studies of Routes to Synthesis of Tetrahedral N₄

A paper [Chem. Phys. Lett. 345, 295 (2001)] describes theoretical studies of excited electronic states of nitrogen molecules, with a view toward utilizing those states in synthesizing tetrahedral N₄ or T₄ N₄ — a metastable substance under consideration as a high-energy-density rocket fuel. Several ab initio theoretical approaches were followed in these studies, including complete active space self-consistent field (CASSCF), state-averaged CASSCF (SA-CASSCF), singles configuration interaction (CIS), CIS with second-order and third-order correlation corrections [CIS(D) and CIS(3)], and linear response singles and doubles coupled-cluster (LRCCSD). Standard double zeta polarized and triple zeta double polarized one-particle basis sets were used.

The CASSCF calculations overestimated the excitation energies, while SA-CASSCF calculations partly corrected these overestimates. The accuracy of the CIS calculations varied, depending on the particular state, while the CIS(D), CIS(3), and LRCCSD results were in generally good agreement. The energies of the lowest six excited singlet states of T₄ N₄ as calculated by the LRCCSD were compared with the energies of possible excited states of N₂ + N₂ fragments, leading to the conclusion that the most likely route for synthesis of T₄ N₄ would involve a combination of two bound quintet states of N₂.

This work was done by Timothy J. Lee of Ames Research Center and Christopher E. Dateo of Elionet Corp.

Inquiries concerning rights for the commercial use of this invention should be addressed to the Ames Technology Partnerships Division at (650) 604-2954. Refer to ARC-15125-1.

Antenna for Measuring Electric Fields Within the Inner Heliosphere

A document discusses concepts for the design of an antenna to be deployed from a spacecraft for measuring the ambient electric field associated with plasma waves at a location within 3 solar radii from the solar photosphere. The antenna must be long enough to extend beyond the photosphere and plasma sheaths of the spacecraft (expected to be of the order of meters thick) and to enable measurements at frequencies from 20 Hz to 10 MHz without contamination by spacecraft electric-field noise. The antenna must, therefore, extend beyond the thermal protection system (TPS) of the main body of the spacecraft and must withstand solar heating to a temperature as high as 2,000 °C while not conducting excessive heat to the interior of the spacecraft.

The TPS would be conical and its axis would be pointed toward the Sun. The antenna would include monopole halves of dipoles that would be deployed from within the shadow of the TPS. The outer portion of each monopole would be composed of a carbon-carbon (C-C) composite surface exposed to direct sunlight (hot side) and a C-C side in shadow (cold side) with yttria-stabilized zirconia spacers in-between. The hot side cannot view the spacecraft bus, while the cold side can. The booms also can be tilted to minimize heat input to spacecraft bus. This design allows one to reduce heat input to the spacecraft bus to acceptable levels.

This work was done by Edward Charles Sitlter, Jr., of Goddard Space Flight Center. Further information is contained in a TSP (see page 1). GSC-15052-1.

Improved High-Voltage Gas Isolator for Ion Thruster

A report describes an improved high-voltage isolator for preventing electrical discharge along the flow path of a propellant gas being fed from a supply to a spacecraft chassis electrical potential to an ion thruster at a potential as high as multiple kilovolts. The isolator must survive launch vibration and must remain electrically nonconductive for thousands of hours under conditions that, in the absence of proper design, would cause formation of electrically conductive sputtered metal, carbon, and/or decomposed hydrocarbons on its surfaces.

The isolator includes an alumina cylinder containing a spiral channel filled with a porous medium made from alumina microbeads fired together with an alumina slurry. Connections to gas-transport tubes are made at both ends of the alumina cylinder by means of metal caps containing fine-mesh screens to prevent passage of loose alumina particles. The outer surface of the alumina cylinder is convoluted to lengthen the electrical path between the metal caps and to afford shadow shielding to minimize the probability of formation of a continuous deposit that would electrically connect the ends. A flanged cylindrical metal cap that surrounds the alumina cylinder without