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COMET HALLEY, PARAMETER STUDY I

by

W. F. Huebner and M. M. Fikani

ABSTRACT

To aid in defining a mission to comet P/Halley, its inner coma is simulated by a computer program that models time-dependent chemical reactions in a radially and isentropically expanding gas, taking into account attenuation of solar ultraviolet radiation in the subsolar direction. Column density predictions are based on intelligently selected combinations of poorly known values for nucleus parameters that include size, visual albedo, and infrared emissivity. Only one chemical composition and a minor modification of it are considered here; the dust-to-gas ratio in this model is zero. Although the somewhat optimistically volatile composition chosen here favors a smaller nucleus, a mean nuclear radius of only 0.5 km is unlikely. No significant increase of molecular column density is predicted by this model as a spacecraft approaches, once it is less than a few 10^4 km from the nucleus. Predictions are made for various heliocentric distances of interest for comet missions and for ground observations.

I. SUMMARY OF RELEVANT DATA OF P/HALLEY (1910 II)

Presented in Table I are observational data from the 1910 apparition of periodic comet Halley that are of primary interest for comparison with the model's predictions. In particular, three species (CN, C₂, and C₃) are traced through an important segment of comet Halley's orbit -- roughly 3 AU heliocentric distance pre-perihelion to 1.4 AU post-perihelion. Given are the physical extent in the coma of the species based on spectral images in thousands of kilometers, as well as their relative logarithmic intensity (determined by photographic densities as discussed by Bobrovnikoff¹). Relevant comments are included for clarity where needed along with those references that proved most valuable in making the trace. It should be borne in mind that, because of the observational quality that existed around the time of the 1910 apparition (and to purported corrections made thereafter), the values presented are not absolute. It is felt that the proper behavior is intact and it is this which is important for comparison.

General observational features include an apparent spectral change -- solar ($\lambda \approx 4700\text{\AA}$) -- violet ($\lambda \approx 4000\text{\AA}$) -- occurring at approximately 1.2 AU. Comparison with the cometary average² at ~ 0.8 AU indicates this possibly to be an important effect. However, the reality of this spectral change appears to be in some doubt. It is felt by some¹ that, in the pre-perihelion approach (constituting a violet-to-solar change), the decrease in brightness of CN, i.e., the violet spectrum, was only apparent -- CN and C₃ actually do increase but are overshadowed by the reflection spectrum and not by a significant increase in the C₂/CN and C₂/C₃ ratios. Others³ feel the spectral change can be attributed to "bad procedures," i.e., poor quality of observations as well as fallacious corrections. In any event, the face value of the observations shows a spectral change that must be accounted for.

Among other observational features were noted: Na-D lines observed in envelopes and extending into the tail during perihelion passage; CH and various bands of C₂, C₃, and CN were positively identified; no CO⁺ found in envelopes (parabolic or elliptical) but definitely in tail along with N₂⁺. It should be mentioned in conjunction with the last statement that both the parabolic and elliptical envelopes were essentially uniform in mixture of CN and C₂.

Table I

Extent $\rho(10^3\text{km})$ /Intensity [log I] of Spectral Images of P/Halley (1910 II)

<u>r/date</u>	<u>CN</u>	<u>C₂</u>	<u>C₃</u>	<u>References and Comments^a</u>
2.95 AU (Oct 22, 1909)	Faint uniform continuum, CN and C ₂ suspect (faint), C ₃ (4050A) observed faintly			2/2; doubtful that C ₂ could be seen at this distance
~2.5 AU (Dec 18, 1909)	71.9/0.25	49.5/0.05	49.6/-	1/
~2.3 AU (Dec 30, 1909)	95.2/0.35	74.6/0.2	77.1/-	1/
~2.1 AU (Jan 09, 1910)	135/0.45	97/0.08	64.9/-	1/; note: maximum extension of CN
~2.0 AU (Jan 15, 1910)	90/0.25	84.5/0.17	64.5/-	1/
1.7 - 1.6 AU (Feb 04, 1910)	65.2/0.4	57.7/0.3	42.0/-	1/
1.6 AU (Feb 10, 1910)	62.5/0.25	69/0.15	42.8/-	1/2; CN and C ₂ become comparable in strength
1.2 - 1.1 AU (Mar 08, 1910)	69.1/0.05	106.6/0.05	(35) ^b /-	1/1; reported spectral change; note: max extension of C ₂
0.6 AU (Apr 21, 1910)	(38) ^b /0.65	46.1/0.8	(20) ^b /-	1/; near perihelion (Apr 19, 1910)
0.7 AU (May 05, 1910)	21.2/0.55	40.5/1.0	8.0/-	1/1; primarily in reflected light, <u>fluctuations</u> ; note: throughout May envelopes are at minimum extension
~0.85 AU (May 27, 1910)	15.4/1.0	14.3/1.4	9.4/-	1/
1.0 AU (Jun 06, 1910)	23.2/1.3	37.3/1.4	16.7/-	1/
1.4 AU (Jun 26, 1910)	59.7/0.15	48.1/0.1	46.5/-	1/1; CN becomes dominant, C ₃ and CN exhibit similar behavior

^a First number is reference for extent; second number is reference for intensity.

^b Estimate from supplied graph in Ref. 1.

II. THE COMPUTER MODEL

A. Physics

The model nucleus is assumed to be a homogenous mixture of volatile frozen gases assembled into a spherical shape of radius R_0 . Solar radiation, mostly in the visual range, impinges on the surface. Depending on the albedo, A , part of the radiation is reflected, the rest is absorbed. The infrared emissivity, ϵ , determines the fraction of absorbed energy that is re-emitted. The rest of the absorbed energy causes sublimation (phase change from solid to gas) of the frozen gases. Because the nucleus rotates, it is assumed that energy for sublimation is distributed uniformly over the surface of the sphere.

Using the adiabatic exponent as the polytropic exponent, the supersonic von Mises⁴ solution describes the isentropic outflow of the coma gas. Solar ultraviolet attenuation is calculated, in wavelength bins a few to 50Å wide, from the density-distance relationship of the coma gas,

$$n = n_0 \frac{v_0 R_0}{vR}, \quad (1)$$

and the photoelectric cross sections and abundances of the mother molecules. In Eq.(1) n is the gas density and v is the outstream speed in the subsolar direction at a distance R from the center of the nucleus. The symbols with subscript o indicate corresponding variables at the nucleus surface. Two-dimensional test calculations of attenuation indicate no large deviation of the chemistry from the subsolar direction except in a narrow cone in the antisolar direction. Solar ultraviolet radiation causes dissociation, ionization, and dissociative ionization producing radicals and ions that initiate a complex network of chemical reactions. For more details on the physics see Refs. 5-7.

B. Chemistry

The nucleus is assumed to have composition 6a (according to our numbering scheme, see Ref. 8). This composition is reproduced in Table II.

Table II

Initial Composition

<u>Species</u>	<u>Percent Number Abundance</u>
H ₂ O	43.0
H ₂ CO	22.1
CH ₄	13.4
CO ₂	12.0
N ₂	5.2
CO	2.8
HCN	0.5
CH ₃ CN	0.4
CH ₃ NH ₂	0.2
H ₂ C ₃ H ₂	0.2
NH ₃	0.1
C ₂ H ₂	0.1

It was pointed out by A'Hearn in a private communication⁹ that a recently quoted oscillator strength used by him and others is too low by a factor of about 40. For this reason we have revised the relative abundance of two trace molecules C₂H₂ from 0.1% to 0.16% and H₂C₃H₂ from 0.2% to 0.005%. This modified composition will be referred to as 6a'. These modifications do not change the relative elemental abundances (see Ref. 8).

The list of species used in the time-dependent chemical kinetics is given in Table III, and the reactions and the associated coefficients A, B, and C for the Arrhenius equation are given in Table IV. The reactions and associated rate coefficients are a summary of those that have been compiled and listed in Refs. 5, 6, and 8. The rate coefficients for the chemical reactions are of the form

$$k = A\left(\frac{T}{300}\right)^B e^{-C/T} . \quad (2)$$

For photolytic processes the rate coefficient is independent of B and C but has to be corrected for ultraviolet attenuation.

Table III

Species Included in ModelsElectrons and Monatomics

e	H	H ⁺	C	C(¹ D)	C ⁺	N	N ⁺
O	O(¹ D)	O ⁺					

Diatomics

H ₂	H ₂ ⁺	CH	CH ⁺	NH	NH ⁺	OH	OH ⁺
C ₂	C ₂ ⁺	CN	CN ⁺	CO	CO(a ³ Π)	CO ⁺	N ₂
N ₂ ⁺	NO	NO ⁺	O ₂	O ₂ ⁺			

Triatomics

H ₃ ⁺	CH ₂	CH ₂ ⁺	NH ₂	NH ₂ ⁺	N ₂ H	H ₂ O	H ₂ O ⁺
C ₂ H	C ₂ H ⁺	HCN	HCN ⁺	HNC	HCO	HCO ⁺	N ₂ H ⁺
HNO	HNO ⁺	HO ₂ ⁺	NCO	C ₃	C ₃ ⁺	C ₂ N ⁺	CO ₂
CO ₂ ⁺							

Tetratomics

C ₄	CH ₃	CH ₃ ⁺	NH ₃	NH ₃ ⁺	H ₃ O ⁺	C ₂ H ₂	C ₂ H ₂ ⁺
H ₂ CN ⁺	H ₂ CO	H ₂ CO ⁺	C ₃ H ⁺	CO ₂ H ⁺			

Pentatomics

H ₅ ⁺	CH ₄	CH ₄ ⁺	C ₄ H	N ₂ H ₂	NH ₄ ⁺	CH ₃ O ⁺	C ₂ H ₃
C ₂ H ₃ ⁺	C ₃ H ₂ ⁺	CH ₂ OH ⁺	H ₂ CO ₂	H ₂ CO ₂ ⁺	CH ₂ CN ⁺	CH ₃ N	

Hexatomics

CH ₅ ⁺	C ₂ H ₄	C ₂ H ₄ ⁺	CH ₄ N ⁺ (=CH ₂ NH ₂ ⁺)	C ₃ H ₃ ⁺	CH ₃ OH	CH ₃ OH ⁺
CH ₃ CN	CH ₃ CO ⁺	HC ₄ H	C ₄ H ₂ ⁺	N ₂ H ₃	C ₃ H ₂ N ⁺ (=C ₂ H ₂ CN ⁺ ?)	H ₂ N ₂ H ₂

Suprahexatomics

CH ₃ NH ₂	C ₂ H ₅	C ₂ H ₅ ⁺	H ₂ C ₃ H ₂	C ₃ H ₄ ⁺	C ₄ H ₃ ⁺	C ₃ H ₃ O ⁺	H ₃ O ⁺ ·H ₂ O(=H ₃ O ⁺ ·W)
C ₂ H ₆	C ₂ H ₆ ⁺	C ₃ H ₅ ⁺	C ₂ H ₇ ⁺	C ₃ H ₆ ⁺	C ₄ H ₅ ⁺	C ₃ H ₇ ⁺	C ₂ H ₉ ⁺
C ₃ H ₈ ⁺	C ₄ H ₇ ⁺	C ₃ H ₉ ⁺	C ₃ H ₁₀ ⁺	C ₄ H ₉ ⁺	C ₃ H ₁₁ ⁺		

Table IV
Reactions

Reactants	Products	A	B	C	Refs. and Notes
H	H ⁺ e	7.31E-08			25
C	C ⁺ e	4.10E-07			25
C(1D)	C ⁺ e	3.58E-06			25
N	N ⁺ e	1.85E-07			25
O	O ⁺ e	2.12E-07			25
O(1D)	O ⁺ e	1.82E-07			25
H ₂	H ₂ ⁺ e	5.41E-08			25
CH	CH ⁺ e	7.56E-07			25
CO	CO ⁺ e	3.10E-07			25
O ₂	O ₂ ⁺ e	5.15E-07			25
CO(3)	CO ⁺ e	8.65E-06			25
N ₂	N ₂ ⁺ e	3.52E-07			25
NO	NO ⁺ e	1.28E-06			25
H ₂ O	H ₂ O ⁺ e	3.34E-07			25
CO ₂	CO ₂ ⁺ e	6.55E-07			25
NH ₃	NH ₃ ⁺ e	6.10E-07			25
H ₂ CO	H ₂ CO ⁺ e	3.79E-07			25
C ₂ H ₂	C ₂ H ₂ ⁺ e	7.81E-07			25
C ₂ H ₄	C ₂ H ₄ ⁺ e	5.80E-07			25
CH ₄	CH ₄ ⁺ e	3.60E-07			25
H ₂ CO ₂	H ₂ CO ₂ ⁺ e	9.11E-07			25
CH ₃ OH	CH ₃ OH ⁺ e	5.01E-07			25
H ₂	H H	4.45E-08			25
CH	C H	1.16E-02			25
NH	N H	2.50E-06			a
OH	O H	5.00E-06			a
CN	C N	5.00E-06			a
CO	C O	2.82E-07			25
CO	C(1D) O(1D)	4.15E-08			25
N ₂	N N	6.61E-07			25
O ₂	O O	6.00E-08			25

Table IV (cont)

Reactants	Products		A	B	C	Refs. and Notes
O ₂	O	O(1D)	4.19E-06			25
C ₂	C	C	5.00E-06			a
CO(3)	C	O	7.87E-05			25
NO	N	O	2.20E-06			25
CH ₂	CH	H	2.00E-05			a
C ₂ H	C ₂	H	3.00E-05			a
C ₃	C ₂	C	1.00E-05			a
NH ₂	NH	H	2.00E-04			a
NH ₂	H ₂	N	5.00E-05			a
H ₂ O	O(1D)	H ₂	3.10E-06			28
H ₂ O	H	OH	8.51E-06			28
HCN	H	CN	1.30E-05			25
HNC	H	CN	2.00E-05			a
CO ₂	CO	O(1D)	9.40E-07			25
CO ₂	CO(3)	O	2.83E-07			25
HCO	CO	H	4.00E-05			a
NH ₃	NH ₂	H	1.13E-04			25
NH ₃	NH	H ₂	6.31E-05			25
H ₂ CO	CO	H ₂	1.62E-04			25
H ₂ CO	HCO	H	8.50E-05			25
H ₂ CO	CO	H	3.23E-05		H	25
C ₂ H ₂	C ₂ H	H	2.98E-05			25
CH ₄	CH ₃	H	1.17E-06			25
CH ₄	CH ₂	H ₂	5.44E-06			25
CH ₄	CH	H ₂	5.01E-07		H	25
H ₂ CO ₂	CO ₂	H ₂	2.73E-04			25
H ₂ CO ₂	OH	HCO	4.87E-04			25
HC ₃ N	C ₂ H	CN	2.77E-05			25
C ₂ H ₄	C ₂ H ₂	H ₂	4.13E-05			25
CH ₃ OH	H ₂	H ₂ CO	2.53E-04			25
CH ₃ OH	OH	CH ₃	1.34E-05			25
CH ₃ CN	CH ₃	CN	5.00E-05			a
H ₂ C ₃ H ₂	C ₃	H ₂	5.00E-05		H ₂	a
CH ₃ NH ₂	NH ₂	CH ₃	3.00E-05			a

Table IV (cont)

Reactants	Products			A	B	C	Refs. and Notes
HC ₄ H	C ₂ H	C ₂ H		5.00E-05			a
HC ₄ H	C ₄ H	H		5.00E-05			a
HC ₄ H	C ₄	H ₂		1.00E-05			a
HC ₄ H	C ₂	C ₂	H ₂	5.00E-06			a
C ₄ H	C ₄	H		1.00E-04			a
C ₄ H	C ₂	C ₂ H		5.00E-05			a
C ₄ H	C ₂	C ₂	H	2.00E-05			a
H ₂ N ₂ H ₂	N ₂ H ₂	H ₂		5.00E-05			a
H ₂ N ₂ H ₂	N ₂ H ₃	H		5.00E-05			a
H ₂ N ₂ H ₂	N ₂	H ₂	H ₂	1.00E-05			a
C ₄	C ₂	C ₂		5.00E-05			a
C ₄	C ₃	C		2.00E-05			a
N ₂ H ₂	N ₂ H	H		5.00E-05			a
N ₂ H ₂	N ₂	H ₂		5.00E-05			a
N ₂ H ₃	N ₂ H ₂	H		1.00E-04			a
N ₂ H ₃	N ₂	H ₂	H	5.00E-05			a
N ₂ H	N ₂	H		1.00E-04			a
H ₂	H ⁺	H	e	9.52E-09			25
N ₂	N ⁺	N	e	1.50E-08			25
O ₂	O ⁺	O	e	5.06E-08			25
CO	C ⁺	O	e	8.01E-09			25
CO	C	O ⁺	e	5.97E-09			25
CO(3)	C ⁺	O	e	1.13E-08			25
CO(3)	O ⁺	C	e	8.38E-09			25
NO	O ⁺	N	e	1.81E-09			25
NO	N ⁺	O	e	3.18E-08			25
H ₂ O	OH ⁺	H	e	5.54E-08			25
H ₂ O	O ⁺	H ₂	e	5.85E-09			25
H ₂ O	H ⁺	OH	e	1.31E-08			25
CO ₂	CO ⁺	O	e	5.02E-08			25
CO ₂	O ⁺	CO	e	6.38E-08			25
CO ₂	C ⁺	O	O e	2.89E-08			25
H ₂ CO	HCO ⁺	H	e	2.05E-07			25
H ₂ CO	CO ⁺	H ₂	e	1.21E-07			25

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
C_2H_2	$C_2H^+ \quad H \quad e$	7.50E-08			25
NH_3	$NH_2^+ \quad H \quad e$	1.77E-07			25
NH_3	$NH^+ \quad H_2 \quad e$	6.90E-09			25
NH_3	$N^+ \quad H_2 \quad H \quad e$	3.25E-09			25
NH_3	$H^+ \quad NH_2 \quad e$	3.38E-09			25
CH_4	$CH_3^+ \quad H \quad e$	1.98E-07			25
CH_4	$CH_2^+ \quad H_2 \quad e$	2.09E-08			25
CH_4	$CH^+ \quad H_2 \quad H \quad e$	4.16E-09			25
CH_4	$H^+ \quad CH_3 \quad e$	9.09E-09			25
H_2CO_2	$OH \quad HCO^+ \quad e$	2.82E-07			25
C_2H_4	$C_2H_3^+ \quad H \quad e$	2.27E-07			25
C_2H_4	$C_2H_2^+ \quad H_2 \quad e$	2.02E-07			25
CH_3OH	$H \quad CH_3O^+ \quad e$	1.20E-07			25
CH_3OH	$H_2 \quad H_2CO^+ \quad e$	1.15E-07			25
$H^+ \quad e$	H	3.50E-12	-0.7	0.0	11
$H^+ \quad H_2O$	$H_2O^+ \quad H$	8.20E-09	0.0	0.0	10
$H^+ \quad CO_2$	$HCO^+ \quad O$	3.00E-09	0.0	0.0	13
$H^+ \quad NH_3$	$NH_3^+ \quad H$	5.20E-09	0.0	0.0	10
$H^+ \quad CH_4$	$CH_3^+ \quad H_2$	2.28E-09	0.0	0.0	10
$H^+ \quad CH_4$	$CH_4^+ \quad H$	1.52E-09	0.0	0.0	10
$H^+ \quad OH$	$OH^+ \quad H$	1.00E-09	0.0	0.0	a
$H^+ \quad H$	H_2^+	4.43E-19	2.11	0.0	35,a,b
$H^+ \quad O$	$O^+ \quad H$	7.96E-10	-0.155	215.	a,c
$H^+ \quad NO$	$NO^+ \quad H$	1.90E-09	0.0	0.0	11
$H^+ \quad O_2$	$O_2^+ \quad H$	1.17E-09	0.0	0.0	10
$H^+ \quad H_2CO$	$H_2CO^+ \quad H$	1.00E-09	0.0	0.0	13,a
$H_2^+ \quad e$	$H \quad H$	1.00E-07	-0.5	0.0	a
$H_2^+ \quad H_2O$	$H_3O^+ \quad H$	3.43E-09	0.0	0.0	10
$H_2^+ \quad H_2O$	$H_2O^+ \quad H_2$	3.87E-09	0.0	0.0	10
$H_2^+ \quad NH_3$	$NH_3^+ \quad H_2$	5.70E-09	0.0	0.0	10
$H_2^+ \quad CH_4$	$CH_5^+ \quad H$	1.14E-10	0.0	0.0	10
$H_2^+ \quad CH_4$	$CH_4^+ \quad H_2$	1.41E-09	0.0	0.0	10
$H_2^+ \quad CH_4$	$CH_3^+ \quad H_2 \quad H$	2.28E-09	0.0	0.0	10
$H_2^+ \quad H_2$	$H_3^+ \quad H$	2.10E-09	0.0	0.0	10

Table IV (cont)

Reactants		Products		A	B	C	Refs. and Notes
H ₂ ⁺	C	CH ⁺	H	1.00E-09	0.0	0.0	a
H ₂ ⁺	N	NH ⁺	H	1.00E-09	0.0	0.0	a
H ₂ ⁺	O	OH ⁺	H	1.00E-09	0.0	0.0	a
H ₂ ⁺	CO	CO ⁺	H ₂	6.44E-10	0.0	0.0	10
H ₂ ⁺	CO	HCO ⁺	H	2.16E-09	0.0	0.0	10
H ₂ ⁺	O ₂	HO ₂ ⁺	H	1.92E-09	0.0	0.0	10
H ₂ ⁺	N ₂	N ₂ H ⁺	H	2.00E-09	0.0	0.0	10
H ₂ ⁺	O ₂	O ₂ ⁺	H ₂	7.83E-10	0.0	0.0	10
H ₂ ⁺	C ₂ H ₂	C ₂ H ₃ ⁺	H	4.77E-10	0.0	0.0	10
H ₂ ⁺	C ₂ H ₂	C ₂ H ₂ ⁺	H ₂	4.82E-09	0.0	0.0	10
H ₂ ⁺	C ₂ H ₄	C ₂ H ₄ ⁺	H ₂	2.20E-09	0.0	0.0	10
H ₂ ⁺	C ₂ H ₄	C ₂ H ₃ ⁺	H ₂ H	1.81E-09	0.0	0.0	10
H ₂ ⁺	C ₂ H ₄	C ₂ H ₂ ⁺	H ₂ H ₂	8.80E-10	0.0	0.0	10
H ₂ ⁺	C ₂ H ₆	C ₂ H ₆ ⁺	H ₂	2.94E-10	0.0	0.0	10
H ₂ ⁺	C ₂ H ₆	C ₂ H ₅ ⁺	H ₂ H	1.37E-09	0.0	0.0	10
H ₂ ⁺	C ₂ H ₆	C ₂ H ₄ ⁺	H ₂ H ₂	2.35E-09	0.0	0.0	10
H ₂ ⁺	C ₂ H ₆	C ₂ H ₃ ⁺	H ₂ H ₂ H	6.86E-10	0.0	0.0	10
H ₂ ⁺	C ₂ H ₆	C ₂ H ₂ ⁺	H ₂ H ₂ H ₂	1.96E-10	0.0	0.0	10
H ₃ ⁺	e	H ₂	H	2.10E-07	-0.5	0.0	52
H ₃ ⁺	e	H	H H	2.10E-07	-0.5	0.0	52
H ₃ ⁺	H ₂ O	H ₃ O ⁺	H ₂	5.90E-09	0.0	0.0	10
H ₃ ⁺	CO ₂	CO ₂ H ⁺	H ₂	1.90E-09	0.0	0.0	13
H ₃ ⁺	NH ₃	NH ₄ ⁺	H ₂	4.70E-09	0.0	0.0	10
H ₃ ⁺	CH ₄	CH ₅ ⁺	H ₂	2.40E-09	0.0	0.0	10
H ₃ ⁺	C	CH ⁺	H ₂	2.00E-09	0.0	0.0	13,a
H ₃ ⁺	O	OH ⁺	H ₂	8.00E-10	0.0	0.0	16,a
H ₃ ⁺	OH	H ₂ O ⁺	H ₂	2.00E-09	0.0	0.0	13,a
H ₃ ⁺	CO	HCO ⁺	H ₂	1.70E-09	0.0	0.0	10
H ₃ ⁺	O ₂	HO ₂ ⁺	H ₂	6.40E-10	0.0	0.0	10
H ₃ ⁺	H ₂ CO	CH ₂ OH ⁺	H ₂	2.00E-09	0.0	0.0	13,a
H ₃ ⁺	C ₂ H ₂	C ₂ H ₃ ⁺	H ₂	3.50E-09	0.0	0.0	10
H ₃ ⁺	C ₂ H ₄	C ₂ H ₅ ⁺	H ₂	1.44E-09	0.0	0.0	10
H ₃ ⁺	C ₂ H ₄	C ₂ H ₃ ⁺	H ₂ H ₂	2.16E-09	0.0	0.0	10
H ₃ ⁺	C ₂ H ₆	C ₂ H ₅ ⁺	H ₂ H ₂	3.40E-09	0.0	0.0	10

Table IV (cont)

Reactants		Products		A	B	C	Refs. and Notes
H_3^+	HCN	H_2CN^+	H_2	8.00E-09	0.0	0.0	10
H_3^+	HCO	H_2CO^+	H_2	1.00E-09	0.0	0.0	a
H_3^+	NO	HNO^+	H_2	1.40E-09	0.0	0.0	12
H_3^+	N_2	N_2H^+	H_2	1.70E-09	0.0	0.0	10
H_3^+	CN	HCN^+	H_2	2.00E-09	0.0	0.0	13,a
H_3^+	H_2	H_5^+	M	1.00E-30	0.0	0.0	17,a
H_5^+	e	H_2	H_2 H	3.00E-06	-0.5	0.0	18,a
H_5^+	CH_4	CH_5^+	H_2 H_2	2.00E-09	0.0	0.0	17,a
C^+	e	C		3.50E-12	-0.7	0.0	a
C^+	H_2O	HCO^+	H	2.70E-09	0.0	0.0	10
C^+	CO_2	CO^+	CO	1.10E-09	0.0	0.0	10
C^+	NH_3	NH_3^+	C	1.15E-09	0.0	0.0	10
C^+	NH_3	HCN^+	H_2	7.00E-11	0.0	0.0	10
C^+	NH_3	H_2CN^+	H	1.08E-09	0.0	0.0	10
C^+	CH_4	C_2H_3^+	H	1.03E-09	0.0	0.0	10
C^+	CH_4	C_2H_2^+	H_2	4.20E-10	0.0	0.0	10
C^+	NH	H^+	CN	1.00E-09	0.0	0.0	a
C^+	NH	CN^+	H	1.00E-09	0.0	0.0	a
C^+	NH_2	H^+	HCN	1.00E-09	0.0	0.0	a
C^+	NH_2	HCN^+	H	1.00E-09	0.0	0.0	a
C^+	H_2	CH_2^+		3.00E-15	-1.0	0.0	19,a
C^+	OH	CO^+	H	1.00E-09	0.0	0.0	a
C^+	OH	H^+	CO	1.00E-09	0.0	0.0	a
C^+	CH	C_2^+	H	2.00E-09	0.0	0.0	13,a
C^+	CH_2	C_2H^+	H	2.00E-09	0.0	0.0	13,a
C^+	CH_3	C_2H_2^+	H	1.00E-09	0.0	0.0	a
C^+	C_2H	C_3^+	H	1.00E-09	0.0	0.0	a
C^+	H_2CO	CH_2^+	CO	2.11E-09	0.0	0.0	10
C^+	H_2CO	HCO^+	CH	9.20E-10	0.0	0.0	10
C^+	H_2CO	H_2CO^+	C	1.36E-09	0.0	0.0	10
C^+	O_2	CO^+	O	7.80E-10	0.0	0.0	10
C^+	O_2	O^+	CO	4.40E-10	0.0	0.0	10
C^+	NO	NO^+	C	8.50E-10	0.0	0.0	10
C^+	HCN	C_2N^+	H	3.20E-09	0.0	0.0	10

Table IV (cont)

Reactants		Products	A	B	C	Refs. and Notes
C^+	H	CH^+	5.67E-18	-1.0	0.0	33,a
CH^+	e	C H	1.00E-07	-0.5	0.0	20,34,a
CH^+	e	CH	1.05E-10	-0.7	0.0	20,33,a,d
CH^+	H ₂ O	HCO^+ H ₂	2.32E-09	0.0	0.0	38,e
CH^+	H ₂ O	H_2CO^+ H	2.90E-10	0.0	0.0	38,e
CH^+	H ₂ O	H_3O^+ C	2.90E-10	0.0	0.0	38,e
CH^+	CO ₂	HCO^+ CO	1.60E-09	0.0	0.0	38
CH^+	NH ₃	H_2CN^+ H ₂	1.84E-09	0.0	0.0	38
CH^+	NH ₃	NH_3^+ CH	4.60E-10	0.0	0.0	38
CH^+	NH ₃	NH_4^+ C	4.00E-10	0.0	0.0	38
CH^+	CH ₄	$C_2H_4^+$ H	7.70E-11	0.0	0.0	10
CH^+	CH ₄	$C_2H_3^+$ H ₂	1.06E-09	0.0	0.0	10
CH^+	CH ₄	$C_2H_2^+$ H ₂ H	1.55E-10	0.0	0.0	10
CH^+	H ₂ CO	CH_2OH^+ C	1.00E-09	0.0	0.0	a
CH^+	HCN	H_2CN^+ C	1.00E-09	0.0	0.0	a
CH^+	C ₂ H ₂	$C_2H_3^+$ C	1.00E-09	0.0	0.0	a
CH^+	C ₂ H ₄	$C_2H_5^+$ C	1.00E-09	0.0	0.0	a
CH^+	HCO	H_2CO^+ C	1.00E-09	0.0	0.0	a
CH^+	NH ₂	NH_3^+ C	1.00E-09	0.0	0.0	a
CH^+	H ₂	CH_2^+ H	1.01E-09	0.0	0.0	10
CH^+	N	CN^+ H	1.00E-09	0.0	0.0	14,a
CH^+	O	CO^+ H	1.00E-09	0.0	0.0	a
CH^+	O ₂	HCO^+ O	9.22E-10	0.0	0.0	42,e
CH^+	O ₂	O^+ HCO	2.40E-11	0.0	0.0	42,e
CH^+	O ₂	CO^+ OH	2.40E-11	0.0	0.0	42,e
CH_2^+	e	CH H	5.10E-07	-0.5	0.0	52
CH_2^+	H ₂ O	CH_2OH^+ H	1.20E-09	0.0	0.0	10
CH_2^+	CO ₂	H_2CO^+ CO	1.60E-09	0.0	0.0	38
CH_2^+	NH ₃	NH_4^+ CH	5.25E-10	0.0	0.0	10
CH_2^+	NH ₃	CH_4N^+ H	1.98E-09	0.0	0.0	10
CH_2^+	CH ₄	$C_2H_5^+$ H	2.88E-10	0.0	0.0	10
CH_2^+	CH ₄	$C_2H_4^+$ H ₂	5.04E-10	0.0	0.0	10
CH_2^+	CH ₄	$C_2H_3^+$ H ₂ H	2.64E-10	0.0	0.0	10
CH_2^+	CH ₄	$C_2H_2^+$ H ₂ H ₂	1.44E-10	0.0	0.0	10

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$\text{CH}_2^+ \text{H}_2$	$\text{CH}_3^+ \text{H}$	$7.20\text{E}-10$	0.0	0.0	10
$\text{CH}_2^+ \text{O}$	$\text{HCO}^+ \text{H}$	$1.00\text{E}-09$	0.0	0.0	a
$\text{CH}_2^+ \text{O}_2$	$\text{HCO}^+ \text{OH}$	$7.28\text{E}-10$	0.0	0.0	42,e
$\text{CH}_2^+ \text{O}_2$	$\text{H}_2\text{CO}^+ \text{O}$	$1.82\text{E}-10$	0.0	0.0	42,e
$\text{CH}_3^+ \text{e}$	$\text{CH}_2 \text{H}$	$2.53\text{E}-07$	-0.5	0.0	52
$\text{CH}_3^+ \text{e}$	$\text{CH} \text{H}_2$	$2.54\text{E}-07$	-0.5	0.0	52
$\text{CH}_3^+ \text{e}$	$\text{CH} \text{H} \text{H}$	$2.53\text{E}-07$	-0.5	0.0	52
$\text{CH}_3^+ \text{NH}_3$	$\text{NH}_4^+ \text{CH}_2$	$3.20\text{E}-10$	0.0	0.0	10,39,f
$\text{CH}_3^+ \text{NH}_3$	$\text{CH}_4\text{N}^+ \text{H}_2$	$1.28\text{E}-09$	0.0	0.0	10,39,f
$\text{CH}_3^+ \text{CH}_4$	$\text{C}_2\text{H}_5^+ \text{H}_2$	$9.60\text{E}-10$	0.0	0.0	10
$\text{CH}_3^+ \text{C}$	$\text{C}_2\text{H}^+ \text{H}_2$	$1.00\text{E}-09$	0.0	0.0	a
$\text{CH}_3^+ \text{N}$	$\text{H}_2\text{CN}^+ \text{H}$	$3.35\text{E}-11$	0.0	0.0	10,16,a
$\text{CH}_3^+ \text{N}$	$\text{HCN}^+ \text{H}_2$	$3.35\text{E}-11$	0.0	0.0	10,16,a
$\text{CH}_3^+ \text{O}$	$\text{HCO}^+ \text{H}_2$	$4.40\text{E}-10$	0.0	0.0	10,16
$\text{CH}_3^+ \text{O}_2$	$\text{HCO}^+ \text{H}_2\text{O}$	$4.30\text{E}-11$	0.0	0.0	10
$\text{CH}_3^+ \text{NO}$	$\text{NO}^+ \text{CH}_3$	$9.40\text{E}-10$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_2$	$\text{C}_3\text{H}_3^+ \text{H}_2$	$1.15\text{E}-09$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_4$	$\text{C}_2\text{H}_3^+ \text{CH}_4$	$3.50\text{E}-10$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_4$	$\text{C}_3\text{H}_3^+ \text{H}_2 \text{H}_2$	$4.60\text{E}-11$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_4$	$\text{C}_3\text{H}_5^+ \text{H}_2$	$5.24\text{E}-10$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_6$	$\text{C}_2\text{H}_5^+ \text{CH}_4$	$1.48\text{E}-09$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_6$	$\text{C}_3\text{H}_5^+ \text{H}_2 \text{H}_2$	$1.57\text{E}-10$	0.0	0.0	10
$\text{CH}_3^+ \text{C}_2\text{H}_6$	$\text{C}_3\text{H}_7^+ \text{H}_2$	$1.04\text{E}-10$	0.0	0.0	10
$\text{CH}_3^+ \text{H}_2\text{CO}$	$\text{HCO}^+ \text{CH}_4$	$1.00\text{E}-09$	0.0	0.0	10
$\text{CH}_3^+ \text{H}_2 \text{M}$	$\text{CH}_5^+ \text{M}$	$1.30\text{E}-28$	0.0	0.0	17,a
$\text{CH}_4^+ \text{e}$	$\text{CH}_3 \text{H}$	$1.20\text{E}-07$	-0.5	0.0	52
$\text{CH}_4^+ \text{e}$	$\text{CH}_2 \text{H}_2$	$1.20\text{E}-07$	-0.5	0.0	52
$\text{CH}_4^+ \text{e}$	$\text{CH}_2 \text{H} \text{H}$	$1.20\text{E}-07$	-0.5	0.0	52
$\text{CH}_4^+ \text{e}$	$\text{CH} \text{H}_2 \text{H}$	$1.20\text{E}-07$	-0.5	0.0	52
$\text{CH}_4^+ \text{e}$	$\text{CH} \text{H} \text{H} \text{H}$	$1.20\text{E}-07$	-0.5	0.0	52
$\text{CH}_4^+ \text{H}_2\text{O}$	$\text{H}_3\text{O}^+ \text{CH}_3$	$3.50\text{E}-09$	0.0	0.0	10
$\text{CH}_4^+ \text{CO}_2$	$\text{CO}_2\text{H}^+ \text{CH}_3$	$1.20\text{E}-09$	0.0	0.0	38
$\text{CH}_4^+ \text{NH}_3$	$\text{CH}_5^+ \text{NH}_2$	$6.40\text{E}-11$	0.0	0.0	10
$\text{CH}_4^+ \text{NH}_3$	$\text{NH}_4^+ \text{CH}_3$	$1.54\text{E}-09$	0.0	0.0	10

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$\text{CH}_4^+ \text{NH}_3$	$\text{NH}_3^+ \text{CH}_4$	1.60E-09	0.0	0.0	10
$\text{CH}_4^+ \text{CH}_4$	$\text{CH}_5^+ \text{CH}_3$	1.15E-09	0.0	0.0	10
$\text{CH}_4^+ \text{H}_2$	$\text{CH}_5^+ \text{H}$	4.10E-11	0.0	0.0	10
$\text{CH}_4^+ \text{O}$	$\text{H}_2\text{CO}^+ \text{H}_2$	1.00E-09	0.0	0.0	a
$\text{CH}_4^+ \text{O}_2$	$\text{O}_2^+ \text{CH}_4$	4.40E-10	0.0	0.0	42
$\text{CH}_4^+ \text{CO}$	$\text{CH}_3\text{CO}^+ \text{H}$	7.02E-11	0.0	0.0	39,f
$\text{CH}_4^+ \text{CO}$	$\text{HCO}^+ \text{CH}_3$	7.10E-10	0.0	0.0	39,f
$\text{CH}_4^+ \text{C}_2\text{H}_2$	$\text{C}_2\text{H}_2^+ \text{CH}_4$	1.13E-09	0.0	0.0	10
$\text{CH}_4^+ \text{C}_2\text{H}_2$	$\text{C}_2\text{H}_3^+ \text{CH}_3$	1.24E-09	0.0	0.0	10
$\text{CH}_4^+ \text{C}_2\text{H}_2$	$\text{C}_3\text{H}_3^+ \text{H}_2$	1.51E-10	0.0	0.0	10
$\text{CH}_4^+ \text{C}_2\text{H}_4$	$\text{C}_2\text{H}_4^+ \text{CH}_4$	1.38E-09	0.0	0.0	10
$\text{CH}_4^+ \text{C}_2\text{H}_4$	$\text{C}_2\text{H}_5^+ \text{CH}_3$	4.23E-10	0.0	0.0	10
$\text{CH}_4^+ \text{C}_2\text{H}_4$	$\text{C}_3\text{H}_5^+ \text{H}_2$	5.50E-11	0.0	0.0	10
$\text{CH}_4^+ \text{C}_2\text{H}_6$	$\text{C}_2\text{H}_4^+ \text{CH}_4$	1.91E-09	0.0	0.0	10
$\text{CH}_5^+ \text{e}$	$\text{CH}_4^+ \text{H}$	7.00E-07	-0.5	0.0	52
$\text{CH}_5^+ \text{H}_2\text{O}$	$\text{H}_3\text{O}^+ \text{CH}_4$	3.70E-09	0.0	0.0	a
$\text{CH}_5^+ \text{NH}_3$	$\text{NH}_4^+ \text{CH}_4$	2.50E-09	0.0	0.0	a
$\text{CH}_5^+ \text{CO}$	$\text{HCO}^+ \text{CH}_4$	1.00E-09	0.0	0.0	42,a
$\text{CH}_5^+ \text{CH}_3$	$\text{C}_2\text{H}_6^+ \text{H}_2$	5.00E-10	0.0	0.0	17,a
$\text{CH}_5^+ \text{C}_2\text{H}_6$	$\text{C}_2\text{H}_7^+ \text{CH}_4$	1.50E-09	0.0	0.0	17,a
$\text{CH}_5^+ \text{CH}_4$	$\text{C}_2\text{H}_9^+ \text{M}$	1.00E-29	0.0	0.0	17,a
$\text{N}^+ \text{e}$	N	3.50E-12	-0.7	0.0	11
$\text{N}^+ \text{H}_2\text{O}$	$\text{H}_2\text{O}^+ \text{N}$	2.60E-09	0.0	0.0	11
$\text{N}^+ \text{CO}_2$	$\text{CO}_2^+ \text{N}$	1.10E-09	0.0	0.0	10
$\text{N}^+ \text{CH}_4$	$\text{CH}_3^+ \text{N}$	7.16E-10	0.0	0.0	10
$\text{N}^+ \text{CH}_4$	$\text{CH}_4^+ \text{N}$	5.40E-11	0.0	0.0	10
$\text{N}^+ \text{CH}_4$	$\text{H}_2\text{CN}^+ \text{H}$	4.32E-10	0.0	0.0	10
$\text{N}^+ \text{CH}_4$	$\text{HCN}^+ \text{H}_2$	1.35E-10	0.0	0.0	10
$\text{N}^+ \text{H}_2$	$\text{NH}^+ \text{H}$	4.80E-10	0.0	0.0	10
$\text{N}^+ \text{CO}$	$\text{CO}^+ \text{N}$	4.90E-10	0.0	0.0	10
$\text{N}^+ \text{CO}$	$\text{NO}^+ \text{C}$	6.00E-11	0.0	0.0	10
$\text{N}^+ \text{NH}$	$\text{N}_2^+ \text{H}$	1.00E-09	0.0	0.0	a
$\text{N}^+ \text{O}_2$	$\text{O}^+ \text{NO}$	3.60E-11	0.0	0.0	10
$\text{N}^+ \text{O}_2$	$\text{NO}^+ \text{O}$	1.70E-10	0.0	0.0	10

Table IV (cont)

Reactants		Products		A	B	C	Refs. and Notes
N^+	O_2	O_2^+	N	4.00E-10	0.0	0.0	10
N^+	NO	NO^+	N	5.20E-10	0.0	0.0	10
N^+	NO	N_2^+	O	4.50E-11	0.0	0.0	10
N^+	O	O^+	N	1.00E-12	0.0	0.0	11,a
NH^+	e	N	H	1.08E-07	-0.5	0.0	52
NH^+	H_2O	H_3O^+	N	1.40E-09	0.0	0.0	39,42
NH^+	NH_3	NH_3^+	NH	1.05E-09	0.0	0.0	10,a
NH^+	NH_3	NH_4^+	N	1.05E-09	0.0	0.0	10,a
NH^+	H_2	NH_2^+	H	9.50E-10	0.0	0.0	10
NH_2^+	e	NH	H	3.00E-07	-0.5	0.0	a
NH_2^+	H_2O	H_3O^+	NH	1.58E-09	0.0	0.0	10
NH_2^+	H_2O	NH_4^+	O	3.40E-11	0.0	0.0	10
NH_2^+	H_2O	NH_3^+	OH	1.02E-10	0.0	0.0	10
NH_2^+	NH_3	NH_4^+	NH	9.68E-10	0.0	0.0	10
NH_2^+	NH_3	NH_3^+	NH_2	1.45E-09	0.0	0.0	10
NH_2^+	H_2	NH_3^+	H	1.20E-10	0.0	0.0	10
NH_3^+	e	NH_2	H	1.00E-07	-0.5	0.0	a,g
NH_3^+	e	NH	H_2	1.00E-07	-0.5	0.0	a,g
NH_3^+	e	NH	H H	1.90E-07	-0.5	0.0	13,a,h
NH_3^+	H_2O	NH_4^+	OH	1.10E-10	0.0	0.0	10
NH_3^+	NH_3	NH_4^+	NH_2	2.30E-09	0.0	0.0	10
NH_3^+	CH_4	NH_4^+	CH_3	3.90E-10	0.0	0.0	10
NH_3^+	OH	NH_4^+	O	1.00E-09	0.0	0.0	a
NH_3^+	H_2	NH_4^+	H	1.70E-11	0.0	1043.1	10,22
NH_3^+	H_2CO	NH_4^+	HCO	4.90E-10	0.0	0.0	10
NH_3^+	CH_2	CH_3^+	NH_2	1.00E-09	0.0	0.0	a
NH_4^+	e	NH_3	H	1.17E-06	-0.5	0.0	11,13,a
NH_4^+	e	NH_2	H H	1.30E-07	-0.5	0.0	11,13,a
O^+	e	O		3.50E-12	-0.7	0.0	11
O^+	H_2O	H_2O^+	O	2.30E-09	0.0	0.0	11
O^+	CO_2	O_2^+	CO	1.10E-09	-0.3	0.0	11
O^+	NH_3	NH_3^+	O	1.20E-09	0.0	0.0	41
O^+	CH_4	CH_4^+	O	8.90E-10	0.0	0.0	41
O^+	CH_4	CH_3^+	OH	1.10E-10	0.0	0.0	41

Table IV (cont)

Reactants		Products		A	B	C	Refs. and Notes
O^+	H_2	OH^+	H	1.58E-09	0.0	0.0	10
O^+	OH	OH^+	O	3.00E-10	0.0	0.0	a
O^+	OH	H^+	O_2	2.70E-11	0.13	0.0	a
O^+	O_2	O_2^+	O	2.00E-11	-0.5	0.0	11
O^+	N_2	NO^+	N	1.20E-12	-1.0	0.0	11
O^+	H	H^+	O	6.80E-10	0.0	0.0	11
OH^+	e	O	H	8.22E-08	-0.5	0.0	52
OH^+	H_2O	H_3O^+	O	1.30E-09	0.0	0.0	10
OH^+	H_2O	H_2O^+	OH	1.59E-09	0.0	0.0	10
OH^+	NH_3	NH_4^+	O	1.19E-09	0.0	0.0	10
OH^+	NH_3	NH_3^+	OH	1.19E-09	0.0	0.0	10
OH^+	CH_4	H_3O^+	CH_2	1.32E-10	0.0	0.0	39,f
OH^+	CH_4	CH_4^+	OH	9.68E-10	0.0	0.0	39,f
OH^+	H_2CO	CH_2OH^+	O	1.12E-09	0.0	0.0	15
OH^+	H_2CO	H_2CO^+	OH	7.44E-10	0.0	0.0	15
OH^+	CO_2	CO_2H^+	O	1.10E-09	0.0	0.0	39,f
OH^+	HCN	H_2CN^+	O	1.00E-09	0.0	0.0	a
OH^+	CO	HCO^+	O	6.50E-10	0.0	0.0	39,f
OH^+	N_2	N_2H^+	O	1.90E-10	0.0	0.0	15
OH^+	OH	H_2O^+	O	1.00E-09	0.0	0.0	a
OH^+	H_2	H_2O^+	H	1.05E-09	0.0	0.0	10
OH^+	C	CO^+	H	1.00E-09	0.0	0.0	14,a
OH^+	C	CH^+	O	1.00E-09	0.0	0.0	a
OH^+	O_2	O_2^+	OH	2.00E-10	0.0	0.0	11
OH^+	C_2H_5	$C_2H_6^+$	O	1.00E-09	0.0	0.0	a
H_2O^+	e	OH	H	5.32E-07	-0.5	0.0	52
H_2O^+	e	O	H_2	1.52E-07	-0.5	0.0	52
H_2O^+	e	H_2	$O(1D)$	7.60E-08	-0.5	0.0	52
H_2O^+	H_2O	H_3O^+	OH	2.05E-09	0.0	0.0	10
H_2O^+	NH_3	NH_3^+	H_2O	2.20E-09	0.0	0.0	10
H_2O^+	NH_3	NH_4^+	OH	9.45E-10	0.0	0.0	10
H_2O^+	CH_4	H_3O^+	CH_3	1.10E-09	0.0	0.0	10
H_2O^+	H_2CO	CH_2OH^+	OH	6.62E-10	0.0	0.0	15
H_2O^+	H_2CO	H_2CO^+	H_2O	1.41E-09	0.0	0.0	15

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
H_2O^+ HCN	H_2CN^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ C_2H_2	C_2H_3^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ C_2H_4	C_2H_5^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ CO	HCO^+ OH	2.52E-10	0.309	180.	a
H_2O^+ HCO	H_2CO^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ NH_2	NH_3^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ CH_2	CH_3^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ CH	CH_2^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ C	CH^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ C_2	C_2H^+ OH	1.00E-09	0.0	0.0	a
H_2O^+ H_2	H_3O^+ H	6.10E-10	0.0	0.0	10
H_2O^+ O_2	O_2^+ H_2O	2.00E-10	0.0	0.0	11
H_3O^+ e	H_2O H	2.34E-07	-0.5	0.0	52
H_3O^+ e	OH H_2	2.33E-07	-0.5	0.0	52
H_3O^+ e	OH H H	2.33E-07	-0.5	0.0	52
H_3O^+ NH_3	NH_4^+ H_2O	2.20E-09	0.0	0.0	10
H_3O^+ H_2CO	CH_2OH^+ H_2O	3.40E-09	0.0	0.0	43
H_3O^+ HCN	H_2CN^+ H_2O	1.00E-09	0.0	0.0	a
H_3O^+ NH_2	NH_3^+ H_2O	1.00E-09	0.0	0.0	a
H_3O^+ CH_2	CH_3^+ H_2O	1.00E-09	0.0	0.0	a
H_3O^+ CH	CH_2^+ H_2O	1.00E-09	0.0	0.0	a
H_3O^+ C	HCO^+ H_2	2.00E-09	0.0	0.0	13,a
H_3O^+ C_2H_3	C_2H_4^+ H_2O	1.00E-09	0.0	0.0	a
H_3O^+ H_2O M	H_3O^+ 1WM	3.50E-27	-3.0	0.0	11
H_3O^+ 1we	H_2O H_2O H	2.80E-06	-0.15	0.0	11
C_2^+ e	C C	5.90E-07	-0.5	0.0	52
C_2^+ CH_4	C_3H_2^+ H_2	5.74E-10	0.0	0.0	38
C_2^+ CH_4	C_2H^+ CH_3	2.38E-10	0.0	0.0	38
C_2^+ CH_4	C_3H_3^+ H	2.10E-10	0.0	0.0	38
C_2^+ CH_4	C_3H^+ H_2 H	1.96E-10	0.0	0.0	38
C_2^+ CH_4	C_2H_2^+ CH_2	1.82E-10	0.0	0.0	38
C_2^+ H_2	C_2H^+ H	1.12E-09	0.0	0.0	10
C_2H^+ e	C_2 H	1.90E-06	-0.5	0.0	a
C_2H^+ CH_4	C_2H_2^+ CH_3	3.74E-10	0.0	0.0	38,1

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$C_2H^+ CH_4$	$C_3H_3^+ H_2$	3.74E-10	0.0	0.0	38,i
$C_2H^+ CH_4$	$C_3H_4^+ H$	1.32E-10	0.0	0.0	38,i
$C_2H^+ NH_3$	$NH_4^+ C_2$	1.00E-09	0.0	0.0	a
$C_2H^+ H_2CO$	$CH_2OH^+ C_2$	1.00E-09	0.0	0.0	a
$C_2H^+ HCN$	$H_2CN^+ C_2$	1.00E-09	0.0	0.0	a
$C_2H^+ H_2$	$C_2H_2^+ H$	7.80E-10	0.0	0.0	10
$C_2H_2^+ e$	$C_2H H$	2.95E-07	-0.5	0.0	52
$C_2H_2^+ e$	$C_2 H H$	2.95E-07	-0.5	0.0	52
$C_2H_2^+ H_2O$	$H_3O^+ C_2H$	2.20E-10	0.0	0.0	10
$C_2H_2^+ NH_3$	$NH_3^+ C_2H_2$	2.14E-09	0.0	0.0	10
$C_2H_2^+ NH_3$	$NH_4^+ C_2H$	9.61E-10	0.0	0.0	10
$C_2H_2^+ CH_4$	$C_3H_4^+ H_2$	1.76E-10	0.0	0.0	10
$C_2H_2^+ CH_4$	$C_3H_5^+ H$	6.64E-10	0.0	0.0	10
$C_2H_2^+ C_2H_2$	$C_4H_2^+ H_2$	5.22E-10	0.0	0.0	10
$C_2H_2^+ C_2H_2$	$C_4H_3^+ H$	8.88E-10	0.0	0.0	10
$C_2H_2^+ C_2H_4$	$C_2H_4^+ C_2H_2$	4.01E-10	0.0	0.0	10
$C_2H_2^+ C_2H_4$	$C_3H_3^+ CH_3$	5.07E-10	0.0	0.0	10
$C_2H_2^+ C_2H_4$	$C_4H_5^+ H$	2.71E-10	0.0	0.0	10
$C_2H_2^+ C_2H_6$	$C_2H_4^+ C_2H_4$	2.63E-10	0.0	0.0	10
$C_2H_2^+ C_2H_6$	$C_2H_5^+ C_2H_3$	1.31E-10	0.0	0.0	10
$C_2H_2^+ C_2H_6$	$C_3H_3^+ CH_3 H_2$	8.80E-11	0.0	0.0	10
$C_2H_2^+ C_2H_6$	$C_3H_5^+ CH_3$	7.88E-10	0.0	0.0	10
$C_2H_2^+ C_2H_6$	$C_4H_5^+ H_2 H$	7.30E-11	0.0	0.0	10
$C_2H_2^+ C_2H_6$	$C_4H_7^+ H$	1.31E-10	0.0	0.0	10
$C_2H_2^+ H_2CO$	$HCO^+ C_2H_3$	5.38E-10	0.0	0.0	10
$C_2H_2^+ H_2CO$	$H_2CO^+ C_2H_2$	8.60E-10	0.0	0.0	10
$C_2H_2^+ H_2CO$	$CH_2OH^+ C_2H$	4.09E-10	0.0	0.0	10
$C_2H_2^+ H_2CO$	$C_3H_3O^+ H$	6.50E-11	0.0	0.0	10
$C_2H_2^+ H_2CO$	$C_2H_4^+ CO$	2.80E-10	0.0	0.0	10
$C_2H_2^+ HCN$	$H_2CN^+ C_2H$	2.20E-11	0.0	0.0	10
$C_2H_2^+ HCN$	$C_3H_2N^+ H$	3.10E-11	0.0	0.0	10
$C_2H_2^+ H_2 M$	$C_2H_4^+ M$	1.20E-27	0.0	0.0	17,a
$C_2H_3^+ e$	$C_2H_2 H$	9.50E-07	-0.5	0.0	52
$C_2H_3^+ H_2O$	$H_3O^+ C_2H_2$	1.11E-09	0.0	0.0	10

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$C_2H_3^+ + NH_3$	$NH_4^+ + C_2H_2$	2.48E-09	0.0	0.0	10
$C_2H_3^+ + CH_4$	$C_3H_5^+ + H_2$	2.20E-10	0.0	0.0	10
$C_2H_3^+ + H_2CO$	$CH_2OH^+ + C_2H_2$	1.00E-09	0.0	0.0	a
$C_2H_3^+ + HCN$	$H_2CN^+ + C_2H_2$	1.00E-09	0.0	0.0	a
$C_2H_3^+ + C_2H_2$	$C_4H_3^+ + H_2$	2.50E-10	0.0	0.0	10
$C_2H_3^+ + C_2H_4$	$C_2H_5^+ + C_2H_2$	9.30E-10	0.0	0.0	10
$C_2H_3^+ + C_2H_6$	$C_2H_5^+ + C_2H_4$	2.91E-10	0.0	0.0	10
$C_2H_3^+ + C_2H_6$	$C_3H_5^+ + CH_4$	2.48E-10	0.0	0.0	10
$C_2H_3^+ + C_2H_6$	$C_4H_7^+ + H_2$	8.10E-11	0.0	0.0	10
$C_2H_3^+ + H_2$ M	$C_2H_5^+ + M$	1.50E-29	0.0	0.0	17
$C_2H_4^+ + e$	$C_2H_2 + H_2$	1.90E-06	-0.5	0.0	a
$C_2H_4^+ + NH_3$	$NH_3^+ + C_2H_4$	1.24E-10	0.0	0.0	10
$C_2H_4^+ + NH_3$	$NH_4^+ + C_2H_3$	1.94E-09	0.0	0.0	10
$C_2H_4^+ + H$	$C_2H_3^+ + H_2$	1.00E-10	0.0	0.0	17,a
$C_2H_4^+ + CH_3$	$CH_3^+ + C_2H_4$	1.00E-09	0.0	0.0	17,a
$C_2H_4^+ + C_2H_2$	$C_3H_3^+ + CH_3$	6.32E-10	0.0	0.0	10
$C_2H_4^+ + C_2H_2$	$C_4H_5^+ + H$	1.58E-10	0.0	0.0	10
$C_2H_4^+ + C_2H_4$	$C_3H_5^+ + CH_3$	7.28E-10	0.0	0.0	10
$C_2H_4^+ + C_2H_4$	$C_4H_7^+ + H$	7.20E-11	0.0	0.0	10
$C_2H_4^+ + C_2H_6$	$C_3H_6^+ + CH_4$	3.71E-13	0.0	0.0	10
$C_2H_4^+ + C_2H_6$	$C_3H_7^+ + CH_3$	4.93E-12	0.0	0.0	10
$C_2H_4^+ + CH_4$ M	$C_3H_8^+ + M$	1.00E-29	0.0	0.0	17,a
$C_2H_5^+ + e$	$C_2H_2 + H_2$ H	1.90E-06	-0.5	0.0	21,23,a
$C_2H_5^+ + H_2O$	$H_3O^+ + C_2H_4$	7.50E-10	0.0	0.0	10
$C_2H_5^+ + NH_3$	$NH_4^+ + C_2H_4$	2.18E-09	0.0	0.0	10
$C_2H_5^+ + H_2CO$	$CH_2OH^+ + C_2H_4$	1.00E-09	0.0	0.0	a
$C_2H_5^+ + HCN$	$H_2CN^+ + C_2H_4$	1.00E-09	0.0	0.0	a
$C_2H_5^+ + CH_3$	$C_2H_4^+ + CH_4$	5.00E-10	0.0	0.0	17,a
$C_2H_5^+ + C_2H_2$	$C_3H_3^+ + CH_4$	6.80E-11	0.0	0.0	10
$C_2H_5^+ + C_2H_2$	$C_4H_5^+ + H_2$	1.22E-10	0.0	0.0	10
$C_2H_5^+ + C_2H_4$	$C_3H_5^+ + CH_4$	3.90E-10	0.0	0.0	10
$C_2H_5^+ + C_2H_6$	$C_4H_9^+ + H_2$	4.00E-11	0.0	0.0	10
$C_2H_5^+ + CH_4$ M	$C_3H_9^+ + M$	1.00E-29	0.0	0.0	17,a
$C_2H_6^+ + e$	$C_2H_4 + H_2$	1.90E-06	-0.5	0.0	a

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$C_2H_6^+ H_2O$	$H_3O^+ C_2H_5$	2.95E-09	0.0	0.0	10
$C_2H_6^+ NH_3$	$NH_3^+ C_2H_6$	6.24E-10	0.0	0.0	10
$C_2H_6^+ NH_3$	$NH_4^+ C_2H_5$	1.61E-09	0.0	0.0	10
$C_2H_6^+ H_2CO$	$CH_2OH^+ C_2H_5$	1.00E-09	0.0	0.0	a
$C_2H_6^+ HCN$	$H_2CN^+ C_2H_5$	1.00E-09	0.0	0.0	a
$C_2H_6^+ CH_3$	$CH_3^+ C_2H_6$	1.00E-09	0.0	0.0	17,a
$C_2H_6^+ H$	$C_2H_5^+ H_2$	1.00E-10	0.0	0.0	17,a
$C_2H_6^+ C_2H_2$	$C_2H_5^+ C_2H_3$	2.22E-10	0.0	0.0	10
$C_2H_6^+ C_2H_2$	$C_3H_5^+ CH_3$	8.19E-10	0.0	0.0	10
$C_2H_6^+ C_2H_2$	$C_4H_7^+ H$	1.29E-10	0.0	0.0	10
$C_2H_6^+ C_2H_4$	$C_2H_4^+ C_2H_6$	1.15E-09	0.0	0.0	10
$C_2H_6^+ C_2H_6$	$C_3H_8^+ CH_4$	7.98E-12	0.0	0.0	10
$C_2H_6^+ C_2H_6$	$C_3H_9^+ CH_3$	1.10E-11	0.0	0.0	10
$C_2H_6^+ CH_4$ M	$C_3H_{10}^+ M$	1.00E-29	0.0	0.0	17,a
$C_2H_7^+ e$	$C_2H_6^+ H$	1.90E-06	-0.5	0.0	a
$C_2H_7^+ CH_3$	$C_2H_6^+ CH_4$	5.00E-10	0.0	0.0	17,a
$C_2H_7^+ H$	$C_2H_6^+ H_2$	1.00E-10	0.0	0.0	17,a
$C_2H_7^+ CH_4$ M	$C_3H_{11}^+ M$	1.00E-29	0.0	0.0	17,a
$C_2H_9^+ e$	$C_2H_6^+ H_2$ H	1.90E-06	-0.5	0.0	a
$C_3^+ e$	$C_2^+ C$	5.00E-07	-0.5	0.0	a
$C_3^+ H_2$	$C_3H^+ H$	1.00E-09	0.0	0.0	a
$C_3H^+ e$	$C_3^+ H$	1.90E-06	-0.5	0.0	a
$C_3H_2^+ e$	$C_3^+ H$ H	5.00E-07	-0.5	0.0	a
$C_3H_3^+ e$	$C_3^+ H$ H H	5.00E-07	-0.5	0.0	a
$C_3H_4^+ e$	$C_3^+ H_2$ H ₂	5.00E-07	-0.5	0.0	a
$C_3H_5^+ e$	$C_3^+ H_2$ H ₂ H	2.50E-07	-0.5	0.0	a
$C_3H_5^+ e$	$H_2C_3H_2H$	2.50E-07	-0.5	0.0	a
$N_2^+ e$	$N^+ N$	3.60E-07	-0.5	0.0	52
$N_2^+ H_2O$	$N_2H^+ OH$	4.62E-10	0.0	0.0	39,f
$N_2^+ H_2O$	$H_2O^+ N_2$	1.64E-09	0.0	0.0	39,f
$N_2^+ CO_2$	$CO_2^+ N_2$	7.70E-10	0.0	0.0	11
$N_2^+ NH_3$	$NH_3^+ N_2$	2.08E-09	0.0	0.0	39,f
$N_2^+ NH_3$	$N_2H^+ NH_2$	2.10E-11	0.0	0.0	39,f
$N_2^+ CH_4$	$CH_4^+ N_2$	1.65E-10	0.0	0.0	39,f

Table IV (cont)

Reactants		Products		A	B	C	Refs. and Notes
N_2^+	CH_4	CH_3^+	H N_2	7.66E-10	0.0	0.0	39,f
N_2^+	CH_4	CH_2^+	H_2 N_2	3.88E-11	0.0	0.0	39,f
N_2^+	H_2	N_2H^+	H	1.73E-09	0.0	0.0	10
N_2^+	CO	CO^+	N_2	7.00E-11	0.0	0.0	12
N_2^+	O	NO^+	N	1.30E-10	-0.46	0.0	11
N_2^+	O	O^+	N_2	1.00E-11	-0.23	0.0	11
N_2^+	H	H^+	N_2	1.20E-10	0.0	0.0	44
N_2^+	O_2	O_2^+	N_2	5.00E-11	-0.8	0.0	11,12
N_2^+	NO	NO^+	N_2	3.30E-10	0.0	0.0	11
N_2H^+	e	N_2	H	7.60E-07	-0.5	0.0	52
N_2H^+	H_2O	H_3O^+	N_2	2.60E-09	0.0	0.0	43
N_2H^+	CO_2	CO_2H^+	N_2	9.20E-10	0.0	0.0	12
N_2H^+	NH_3	NH_4^+	N_2	2.30E-09	0.0	0.0	43
N_2H^+	CH_4	CH_5^+	N_2	8.90E-10	0.0	0.0	12
N_2H^+	CO	HCO^+	N_2	8.80E-10	0.0	0.0	24
N_2H^+	O	OH^+	N_2	1.40E-10	0.0	0.0	43
O_2^+	e	O	O	1.90E-07	-0.5	0.0	52
O_2^+	e	O_2		4.00E-12	-0.7	0.0	11,a
O_2^+	NH_3	NH_3^+	O_2	2.40E-09	0.0	0.0	12
O_2^+	NO	NO^+	O_2	4.40E-10	0.0	0.0	11
O_2^+	C	C^+	O_2	1.00E-09	0.0	0.0	13,a
O_2^+	N	NO^+	O	1.80E-10	0.0	0.0	11
HO_2^+	e	O_2	H	5.00E-07	-0.5	0.0	a
HO_2^+	H_2	H_3^+	O_2	3.20E-10	0.0	0.0	10
CO^+	e	C	O(1D)	2.50E-07	-0.5	0.0	a
CO^+	e	C(1D)	O	2.50E-07	-0.5	0.0	a
CO^+	H_2O	H_2O^+	CO	1.72E-09	0.0	0.0	39,f
CO^+	H_2O	HCO^+	OH	8.84E-10	0.0	0.0	39,f
CO^+	CO_2	CO_2^+	CO	1.10E-09	0.0	0.0	45,e,j
CO^+	NH_3	NH_3^+	CO	2.06E-09	0.0	0.0	39,f
CO^+	NH_3	HCO^+	NH_2	4.20E-11	0.0	0.0	39,f
CO^+	CH_4	CH_4^+	CO	1.16E-09	0.0	0.0	39,f
CO^+	CH_4	HCO^+	CH_3	2.10E-10	0.0	0.0	39,f
CO^+	CH_4	CH_3CO^+	H	2.80E-11	0.0	0.0	39,f

Table IV (cont)

Reactants		Products	A	B	C	Refs. and Notes
CO ⁺	H ₂ CO	H ₂ CO ⁺ CO	2.00E-09	0.0	0.0	a
CO ⁺	H ₂ CO	HCO ⁺ HCO	1.00E-09	0.0	0.0	a
CO ⁺	H ₂ CO ₂	H ₂ CO ₂ ⁺ CO	3.00E-09	0.0	0.0	a
CO ⁺	HCN	HCN ⁺ CO	1.00E-09	0.0	0.0	a
CO ⁺	HCN	HCO ⁺ CN	5.00E-10	0.0	0.0	a
CO ⁺	H ₂	HCO ⁺ H	1.39E-09	0.0	0.0	10
CO ⁺	OH	OH ⁺ CO	3.25E-10	-0.127	0.0	a
CO ⁺	NO	NO ⁺ CO	3.30E-10	0.0	0.0	11
CO ⁺	O ₂	O ₂ ⁺ CO	2.00E-10	0.0	0.0	12
CO ⁺	O	O ⁺ CO	1.40E-10	0.0	0.0	11
CO ⁺	H	H ⁺ CO	9.00E-11	0.0	0.0	37
HCO ⁺	e	H CO	2.00E-07	-1.0	0.0	13,32,a
HCO ⁺	H ₂ O	H ₃ O ⁺ CO	2.70E-09	0.0	0.0	40
HCO ⁺	NH ₃	NH ₄ ⁺ CO	2.60E-09	0.0	0.0	10
HCO ⁺	OH	CO ₂ H ⁺ H	1.00E-09	0.0	0.0	13,a
HCO ⁺	OH	H ₂ O ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	NH ₂	NH ₃ ⁺ CO	1.00E-09	0.0	0.0	13,a
HCO ⁺	H ₂ CO	CH ₂ OH ⁺ CO	1.00E-09	0.0	0.0	13,a
HCO ⁺	HCN	H ₂ CN ⁺ CO	1.14E-09	0.0	0.0	10
HCO ⁺	C ₂ H	C ₂ H ₂ ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	C ₂ H ₂	C ₂ H ₃ ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	C ₂ H ₄	C ₂ H ₅ ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	HCO	H ₂ CO ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	CH ₂	CH ₃ ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	CH	CH ₂ ⁺ CO	1.00E-09	0.0	0.0	a
HCO ⁺	NH	NH ₂ ⁺ CO	1.00E-09	0.0	1007.	a
HCO ⁺	C	CH ⁺ CO	1.00E-09	0.0	0.0	10
H ₂ CO ⁺	e	CO H H	1.90E-07	-0.5	0.0	13,a,h
H ₂ CO ₂ ⁺	e	CO H OH	2.00E-07	-0.5	0.0	a
H ₂ CO ⁺	H ₂ O	H ₃ O ⁺ HCO	1.60E-09	0.0	0.0	44
H ₂ CO ⁺	H ₂ CO	CH ₂ OH ⁺ HCO	1.00E-09	0.0	0.0	a
H ₂ CO ⁺	NH ₃	NH ₃ ⁺ H ₂ CO	1.15E-09	0.0	0.0	10
H ₂ CO ⁺	NH ₃	NH ₄ ⁺ HCO	1.15E-09	0.0	0.0	10
H ₂ CO ⁺	HCN	H ₂ CN ⁺ HCO	1.40E-09	0.0	0.0	10

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$\text{H}_2\text{CO}^+ \text{C}_2\text{H}_4$	$\text{C}_2\text{H}_5^+ \text{HCO}$	1.00E-09	0.0	0.0	a
$\text{H}_2\text{CO}^+ \text{CH}$	$\text{CH}_2^+ \text{HCO}$	1.00E-09	0.0	0.0	a
$\text{H}_2\text{CO}^+ \text{CH}_2$	$\text{CH}_3^+ \text{HCO}$	1.00E-09	0.0	0.0	a
$\text{H}_2\text{CO}^+ \text{NH}_2$	$\text{NH}_3^+ \text{HCO}$	1.00E-09	0.0	0.0	a
$\text{H}_2\text{CO}^+ \text{C}_2$	$\text{C}_2\text{H}^+ \text{HCO}$	1.00E-09	0.0	0.0	a
$\text{CH}_2\text{OH}^+ \text{e}$	$\text{H}_2\text{CO} \text{H}$	3.20E-07	-0.5	0.0	13,a,h
$\text{CH}_2\text{OH}^+ \text{e}$	$\text{CO} \text{H} \text{H} \text{H}$	3.20E-07	-0.5	0.0	13,a,h
$\text{CH}_2\text{OH}^+ \text{H}_2\text{O}$	$\text{H}_3\text{O}^+ \text{H}_2\text{CO}$	2.00E-09	0.0	648.8	44,k
$\text{CH}_2\text{OH}^+ \text{NH}_3$	$\text{NH}_4^+ \text{H}_2\text{CO}$	2.30E-09	0.0	0.0	10
$\text{CH}_2\text{OH}^+ \text{HCN}$	$\text{H}_2\text{CN}^+ \text{H}_2\text{CO}$	1.00E-09	0.0	0.0	a
$\text{CH}_2\text{OH}^+ \text{CH}$	$\text{CH}_2^+ \text{H}_2\text{CO}$	1.00E-09	0.0	0.0	a
$\text{CH}_2\text{OH}^+ \text{CH}_2$	$\text{CH}_3^+ \text{H}_2\text{CO}$	1.00E-09	0.0	0.0	a
$\text{CH}_2\text{OH}^+ \text{NH}_2$	$\text{NH}_3^+ \text{H}_2\text{CO}$	1.00E-09	0.0	0.0	a
$\text{CN}^+ \text{e}$	$\text{C} \text{N}$	5.00E-07	-0.5	0.0	a
$\text{CN}^+ \text{CH}_4$	$\text{CH}_2\text{CN}^+ \text{H}_2$	1.00E-09	0.0	0.0	a
$\text{CN}^+ \text{H}_2$	$\text{HCN}^+ \text{H}$	1.24E-09	0.0	0.0	10
$\text{HCN}^+ \text{e}$	$\text{CN} \text{H}$	5.00E-07	-0.5	0.0	a
$\text{HCN}^+ \text{H}_2$	$\text{H}_2\text{CN}^+ \text{H}$	9.00E-10	0.0	0.0	10
$\text{H}_2\text{CN}^+ \text{e}$	$\text{HCN} \text{H}$	2.13E-07	-0.5	0.0	a
$\text{H}_2\text{CN}^+ \text{e}$	$\text{HNC} \text{H}$	2.13E-07	-0.5	0.0	a
$\text{H}_2\text{CN}^+ \text{e}$	$\text{CN} \text{H} \text{H}$	2.13E-07	-0.5	0.0	a
$\text{H}_2\text{CN}^+ \text{NH}_3$	$\text{NH}_4^+ \text{HNC}$	1.10E-09	0.0	0.0	10,a
$\text{H}_2\text{CN}^+ \text{NH}_3$	$\text{NH}_4^+ \text{HCN}$	1.10E-09	0.0	0.0	10,a
$\text{NO}^+ \text{e}$	$\text{N} \text{O}$	2.30E-07	-0.5	0.0	52
$\text{CO}_2^+ \text{e}$	$\text{CO}(3) \text{O}$	8.79E-08	-0.5	0.0	11,a
$\text{CO}_2^+ \text{e}$	$\text{CO} \text{O}(1\text{D})$	2.92E-07	-0.5	0.0	11,a
$\text{CO}_2^+ \text{H}_2\text{O}$	$\text{H}_2\text{O}^+ \text{CO}_2$	2.04E-09	0.0	0.0	39,f
$\text{CO}_2^+ \text{H}_2\text{O}$	$\text{CO}_2\text{H}^+ \text{OH}$	7.56E-10	0.0	0.0	39,f
$\text{CO}_2^+ \text{CH}_4$	$\text{CH}_4^+ \text{CO}_2$	8.80E-10	0.0	0.0	39,f
$\text{CO}_2^+ \text{CH}_4$	$\text{CO}_2\text{H}^+ \text{CH}_3$	2.20E-10	0.0	0.0	39,f
$\text{CO}_2^+ \text{NH}_3$	$\text{NH}_3^+ \text{CO}_2$	2.00E-09	0.0	0.0	39,f
$\text{CO}_2^+ \text{OH}$	$\text{OH}^+ \text{CO}_2$	3.00E-10	0.0	0.0	a
$\text{CO}_2^+ \text{H}_2$	$\text{CO}_2\text{H}^+ \text{H}$	1.40E-09	0.0	0.0	12
$\text{CO}_2^+ \text{H}$	$\text{H}^+ \text{CO}_2$	1.10E-10	0.0	0.0	44

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
$\text{CO}_2^+ \text{ O}$	$\text{O}^+ \text{ CO}_2$	1.00E-10	0.0	0.0	11
$\text{CO}_2^+ \text{ O}$	$\text{O}_2^+ \text{ CO}$	1.60E-10	0.0	0.0	11
$\text{CO}_2^+ \text{ O}_2$	$\text{O}_2^+ \text{ CO}_2$	5.00E-11	0.0	0.0	11
$\text{CO}_2^+ \text{ NO}$	$\text{NO}^+ \text{ CO}_2$	1.20E-10	0.0	0.0	11
$\text{CO}_2\text{H}^+ \text{ e}$	$\text{CO}_2 \text{ H}$	3.20E-07	-0.5	0.0	13,a,h
$\text{CO}_2\text{H}^+ \text{ e}$	$\text{CO} \text{ O} \text{ H}$	3.20E-07	-0.5	0.0	13,a,h
$\text{CO}_2\text{H}^+ \text{ H}_2\text{O}$	$\text{H}_3\text{O}^+ \text{ CO}_2$	3.00E-09	0.0	0.0	43
$\text{CO}_2\text{H}^+ \text{ NH}_3$	$\text{NH}_4^+ \text{ CO}_2$	1.00E-09	0.0	0.0	43,a
$\text{CO}_2\text{H}^+ \text{ CH}_4$	$\text{CH}_5^+ \text{ CO}_2$	7.80E-10	0.0	0.0	43
$\text{CO}_2\text{H}^+ \text{ H}_2\text{CO}$	$\text{CH}_2\text{OH}^+ \text{ CO}_2$	1.00E-09	0.0	0.0	a
$\text{CO}_2\text{H}^+ \text{ HCN}$	$\text{H}_2\text{CN}^+ \text{ CO}_2$	1.00E-09	0.0	0.0	a
$\text{CO}_2\text{H}^+ \text{ CH}_2$	$\text{CH}_3^+ \text{ CO}_2$	1.00E-09	0.0	0.0	a
$\text{CO}_2\text{H}^+ \text{ CO}$	$\text{HCO}^+ \text{ CO}_2$	1.00E-09	0.0	0.0	a
$\text{CH}_4\text{N}^+ \text{ e}$	$\text{HCN} \text{ H}_2 \text{ H}$	2.50E-07	-0.5	0.0	a
$\text{CH}_4\text{N}^+ \text{ e}$	$\text{CN} \text{ H}_2 \text{ H}_2$	2.50E-07	-0.5	0.0	a
$\text{CH} \text{ CH}_4$	$\text{C}_2\text{H}_4 \text{ H}$	2.50E-12	0.0	0.0	48
$\text{CH}_2 \text{ CH}_2$	$\text{C}_2\text{H}_2 \text{ H}_2$	5.30E-11	0.0	0.0	27
$\text{CH}_2 \text{ CH}_3$	$\text{C}_2\text{H}_4 \text{ H}$	5.00E-11	0.0	0.0	17,a
$\text{C}_2\text{H}_3 \text{ H}_2$	$\text{C}_2\text{H}_4 \text{ H}$	5.00E-12	0.0	3200.	17
$\text{C}_2\text{H}_3 \text{ H}$	$\text{C}_2\text{H}_2 \text{ H}_2$	7.00E-12	0.0	0.0	17
$\text{C} \text{ OH}$	$\text{H} \text{ CO}$	4.00E-11	0.0	0.0	13,a
$\text{O} \text{ CH}_3$	$\text{H}_2\text{CO} \text{ H}$	9.00E-11	0.0	0.0	46
$\text{O} \text{ CH}_2$	$\text{CH} \text{ OH}$	8.00E-12	0.0	0.0	49,a
$\text{O} \text{ CH}_2$	$\text{HCO} \text{ H}$	1.00E-11	0.0	0.0	49,a
$\text{CH}_2 \text{ N}$	$\text{HCN} \text{ H}$	4.00E-11	0.0	0.0	49,a
$\text{O} \text{ HCO}$	$\text{CO} \text{ OH}$	1.23E-10	0.0	0.0	30
$\text{O} \text{ HCO}$	$\text{CO}_2 \text{ H}$	8.79E-11	0.0	0.0	30
$\text{HCO} \text{ H}$	$\text{CO} \text{ H}_2$	7.38E-10	0.0	0.0	30
$\text{O} \text{ OH}$	$\text{H} \text{ O}_2$	4.15E-11	0.0	0.0	51
$\text{N} \text{ NH}$	$\text{N}_2 \text{ H}$	4.00E-11	0.0	0.0	13,a
$\text{NH} \text{ C}$	$\text{CN} \text{ H}$	4.00E-11	0.0	0.0	13,a
$\text{N} \text{ CH}$	$\text{CN} \text{ H}$	4.00E-11	0.0	0.0	13,a
$\text{NH} \text{ O}$	$\text{NO} \text{ H}$	4.00E-11	0.0	0.0	13,a
$\text{NH}_2 \text{ O}$	$\text{OH} \text{ NH}$	1.75E-12	0.0	0.0	50,1

Table IV (cont)

Reactants			Products		A	B	C	Refs. and Notes
NH ₂	O		HNO	H	1.75E-12	0.0	0.0	50,1
NO	N		N ₂	O	2.66E-11	0.0	0.0	30
C	O ₂		CO	O	3.30E-11	0.0	0.0	29
C	NO		CN	O	7.30E-11	0.0	0.0	29
N	OH		NO	H	5.81E-11	0.0	0.0	51
OH	OH		O	H ₂ O	1.05E-11	0.0	550.	30
CO	OH		CO ₂	H	9.30E-13	0.0	540.	11
CH	O		CO	H	4.00E-11	0.0	0.0	13,a
CH	O		HCO ⁺	e	1.00E-11	0.0	0.0	47,m
CH	C		C ₂	H	4.00E-11	0.0	0.0	33,a
C ₂	O		CO	C	3.00E-11	0.0	0.0	33,a
CN	O ₂		NCO	O	7.00E-12	0.0	0.0	46
CH	H		C	H ₂	1.00E-14	0.0	0.0	33,a
N	N	CO ₂	N ₂	CO ₂	1.30E-33	0.0	-500.	30
N	O	H ₂ O	NO	H ₂ O	6.90E-32	-0.5	0.0	30
N	O	CO ₂	NO	CO ₂	3.00E-32	-0.5	0.0	30
H	H	M	H ₂	M	8.00E-32	-0.6	0.0	17
CH ₃	H	M	CH ₄	M	8.50E-29	0.0	0.0	17
CH ₃	CH ₃	M	C ₂ H ₆	M	6.00E-29	0.0	0.0	17
C ₂ H ₂	H	M	C ₂ H ₃	M	2.50E-30	0.0	0.0	17
O	H		OH		1.14E-19	0.807	0.0	36,a,n
C	O		CO		1.00E-16	0.0	0.0	31,a
C	C		C ₂		1.00E-16	0.0	0.0	31,a
C	H		CH		8.00E-19	-1.2	0.0	33,a
C	N		CN		2.00E-17	0.0	0.0	11
O(1D)			O		6.80E-03	0.0	0.0	11
O(1D)	H ₂ O		OH	OH	2.10E-10	0.0	0.0	11,26
O(1D)	CO ₂		O	CO ₂	1.20E-10	0.0	0.0	11
O(1D)	NH ₃		NH ₂	OH	3.40E-10	0.0	0.0	11
O(1D)	CH ₄		CH ₃	OH	1.20E-10	0.0	0.0	11
O(1D)	CH ₄		H ₂ CO	H ₂	1.30E-11	0.0	0.0	11
O(1D)	CO		O	CO	5.50E-10	0.0	625.	53
O(1D)	H ₂		OH	H	1.30E-10	0.0	0.0	11
CO(3)			CO		3.10E+02	0.0	0.0	55

Table IV (cont)

Reactants	Products	A	B	C	Refs. and Notes
CO(3) M	CO M	2.00E-10	0.0	0.0	a
C(1D)	C	3.10E-04	0.0	0.0	11
C(1D) CH ₄	C ₂ H ₂ H ₂	3.20E-11	0.0	0.0	54
C(1D) H ₂	CH H	4.15E-11	0.0	0.0	54
C(1D) NO	CN O	9.20E-11	0.0	0.0	54
C(1D) M	C M	2.00E-10	0.0	0.0	a

a Estimate.

b From extrapolation to low temperature of Bates's Table 2 (Ref. 35).

c From detailed balance of reverse reaction.

d $\sim 10^{-10} \text{ cm}^3 \text{ s}^{-1}$ at 100 K is considered an upper limit by Krauss and Julienne (Ref. 20).

e All branches observed with HCO^+ being the major product ion; branching ratios are our estimate.

f Preliminary result.

g These branches in addition to branches proposed by Herbst and Klemperer (Ref. 13), which doubles the overall rate.

h Assumes Herbst and Klemperer (Ref. 13) rate was estimated for 30 K; $T^{-0.5}$ variation.

i Effect of three-body association removed.

j Huntress (Ref. 39) gives a similar preliminary result in which the rate coefficient is $9.6 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$.

k Our estimate for temperature dependence.

l Branching ratios are our estimate.

m Calculated; perhaps a lower limit, especially for our coma temperatures.

n From fit, $T = 200\text{--}300 \text{ K}$.

C. Combining Physics and Chemistry

In the computer model the physical and chemical processes are analyzed in a thin spherical shell of coma gas as it expands and moves radially outward. Chemical reactions take place in a continually diluting gas exposed to a continually less attenuated solar ultraviolet flux. Because of the motion and progressive dilution of the gas, many reactions will not reach steady-state conditions so that the abundances of some species, that otherwise might have undergone further reactions, will "freeze-in."

III. PARAMETERS

The size of the nucleus, its albedo, and infrared emissivity are not known for P/Halley and most other comets. We have adopted a standard set of values in agreement with other investigators (Ref. 2). For this standard nucleus the mean radius is $R_0 = 2.5$ km, its visual albedo $A = 0.3$, and its infrared emissivity is assumed to be $\epsilon = 1-A = 0.7$. Extreme values for the nuclear mean radius are thought to be 0.5 km and 5.0 km. Extremes for the visual albedo are assumed to be $A = 0.1$ and $A = 0.7$. The corresponding values for the infrared emissivity are assumed to be $\epsilon = 1-A$. Gas production rates, Z , consistent with chemical composition 6a are given in Table V. For this composition and the standard nucleus the total gas production rate at $r = 1$ AU is $Q = 4\pi R_0^2 Z = 2.8 \times 10^{29}$ molecules s^{-1} . This is about 2/3 more than the predicted nominal gas production of $1.7 \times 10^{29} s^{-1}$ (see Ref. 2).

Table V

r(AU)	Gas Production Rates, $Z(10^{17} \text{ Molecules cm}^{-2} \text{ s}^{-1})$			
	A			
	0.1	0.3	0.5	0.7
0.6	13.5	10.5	7.53	4.53
1.0	4.60	3.59	2.58	1.56
1.5		1.47		
2.0		0.715		
3.0	0.262	0.211	0.157	0.0997
5.0		0.00843		

IV. RESULTS

In trying to assimilate a consistent picture of comet Halley from the model presented here, establishment of some type of systematic criterion is required for comparison with the 1910 observations. It is difficult at best to make any direct correlations between intensities of spectral images and column densities. An attempt to compare observational plates from the 1910 apparition (and inferences made thereof) to the computer model's column density predictions would be particularly difficult because of the suspect quality of the 1910 observations as discussed in Sec. I. However, to facilitate understanding and thus determine the correct behavior of the model in relation to the 1910 apparition, a lower cutoff in column density of about 10^{11} CN or C_2 molecules cm^{-2} is somewhat arbitrarily imposed for the purpose of comparing with the observed intensities. It is felt that this limit is entirely reasonable in view of observations of more recent comets. Similar arguments hold for C_3 for the unmodified composition 6a (as given in Table II), assuming the incorrect oscillator strength that is too low by a factor ~ 40 . For the modified composition 6a' (assuming the correct oscillator strength), the cutoff limit for C_3 has to be lowered by a factor of about 40. A further, but somewhat arbitrary, criterion is that when not dealing explicitly with envelope extent as delineated by the coma projection distance ρ , all column density values are given as averaged out to $\rho \approx 10^4$ km. That this approach is meaningful can be seen from the fact that most of the physics and chemistry occurs within this distance, thereby giving credence to this value of ρ and the averaged column densities.

To discuss the results in a logically ordered manner, attention will be focused on the "standard" model of comet Halley; i.e. -- a 2.5-km nuclear radius and visual albedo $A = 0.3$, and a Z of $\sim 10^{17}$ - 10^{18} molecules $cm^{-2}s^{-1}$ at 1 AU. The extremes considered in this study can then be viewed in relation to this standard, allowing for a better picture of P/Halley and thus refinements in the model. As an aid in comparing the model's results to the 1910 observational sketch as given in Table I, a similar, though discussion orientated, trace will be made here.

At a comparable heliocentric distance of 3.0 AU (Fig.1) the standard nucleus exhibits a faint, small halo (~ 4 to 5×10^3 km) of CN. Though below the imposed lower cutoff in column density, C_3 is such that a faint observation is

possible. C_2 on the other hand, being an order of magnitude lower than C_3 , should not be visible, supporting the argument² that C_2 was only doubtfully seen at this distance.

Coming to 2.0 AU (Fig.2) one finds CN and C_3 visible with envelope extensions of ~ 1 to 2×10^5 km and ~ 2 to 3×10^4 km, respectively. C_2 is still below cutoff by roughly a factor of 4.

By 1.0 AU (Fig.2) C_2 becomes visible with a coma dimension of $\sim 2 \times 10^5$ km. For CN and C_3 we have envelope sizes of ~ 4 and 2×10^5 km, respectively. In the inner coma out to approximately 6×10^4 km, C_3 has clear dominance over C_2 , thereafter C_2 becomes dominant and approaches (within a factor of 2 to 3) CN abundances in the far outer regions. One can easily notice (Figs.3 and 4) that for larger nuclear radii this crossing distance (C_3 to C_2 dominance) diminishes, the reverse being true for smaller radii. C_2 production has thus increased in relation to CN, C_3 , and OH as can be seen in Fig.5. Up to this point, CN, C_3 , and OH have exhibited similar behavior, and readily seen is the steepening slope of C_2 in relation to these species; C_2 is on a faster rise, giving some credence to the argument¹ that an actual spectral change occurred around 1 to 1.2 AU. Fig.6 exhibits this rise in C_2 for the extremes in nuclear radii. Note the slightly more acute slope for the larger nuclear radii on approach to the Sun. C_2 production is thus apparently favored by larger nuclear sizes. Referring to the sequential plots (Figs.7 through 10) shows this effect quite nicely, with OH/CN, OH/ C_3 , and CN/ C_3 ratios remaining roughly constant and C_2 rising (sharper for larger R_0) in relation.

Perihelion being at approximately 0.6 AU for P/Halley (Fig.1) shows the standard model exhibiting strong CN and C_2 (comparable) in the outer coma (envelope dimensions both $\leq 5 \times 10^5$ km). The C_3 - C_2 dominance crossing distance has decreased to $\sim 10^4$ km with the C_3 halo having an $\sim 10^5$ -km size.

Thus far discussion has been made concerning only the species CN, C_2 , C_3 , and OH, but what of the ionic behavior? Of particular interest, two ionic species, H_2O^+ and CO^+ should be noted. Fig.11 shows these species' variations with heliocentric distance for three nuclear dimensions; 5.0 km, 2.5 km, and 0.5 km. Note the changes in slope and dominance with respect to nuclear size. In relation to similar plots (Figs.5 and 6) for the neutrals the ionic behavior is noticeably different.

The standard model in these ions is shown in Fig.12 for these heliocentric distances. Again, with approach to the Sun, the dominance crossing distance decreases (a limit being reached at ~ 1.0 AU), CO^+ the stronger in the outer regions. A rather strange effect can easily be seen in this plot; with solar approach CO^+ and H_2O^+ are significantly depleted in the far coma yet increasingly abundant in the inner regions. This could possibly be explained if solar wind loading and ionic sweep out were taken into account, however, in this present model they are not. Evidently, this then is an intrinsic effect, explainable on physio-chemical grounds.

At a given heliocentric distance (such as 1.0 AU in Fig.13) one sees roughly the same behavior in these ions over the ranges of nuclear sizes considered, the only difference being the crossing distance of dominance shift in H_2O^+ and CO^+ ; larger nuclear radii yielding increasing crossing distance (the opposite effect of the neutrals considered).

Figs.14-18 give information on variation with albedo for the neutrals mentioned above. One can see that similar behavior is exhibited by all of these species. No significant variation is apparent with respect to either nuclear size or heliocentric distance. At a given heliocentric distance and for a particular nuclear radius a variation in albedo of 0.1 to 0.7 simply decreases the abundance by roughly a factor of 3 (about the same for all species shown).

The first 18 figures are based on composition 6a. Fig.19 is for composition 6a'. Since the relative abundances of C_2H_2 and $\text{H}_2\text{C}_3\text{H}_2$ are very small, the changes in these abundances affect only the production of C_3 ; the other observable species remain essentially unchanged. The C_3 curves could thus be scaled down by a factor of 40 in Figs. 1-10 and 14-18 without affecting the other curves. This is borne out by the results of test calculations presented in Fig.19 that can be compared with Fig.5.

V. CONCLUSIONS

The model with the standard size nucleus, $R_0 = 2.5$ km, compares favorably with the observations from 1910. The smallest nucleus, $R_0 = 0.5$ km, compares least favorably, giving column densities which are too low even for the relatively volatile composition assumed here. Results from the model are too insensitive to indicate a preference for albedo and emissivity. The column

density profiles are nearly flat, increasing only very slowly with decreasing projected distance from the nucleus. Thus, a spacecraft approaching the nucleus from a distance less than a few 10^4 km will "see" only very small changes in the intensity of C_2 , C_3 , CN, OH, and most other molecular radicals.

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Fig.1
Column density vs. projected distance in coma for the standard model (2.5 km nuclear radius, $A = 0.3$) in CN, C_2 , and C_3 at two heliocentric distances: solid line $r = 3.0$ AU, dashed line $r = 0.6$ AU.

Fig.2
Column density vs. projected distance in coma for the standard model (2.5 km nuclear radius, $A = 0.3$) in CN, C_2 , and C_3 at two heliocentric distances: solid line $r = 2.0$ AU, dashed line $r = 1.0$ AU.

Fig.3
Column density vs. projected distance in coma for the extremes in nuclear radius in CN, C_2 , and C_3 at $r = 1.0$ AU heliocentric distance and with $A = 0.3$: dotted line $R_0 = 5.0$ km, chain-dashed line $R_0 = 0.5$ km.

Fig.4
Column density vs. projected distance in coma for intermediate nuclear radii in CN, C₂, and C₃ at $r = 1.0$ AU heliocentric distance and with $A = 0.3$: dotted line $R_0 = 3.5$ km, chain-dashed line $R_0 = 1.5$ km.

Fig.5
Column densities averaged to $\rho = 10^4$ km of CN, C₂, C₃, and OH as a function of heliocentric distance for the standard model. Note the steepening slope of C₂ relative to the other constituents at small heliocentric distances.

Fig.6
Column densities averaged to $\rho = 10^4$ km of CN, C₂, C₃, and OH as a function of heliocentric distance for the extremes in nuclear radius: dotted line $R_0 = 5.0$ km, chain-dashed line $R_0 = 0.5$ km.

Fig.7
Column densities averaged to $\rho = 10^4$ km of CN, C₂, C₃, and OH as a function of nuclear radius with $A = 0.3$ at a heliocentric distance $r = 3.0$ AU.

Fig.8
Column densities averaged to $\rho = 10^4$ km of CN, C₂, C₃, and OH as a function of nuclear radius with $A = 0.3$ at a heliocentric distance $r = 2.0$ AU.

Fig.9
Column densities averaged to $\rho = 10^4$ km of CN, C₂, C₃, and OH as a function of nuclear radius with $A = 0.3$ at a heliocentric distance $r = 1.0$ AU.

Fig.10
Column densities averaged to $\rho = 10^4$ km of CN, C₂, C₃, and OH as a function of nuclear radius with $A = 0.3$ at a heliocentric distance $r = 0.6$ AU.

Fig.11
Column densities averaged to $\rho = 10^4$ km of H₂O⁺ and CO⁺ as a function of heliocentric distance for three nuclear radii (with $A = 0.3$): dotted line $R_0 = 5.0$ km, solid line $R_0 = 2.5$ km, and chain-dashed line $R_0 = 0.5$ km.

Fig.12
Column density vs. projected distance in coma for the standard model in H₂O⁺ and CO⁺ for three heliocentric distances: dashed line $r = 0.6$ AU, solid line $r = 1.0$ AU, and chain-dotted line $r = 2.0$ AU.

Fig.13
Column density vs. projected distance in coma for the ions H_2O^+ and CO^+ at $r = 1.0$ AU heliocentric distance with $A = 0.3$ for three nuclear radii: dotted line $R_0 = 5.0$ km, solid line $R_0 = 2.5$ km, and chain-dashed line $R_0 = 0.5$ km.

Fig.14
Column density vs. albedo A for a nucleus with radius $R_0 = 2.5$ km at $r = 1.0$ AU heliocentric distance. Column densities averaged to $\rho = 10^4$ km.

Fig.15
Column density vs. albedo A for the extremes in nuclear radii (dotted line $R_0 = 5.0$ km, chain-dashed line $R_0 = 0.5$ km) at $r = 3.0$ AU heliocentric distance. Column densities averaged to $\rho = 10^4$ km.

Fig.16
Column density vs. albedo A for the extremes in nuclear radii (dotted line $R_0 = 5.0$ km, chain-dashed line $R_0 = 0.5$ km) at $r = 0.6$ AU heliocentric distance. Column densities averaged to $\rho = 10^4$ km.

Fig.17
Column density vs. nuclear radius R_0 for the extremes in albedo (solid line $A = 0.7$, chain-dotted line $A = 0.1$) at $r = 3.0$ AU heliocentric distance. Column densities averaged to $\rho = 10^4$ km.

Fig.18
Column density vs. nuclear radius R_0 for the extremes in albedo (solid line $A = 0.7$, chain-dotted line $A = 0.1$) at $r = 0.6$ AU heliocentric distance. Column densities averaged to $\rho = 10^4$ km.

Fig.19
Column densities averaged to $\rho = 10^4$ km of CN, C, C_3 , and OH as a function of heliocentric distance for the standard model composition 6a'. For this, the initial abundance of C_2H_2 has been increased from 0.1% to 0.16% and $H_2C_3H_2$ has been reduced from 0.2% to 0.005% (see Sec. II B). Compare with Fig.5 for the unmodified composition 6a.