



Theoretical Studies of Routes to Synthesis of Tetrahedral N_4

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 N_4 , or $T_d N_4$ — 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 $T_d N_4$ as calculated by the LRCCSD were compared with the energies of possible excited states of $N_2 + N_2$ fragments, leading to the conclusion that the most likely route for synthesis of $T_d N_4$ would involve a combination of two bound quintet states of N_2 .

This work was done by Timothy J. Lee of Ames Research Center and Christopher E. Dato of Eloret 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.

Estimation Filter for Alignment of the Spitzer Space Telescope

A document presents a summary of an onboard estimation algorithm now being used to calibrate the alignment of the Spitzer Space Telescope (formerly known as the Space Infrared Telescope Facility). The algorithm, denoted the S2P calibration filter, recursively generates estimates of the alignment angles between a telescope reference frame and a star-tracker

reference frame. At several discrete times during the day, the filter accepts, as input, attitude estimates from the star tracker and observations taken by the Pointing Control Reference Sensor (a sensor in the field of view of the telescope). The output of the filter is a calibrated quaternion that represents the best current mean-square estimate of the alignment angles between the telescope and the star tracker. The S2P calibration filter incorporates a Kalman filter that tracks six states — two for each of three orthogonal coordinate axes. Although, in principle, one state per axis is sufficient, the use of two states per axis makes it possible to model both short- and long-term behaviors. Specifically, the filter properly models transient learning, characteristic times and bounds of thermomechanical drift, and long-term steady-state statistics, whether calibration measurements are taken frequently or infrequently. These properties ensure that the S2P filter performance is optimal over a broad range of flight conditions, and can be confidently run autonomously over several years of in-flight operation without human intervention.

This work was done by David Bayard of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).

The software used in this innovation is available for commercial licensing. Please contact Karina Edmonds of the California Institute of Technology at (626) 395-2322. Refer to NPO-43375.

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 photoelectron 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 Sittler, 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 at 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