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OBSERVATIONAL DATA NEEDS USEFUL FOR MODELING THE COMA

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Abstract

The present status of our computer model of comet comae is described; results from assumed composition of frozen gases are summarized and compared to coma observations. Restrictions on relative abundance of some frozen constituents are illustrated. Modeling, when tightly coupled to observational data, can be important for comprehensive analysis of observations, for predicting undetected molecular species and for improved understanding of coma and nucleus. To accomplish this, total gas production rates and relative elemental abundances of H:C:N:O:S are needed as a function of heliocentric distance of the comet. Also needed are relative column densities and column density profiles with well defined diaphragm range and pointing position on the coma. Production rates are less desirable since they are model dependent. Total number (or upper limits) of molecules in the coma and analysis of unidentified spectral lines are needed also. An aggressive search for new molecules and new molecular states should be carried out. Most of all, a uniform analysis of all observational data must be encouraged. It would be most effective if such data were frequently and periodically updated at a special data center. Also needed are laboratory data: f-values, rate coefficients (particularly for neutral-neutral interactions), branching ratios (particularly for electron dissociative recombination) and better cross sections for photo-dissociative ionization.

The details of our computer model of the coma have been described earlier (Giguere and Huebner, 1978; Huebner and Giguere, 1980 -- henceforth referred to as papers I and II); only a summary of the processes is presented here.

From energy balance--between insolation on the nuclear surface and vaporization (sublimation) of the frozen gases and reradiation in the infrared--and the Clausius Clapeyron-equation the computer program calculates temperature, gas production rate, sound speed, ratio of specific heats and initial density and outstream speed of the coma gases. Assuming adiabatic expansion into a vacuum, application of the usual fluid dynamic conservation laws results in supersonic outstreaming (von Mises, 1958). Table I shows six assumed compositions of frozen gases in the nucleus. Table II summarizes the physical quantities consistent with the approximations for these chemical compositions. Wavelength dependent attenuation of solar ultraviolet radiation by coma gases is approximated to determine the effectiveness of photolytic processes in the inner coma. Nearly 100 photolytic processes are included in the model calculation; many are considered in great detail (Huebner and Carpenter, 1979). Others, for which cross sections are not available--see Table III--are only estimated. Photodissociative ionization (PDI) is an important process for which improved cross sections may be useful. (See paper II for a list of relevant species.) In addition about 500 chemical reactions are available in the program and used in accordance with the assumed initial chemical composition. See the notes to tables in papers I and II for rate coefficients and branching ratios which need to be improved.

Presently the model assumes spherical symmetry. Preliminary calculations show that attenuation of solar radiation at angles away from the comet-sun axis does not introduce a significant variation from spherical symmetry except in a small sector about the antisolar direction. On the other hand, radiation pressure on neutral coma species and particularly solar wind interaction with coma ions introduces large deviations from spherical symmetry in the outer coma. One can therefore expect significant changes in the ion column density prediction when the solar wind interaction is incorporated into our computer model. Impact ionization and dissociation by photoelectrons will be incorporated next. Except for H_2 and N_2, electron impact dissociation cross sections for which the dissociation products are in their ground state do not exist. Dissociative heating of the coma, which will also be included in our coma model, increases the outstream velocity -- particularly of the light species in the outer coma. This will modify our column density profiles.

Composition 6 is our first attempt to include interstellar molecules. The ratio of C:N:O was assumed to be the same as for cosmic abundances. The ratio of H:O was assumed to be about 2:1. These restrictions are insufficient to define a unique composition. But observational determinations of the abundance ratios of H:C:N:O:S are needed as a first step to determine the chemical composition of comets. It should be noted that composition 6 contains only fractions of one percent of NH_3, HCN, CH_3CN, CH_3NH_2, $H_2C_3H_2$, and C_2H_2. Larger amounts would cause serious over-production of NH_2, CN, C_2, C_3 and possibly NH. CH_3NH_2 was picked as an alternative to NH_3 to produce NH_2 and NH (see Delsemme, 1975). C_2H_2 is an obvious source for C_2 (see Delsemme, 1975). HCN and CH_3CN are prime sources for CN and allene ($H_2C_3H_2$) was assumed as a source for C_3 and C_2. It should be pointed out that chemistry remains an important source for the observed species at heliocentric distances less than about 1 AU, and for some species as far as 3 AU.

An aggressive search should be made to identify new species in the coma. Good candidates are transitions for CO triplet systems (Biermann, 1976), CO Cameron bands (Smith et al., 1980), H_2, NO, H_3O^+, HCO^+, and HCO_2^+.

Table I

Assumed Composition in Percent of Frozen Gases in the Nucleus

Species	Composition 1	2	3	4	5	6
H_2O	55.6	53.3	48.9	61.1	48.9	43.0
CO_2	33.3	33.3	28.9			12.0
NH_3	11.1	11.1	11.1	8.4	11.1	0.1
CH_4		2.2	11.1	30.4	11.1	13.4
CO					28.9	2.8
H_2CO						22.1
N_2						5.2
HCN						0.5
CH_3CN						0.4
CH_3NH_2						0.2
$H_2C_3H_2$						0.2
C_2H_2						0.1

Table IV gives a comparison between observations from several comets at various heliocentric distances and our model composition 6. Since comets show brightness fluctuations, we have averaged some observations made by A'Hearn (1975, 1980) and A'Hearn et al. (1980) over narrow ranges of heliocentric distances. Since the column density profile varies across the coma, it is important that the observations are centered and that the range (radius) in the coma subtended by the diaphragm is clearly stated. Observers should quote column densities averaged over the range of the diaphragm in the coma; a column density reduced to a given distance in the coma is model dependent. It is also important that the f-values are stated that have been used in the conversion from observed brightness to number of emitting molecules in a column. Standardization of filters is very important. More determinations of the ratio of column densities of CO^+ to H_2O^+ are needed. Cooperation with the International Halley Watch (IHW), as organized by Brandt, Friedman and Newburn will be extremely useful. It would be most effective if observational data were frequently and periodically reduced, analyzed and standardized by a special comet data center which could be part of the IHW, or go beyond it if other bright comets become observable.

Table II

Model Parameters at 1 AU Heliocentric Distance for a Nucleus with Radius 1 km, Albedo of 0.3, and IR Emissivity of 0.7

	Composition					
	1	2	3	4	5	6
Mean Sublimation Heat [kcal mol^{-1}]	9.27	9.07	8.48	8.34	7.11	7.84
Gas Production Rate [10^{17} cm^{-2} s^{-1}]	2.90	3.00	3.29	3.31	4.06	3.59
Mean Molecular Weight	26.6	26.5	25.2	17.3	20.6	24.6
Ratio of Specific Heats	1.36	1.36	1.35	1.33	1.35	1.34
Sublimation Temperature [K]	162.	159.	151.	154.	137.	147.
Sound Speed [km s^{-1}]	.262	.260	.259	.314	.273	.258
Final Outstream Speed [km s^{-1}]	.674	.668	.670	.831	.706	.675
Gas Density at Nucleus [10^{13} cm^{-3}]	4.43	4.62	5.07	4.22	5.94	5.56

Table III

Photolytic Processes for Which Cross Sections Are Not Available

OH	→	O	+	H	*	
CN	→	C	+	N		
C_2	→	C	+	C		
NH	→	N	+	H		
HNC	→	H	+	CN		
C_2H	→	C_2	+	H		
CH_2	→	CH	+	H		
HCO	→	H	+	CO		
CH_3CN	→	CH_3	+	CN		
CH_3NH_2	→	CH_3	+	NH_2		
$H_2C_3H_2$	→	C_3	+	H_2	+	H_2
NH_2	→	NH	+	H		
C_3	→	C_2	+	C		

*OH lifetimes for photodissociation at 1 AU and for several radial velocities with respect to the sun have been calculated by Jackson (1980).

Table IV

Some Comparisons of Observed and Model Calculated Column Densities

Species	Comet	Heliocentric Distance [AU]	Distance into Coma [10^4km]	Log Column Density [cm^{-2}] Observed (from A'Hearn)	Composition 6
CN	West	0.6	5	12.3	12.7
		1.0	5	11.8	12.3
C_2	West	0.6	5	12.3	12.3
		0.6	1	13.6*	12.6
		1.0	5	12.2	11.6
	Kohoutek	1.0	3	11.5	11.6
C_3	West	0.6	5	12.0	12.0
		1.0	5	12.2	11.7
NH_2	Kohoutek	1.0	3	10.8	10.7
CH	Kohoutek	0.6**	5	11.5	10.7

* Sivaraman et al., 1979
** Post perihelion

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