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ORGANIC SYNTHESIS IN THE OUTER SOLAR SYSTEM: RECENT LABORATORY SIMULATIONS FOR TITAN, THE JOVIAN PLANETS, TRITON AND COMETS

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The atmosphere of Titan is composed mainly of N_2 , with 3-12% CH₄ (depending on altitude and details of the surface equilibrium). Voyager revealed Titan to be covered by a thick haze; the optical properties of this haze derived by scattering models are consistent with those of organic heteropolymer (tholin) produced in the laboratory by a plasma discharge in 90% N_2 -10% CH₄. Abundant amino acids are produced from this tholin on hydrolysis . We have recently analyzed the volatile products of continuous flow plasma excitation of this atmosphere (generated on Titan primarily by Saturnian magnetospheric electrons and solar and galactic cosmic rays), and find some 60 products, including many multiply-bonded hydrocarbons and nitriles.

We tabulate below the most abundant gases and their radiation yields, for two experimental pressures: 0.24 mb, more relevant to upper atmosphere excitation, and 17 mb, more relevant to tropospheric, cosmic ray excitation. The yields computed in the 0.24 mb experiment combined with measured electronic fluxes and a simple, eddy diffusion model of Titan's atmosphere predict abundances of detected molecules in agreement with those found by Voyager and for heavier products, in somewhat better agreement with observation than photochemical absolute reaction rate kinetics models. All Voyager organics are accounted for and no detectable products are found that Voyager did not detect. A striking increase of products with multiple bonds is found with decreasing pressure. Hydrocarbon abundances decline slowly with increasing carbon number.

Additionally, we list preliminary estimates for the yield of the heteropolymer, which seems to be produced in a quantity comparable (in moles of C+N consumed) to the total amount of gaseous product. The production rate required to sustain Titan's haze against sedimentation also indicates yields of this order. As can be seen from the table, over 10^9 years substantial amounts of these products can accumulate on the surface -- ranging from cm thicknesses for the (C+N=4) species to a meter or more for HCN and C_2H_2 ; we also expect a meter or more of tholins.

Similar analyses have been or are being done for the Jovian planets and Triton.

Charged particle irradiation of hydrocarbon clathrates or mixed hydrocarbon/water ices produces a range of organic products, reddening and darkening of the ices and characteristic infrared spectra. From such spectra, the predicted emission by fine particles in cometary comae well-matches the observed 3.4 μ m emission spectra of Comet Halley and other recent comets. Heliocentric evolution of organic emission features in comets is predicted. Organic products of such ice irradiation may account for colors and albedos on some of the satellites in the outer solar system, especially Triton and Pluto, where solid methane is known to exist.

Titan Continuous Flow Simulation Results (from W.R. Thompson, T. Henry, J. Schwarts, B.N. Khare, and C. Sagan, <u>Icarus</u>, in press)

Species	G, 17 mb molec/100 eV	G, 0.24 mb molec/100 eV	Voyager IRIS	Kinetic Chemical Model [†]	This Work	Column Density gm/cm ² /10 ⁹ y
					•	
НС≡СН	1.6×10^{-1}	3.9×10^{-3}	2×10^{-6}	4.0×10^{-6}	$0.3-1.3 \times 10^{-6}$	150 - 1770
HC≡N	3.3×10^{-2}	1.6×10^{-1}	2 x 10 ⁻⁷	5.6 x 10 ⁻⁷	$1.8-9.0 \times 10^{-7}$	50 - 33 0
N≡C-C≡N	3.6×10^{-3}	2.8×10^{-3}	10 ⁻⁷ - 10 ⁻⁸	1.9×10^{-8}	$1.4-7.0 \times 10^{-8}$	7.3 - 28
HC≡C-C≡N	2.4×10^{-3}	8.8×10^{-3}	10 ⁻⁷ - 10 ⁻⁸	5.6 x 10 ⁻⁸	$1.6-8.0 \times 10^{-8}$	6.1 - 51
CH ₃ C≡N	1.5×10^{-3}	4.6×10^{-3}	·		$0.7 - 3.2 \times 10^{-8}$	2.8
CH ₃ -C≡CH	1.4×10^{-3}	1.9×10^{-2}	3 x 10 ⁻⁸	1.8×10^{-7}	$0.3-1.4 \times 10^{-8}$	5 - 130
$H_2C = CH - CH = CH_2 1.3 \times 10^{-3}$		1.7×10^{-3}			$0.6-3.0 \times 10^{-8}$	2.8
HC≣C-C≣CH	8.2 x 10 ⁻⁴	1.5×10^{-3}	10 ⁻⁷ - 10 ⁻⁸	7.8×10^{-10}	$0.4-1.8 \times 10^{-8}$	1.7
H ₂ C=C=CH ₂	7.7×10^{-4}	1.6×10^{-2}			$1.5-7.5 \times 10^{-9}$	3.8
H ₂ C=CH-C≡C	H 2.4 x 10 ⁻⁴	1.7×10^{-3}			$1.1-5.5 \times 10^{-9}$	0.8
H ₂ C=CH-C≡N	1.9×10^{-4}	1.3×10^{-3}			$0.8-4.1 \times 10^{-9}$	0.6
Heteropolymers	* - 0.2-2	- 0.2-2				100 - 1000

^{*}Units of measure are total atoms (C+N). [†]These volume mixing ratios derive from simple eddy diffusion models of vertical transport. Laboratory results are shown for 0.24 mb, roughly where magnetospheric electrons drive atmospheric chemistry.