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Informal Report

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Final Report

New Research Initiatives Program

Project W-219: Chemistry in Comet Comae

**los alamos
scientific laboratory**

of the University of California

LOS ALAMOS, NEW MEXICO 87545

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Project W-219: Chemistry in Comet Comae

W. F. Huebner, Principal Investigator

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FINAL REPORT
NEW RESEARCH INITIATIVES PROGRAM
Project W-219: Chemistry in Comet Comae

by

W. F. Huebner, Principal Investigator

ABSTRACT

The two main objectives of this program have been substantially successful. (1) A short-term visitors program has led to close interaction and collaboration on relevant and clearly defined astrophysical research. This, together with presentations of papers at astrophysics meetings and publications in astrophysics journals, has helped to focus the astronomical community's attention to astrophysics at the Los Alamos Scientific Laboratory. (2) The scientific objective to investigate theoretically chemical reactions in the comae of comets has been accomplished using a one-dimensional model. Ninety-eight species, which involved 441 reactions in the presence of wavelength-dependent solar radiation, have been considered in a time-dependent calculation, which includes effects resulting from ultraviolet opacity.

Many astronomers and astrophysicists of national and international renown have visited the Los Alamos Scientific Laboratory (LASL) under the sponsorship of the New Research Initiatives Program (NRIP). These interactions led to collaboration on comet chemistry and to exchanges of information on questions related to equation of state and opacities, which are the main responsibilities of LASL Group T-4. The goal to establish an annual short-term visitors program for outstanding astrophysicists has also been accomplished within the constraints of the comet chemistry program, which will be funded by NASA.

The results of the scientific objectives have been submitted for publication in the *Astrophysical Journal*. Therefore, we have chosen to present only one of the final results in this report (see Fig. 1), and the abstracts (see Appendix) of papers that were written

as a result of this project to show the progress of this program in a comprehensive manner. The following paper, a review of the processes occurring in comets, was the initial step of the program.

"Physical Processes in Comets," F. L. Whipple and W. F. Huebner, an invited review in *Annual Review of Astronomy and Astrophysics*, **14**, 143 (1976).

Also, as a result of this program, we have been asked to give seminars at the following:

- University of Rochester, Rochester, New York
- New Mexico State University, Las Cruces, New Mexico
- University of Toledo, Toledo, Ohio
- New Mexico Institute of Technology, Socorro, New Mexico
- University of Arizona, Tucson, Arizona

Fig. 1.

Partial results of a typical calculation, including optical depth effects. Number density of the indicated species is shown as a function of time and distance ($r-R_0$) above the nuclear surface for outstreaming velocity = 0.3 km s^{-1} . The assumed initial mother molecule composition is H_2O : $24 \times 10^{12} \text{ cm}^{-3}$; CO_2 : $15 \times 10^{12} \text{ cm}^{-3}$; NH_3 : $5 \times 10^{12} \text{ cm}^{-3}$; and CH_4 : $1 \times 10^{12} \text{ cm}^{-3}$. Curves for products from the photochemistry rise from lower left.

The following proposals have been made in fulfillment of the main purpose of the NRIP, that is, to initiate research that may become self-supporting.

"A Model of Comet Inner Comae: Their Chemistry and Interaction with the Solar Wind and Radiation." This proposal was submitted to NASA and has been approved for funding. Funding for this project will commence in early 1978.

"Calculation of Dissociation and Ionization Cross Sections of Cometary Radicals." This proposal was submitted to NASA and has been approved for funding. Funding for this project (although less than the requested amount) is expected to commence at the beginning of FY 1979.

"Calculation of Time-Dependent Population Inversions in Gases." This proposal is now being prepared for submission to the Department of Energy.

The last proposal is an outgrowth of the comet chemistry program (Project W-219) and discussions that followed a seminar at the University of Rochester. Three sample calculations were carried out for the Laser Energetics Laboratory at the University of Rochester to illustrate how this program can be used to predict population inversions in gases bombarded by electron beams (Brand-X Laser Program). This work also illustrates the reciprocity between astrophysics and programmatic research. We hope that with such examples, the need to formally establish astrophysics as an "approved" discipline at LASL will be recognized.

APPENDIX

ABSTRACTS FROM PAPERS PRESENTED AT ASTROPHYSICS MEETINGS, ISSUED AS LASL REPORTS, OR SUBMITTED FOR PUBLICATION

TRIPLET TRANSITIONS OF NEUTRAL CO IN THE SPECTRA OF COMETS AND THE ABUNDANCE OF CO₂ OR MOLECULES CONTAINING THE CO GROUP IN COMETS*

by

L. Biermann

The high-dispersion spectra of comet Mrkos (1957 V) taken at Mt. Palomar by J. L. Greenstein and remeasured by A. Woszczyk contain many unidentified weak lines. The possibility that some of these lines belong to transitions between triplet levels of neutral CO molecules is investigated. Their presence would suggest excitation related to the dissociative recombination of a parent containing the CO group, which is first ionized by solar uv. Of 31 CO lines (of the Asundi and Triplet systems), 14 are masked by known or by questionably identified lines as statistically expected. Of the remaining 17, 13 coincide within a few tenths of an Ångström with an unidentified line and 4 do not. These results are contrary to statistical expectations. (Some members of the third positive system of CO, which might be present, have not been included in the figures.)

Although these figures strongly favor the identification proposed, the numbers are not large enough to support entirely the argument of a small statistical probability (0.2%) of the observed state. Also, the rotational structure of the CO bands for the triplet systems needs further investigation.

C. F. Lillie's observations of comet Bennett (1970 II) between 1200 and 1800 Å, especially of the fourth positive system of CO, seem to favor a cometary atmosphere characterized by a large relative abundance of CO₂ and/or molecules containing the CO group. A model outlined for comet Bennett at 0.8 a.u. seems to be approximately consistent with observations. The chemical aspects, however, especially need further consideration. New observations, particularly of the Cameron bands of CO, are needed to settle the questions raised.

*Los Alamos Scientific Laboratory report LA-6289-MS (August 1976).

CHEMISTRY OF THE INNER COMA: A PROGRESS REPORT*

by

W. F. Huebner

The composition of the inner coma is modeled assuming that about 30 chemical species composed of H, C, and O undergo reactions. Ionization and dissociation by solar radiation and over 100 forward and reverse reactions between atoms, molecules, and ions are considered in the kinetics. Vaporization from a simple $\text{H}_2\text{O} - \text{CO}_2$ nucleus provides the initial composition of the gas near the surface.

CHEMICAL KINETICS IN THE INNER COMA OF A COMET**

by

W. F. Huebner

In the inner coma of a comet, out to a distance of 10^4 to 10^5 km, gas densities are such that chemical reactions can be expected. At one astronomical unit heliocentric distance solar ultraviolet radiation dissociates and ionizes the mother molecules evaporated from the icy nucleus. It is found that the so formed ions and radicals do not reach a steady state based on chemical kinetics alone.

CHEMICAL REACTIONS IN COMET COMAE†

by

W. F. Huebner

Sublimation from a simple $\text{H}_2\text{O} - \text{CO}_2 - \text{NH}_3$ icy mixture provides an initial composition and density of the gas just above the nuclear surface. The model calculation assumes an optically thin coma in which the gas dissociates and ionizes under the influence of solar radiation. The ions and radicals react

*Presented at International Astronomical Union Colloquium No. 39, *Relationships Between Comets, Minor Planets, and Meteorites*, held at Lyon, France, August 1976. The complete paper was published in *Comets, Asteroids, Meteorites—Interrelations, Evolution, and Origins*, A. H. Delsemme, Ed., (University of Toledo Bookstore, Toledo, Ohio, 1977), p. 57.

**Invited paper presented at the International Astronomical Union meeting in Grenoble, France, September 1976.

†Presented at the January 1977 meeting of the Division of Planetary Sciences of the American Astronomical Society.

chemically as they move radially outward with a thermal speed of several hundred meters per second. About 60 species composed of H, C, N and O and over 200 reactions are considered in the time-dependent kinetics. The spatial distribution of the various chemical species and free electrons is calculated to a distance of 3×10^6 km. At larger distances the density is too low to cause reactions other than photodissociation and photoionization. The calculations predict that the dissociation products H, OH, O, CO, NH₂ and NH build up to their peak values of the order 10^8 to 10^9 cm⁻³ within seconds. Other species such as H₂, O₂, NH₄⁺, NH₃⁺, NH₂⁺, H₃O⁺, CO₂⁺ and NO reach peak densities of the order 10^4 to 10^5 cm⁻³ within time intervals of a fractional second to a few tens seconds. The peak electron density, 10^6 cm⁻³, is reached within a second. Many other species with smaller peak densities but not necessarily small abundances are present. Additional species and reaction rates and the effects of optical depth and interaction with the solar wind must be considered to improve the model.

GAS PHASE CHEMISTRY OF COMET INNER COMAE*

by

P. T. Giguere and W. F. Huebner

A computer model of gas-phase chemical kinetics has been developed and applied to the chemistry of the inner coma. The chemistry is driven by solar photodissociation and ionization of a mixture of outstreaming mother molecules. Over 300 chemical reactions among mother and daughter species are considered simultaneously. Including chemical reactions tends to shorten predicted lifetimes of coma species. Effects of varying the initial composition of mother molecules will be discussed.

COMETARY NUCLEUS RELEASE EXPERIMENTS AND ICE PHYSICS**

by

W. F. Huebner

Some physical and chemical processes involved in the evaporation and sublimation of mixtures of frozen gases are discussed. Effects of zero gravity, vacuum and solar radiation are emphasized. Relevant experiments that can be carried out with the aid of the Space Shuttle are proposed.

*Presented at the June 1977 meeting of the American Astronomical Society.

**Presented at the Shuttle-Based Cometary Science Workshop, November 1976, NASA, George C. Marshall Space Flight Center.

A MODEL OF COMET COMAE, I: GAS PHASE CHEMISTRY IN ONE DIMENSION*

by

P. T. Giguere and W. F. Huebner

A model of gas phase chemical kinetics in comet comae has been developed. Its purpose is to allow characterization of comet nuclei by predicting abundances of observable coma species. The one-dimensional calculation follows an isothermal shell of outstreaming molecules, positive ions, and atoms that starts at the nucleus with a simple set of mother molecules. Rate equations for 441 photo and chemical reactions are solved simultaneously at many points in the expansion of the shell. The calculation includes effects of the ultraviolet opacity of the mother molecules. Results are presented for four combinations of hypothetical mother molecules H_2O , CO_2 , NH_3 , and CH_4 . Several species that are not simple photodestruction products of the mother molecules reach large abundances. CO^+ , C_2 , C_3 , HCN , N_2^+ and (probably) CN are underproduced by the model. Additional sources for these species are discussed.

THE POTENTIAL OF A DIRECT DISCHARGE $\text{O}(^1\text{S})$ LASER**

by

**J. Wilson,† E. Lozansky,†
P. T. Giguere, and W. F. Huebner**

Calculations are presented of the $\text{O}(^1\text{S})$ production rate in conditions approximating discharges in (i) pure oxygen (ii) oxygen/argon mixtures, to evaluate their potential as fusion lasers.

*Submitted to the Astrophysical Journal.

**Preprint, Laboratory for Laser Energetics, University of Rochester, Rochester, New York.

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