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from

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(NASA-CR-183029) PHOTOCHEMICAL AND THERMAL MODELING IN THE EARLY ATMOSPHERE OF THE EARTH Final Report, 1 Oct. 1981 - 31 Dec. 1987 (California Inst. of Tech.) 3 p CSCL 04A G3/46

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PHOTOCHEMICAL AND THERMAL MODELING IN THE EARLY ATMOSPHERE OF THE EARTH

(formerly Photochemical Processes in the Primitive Atmosphere of the Earth)

Period of Research October 1, 1981 to December 31, 1987

NASA Technical Officer
John Rummel

Yuk L. Yung
Principal Investigator

FINAL TECHNICAL REPORT

A number of research projects were completed under this proposal in the past fiscal year. They are briefly summarized as follows:

<u>Estimation of the reaction rate for the formation of CH_3O from $H + H_2CO$: Implications for chemistry in the solar system.</u>

The simplest carbon compounds, present in the terrestrial and planetary atmospheres, exhibit a wide range of oxidation states, carbon dioxide and methane being the most oxidized and the most reduced form of carbon, respectively. The question arises as to the origin of and the interconversion among the carbon species. The chemical pathways for the conversion of CH_4 to CO and CO_2 are for the post part known. The reverse process, the reduction of CO to CH_4 is however, poorly understood. We propose a new reaction $H_2CO + H + M \rightarrow CH_3O + M$, which might play a fundamental role in the reduction of CO to CH_4.

<u>An update of nitrile photochemistry on Titan</u>

According to Yung et al. (1984), the primary source of nitrile compounds in the atmosphere of Titan is the reaction

$$N + CH_3 \rightarrow HCN + H_2 \quad ,$$

where the nitrogen atoms are derived from electron impact dissociation of N_2,

$$N_2 + e \rightarrow N + N(^2D) + e$$

Cyanogen (C_2N_2) was thought to form via

$$CN + HCN \rightarrow H + X_2N_2 \quad ,$$

and the authors showed that this reaction could account for the observed abundance of C_2N_2 (Kunde *et al.* (1981) if the rate coefficient, k, were as large as $3.1 \times 10^{-11} cm^3 s^{-1}$. Recent experiments by Li *et al.* (1984) suggested that $k = 1.8 \times 10^{-14} cm^3 s^{-1}$ at 300 K, which is considerably lower than the original estimate..

So a new scheme has to be explored to explain the Voyager observations. The postulated new scheme is as follows:

$$N_2 + e \rightarrow N(^2D) + N + e$$

$$N(^2D) + C_2H_2 \rightarrow CHCN + H$$

$$CHCN + N \rightarrow H + C_2N_2$$

$$\text{net} \quad N_2 + C_2H_2 \rightarrow C_2N_2 + 2H$$

Publications

Y.L. Yung. An Update of Nitrile Photochemistry on Titan. *Icarus* **72**, 468-472 (1987).

Y.L. Yung, W.A. Drew, J.P. Pinto, and R.R. Friedl. Estimation of the Reaction Rate for the Formation of CH^3O from H + H_2CO: Implications for Chemistry in the Solar System. *Icarus* **73**, 516-526 (1988).

Y.L. Yung, R.R. Friedl, J.P. Pinto, K.D. Bayes, and J.-S. Wen. Kinetic Isotopic Fractionation and the Origin of HDO and CH^3D in the Solar System. *Icarus* **74**, 121-132 (1988).