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CALCULATION OF THERMODYNAMIC AND OPTICAL PROPERTIES OF THE VAPORS OF COSMIC BODIES ENTERING THE EARTH'S ATMOSPHERE

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A procedure for calculating thermodynamic and optical properties of the vapors of cosmic bodies entering the earth's atmosphere is described. Calculations were carried out on the basis of a mixture of the 16 elements Fe–O–Mg–Si–C–N–H–S–Al–Ca–Na–K–Ti–Cr–Mn–Ni for bodies of different chemical composition: H-, LL-, and C-chondrites, comet matter, and ice in the temperature range of 2–40 kK. The scale of quanta energies used in calculations of spectral absorption coefficients numbered approximately 22 thousand points. Examples of calculations are given.

In order to calculate thermal radiation and determine the rate of ablation of cosmic bodies entering the atmospheres of planets it is necessary to know the optical properties of the vapors of these bodies.

In [1] thermodynamic and optical characteristics are given for a number of multicomponent gas mixtures in a wide range of the parameters, including those of the planetary atmosphere. Below, a procedure is developed for calculating these properties for some particular types of cosmic bodies.

Earlier, optical properties of the vapors of cosmic bodies were calculated for an iron body [2] and H-chondrite [3]. We increased the number of types of substances considered. Moreover, calculation of the chemical composition and optical properties was carried out on the basis of 16 elements: Fe–O–Mg–Si–C–N–H–S–Al–Ca–Na–K–Ti–Cr–Mn–Ni. The addition of several elements, especially metals, is due to the fact that the spectra of meteoroids display a considerable number of bright lines of the atoms of these metals and their ions [4].

For the purpose of the most inclusive coverage of cosmic bodies that differ in their strength and thermophysical characteristics and chemical composition, calculations were carried out for the following types of bodies: H-, L-, and LL-chondrites, which are distinguished by a high content of iron and its oxide [5], carbonaceous (C-) chondrites, ice, and comet matter. The latter is understood here to represent a mixture of ice and chondrite dust; it was suggested earlier for modeling the properties of the matter of Halley's comet [6] (see Table 1).

The composition of a chemically reacting, dissociating, and ionizable medium is calculated under the assumption of local thermodynamic equilibrium. In the molecular region, at a temperature $T \leq 10^4$ K about 230 gaseous components are taken into account (see Table 2). A specific chemical composition for each pair of values of density and temperature is determined by solving a system of equations of chemical and ionization equilibrium with account taken of electroneutrality and preservation of the number of nuclei of each element.

Here the system considered can be written in the form

$$\sum_m b_{k,m} \sum_q n_{m,q} = N_k \, , \quad \sum_m \sum_q q n_{m,q} = N_e \, ,$$

$$n_{m,0} = K_{m,0} \prod_{k=1} n_{k,0}^{b_{k,m}} \, ,$$

$$n_{m,q} = K_{m,q} n_{m,q-1} / N_e \quad \text{for } q > 0 \text{ (positive ions)} \, ,$$

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TABLE 1. Weight Content of Chemical Elements for Various Types of Cosmic Bodies (%)

Element	H-chondrite	LL-chondrite	C1-chondrite	Comet matter
1. Fe	27.54	19.74	18.7	4.54
2. O	33.65	38.59	45.58	51.01
3. Mg	14.08	15.29	9.73	3.8
4. Si	17.17	19.08	10.45	8.12
5. C	0.11	0.22	3.38	18.94
6. H	0.049	0.079	1.97	6.35
7. S	1.99	2.12	6.14	3.61
8. N	–	–	0.31	2.08
9. Al	1.137	1.19	0.85	0.287
10. Ca	1.248	1.38	0.91	0.395
11. Na	0.64	0.709	0.49	0.359
12. K	0.075	0.084	0.055	0.012
13. Cr	0.271	0.282	0.262	0.073
14. Mn	0.237	0.087	0.048	0.034
15. Ti	0.072	0.078	0.043	0.03
16. Ni	1.72	1.06	1.06	0.37

$$n_{m,-1} = K_{m,-1} n_{m,0} N_e \quad \text{for } q = -1 \quad \text{(negative ions)}.$$

In these equations the equilibrium constants are functions of temperature and density; they are proportional to the ratio of the statistical sums of the corresponding components. The values of the quantities $K_{m,q}$ are taken from the tables of [7, 8] or are calculated in the "harmonic oscillator–rigid rotator" approximation for molecules or in the Debye approximation in a large canonical ensemble for the Saha ionization equations [9].

To solve this system of nonlinear algebraic equations, an efficient algorithm that employs inserted iterations over electrons and the concentrations of the particles that predominate in the mixture is used.

The thermodynamic functions of one mole of gas of the i-th component consisting of identical molecules are connected with the values of the statistical sum and its derivatives by the following relations [6]:

$$\text{entropy of gas} \quad S(T) = R \ln \frac{Q(T)}{N_A} + RT \frac{\partial \ln Q(T)}{\partial T},$$

$$\text{enthalpy} \quad H(T) = H(0) + RT^2 \frac{\partial \ln Q(T)}{\partial T},$$

$$\text{internal energy} \quad E(T) = H(T) - RT.$$

In the present work the absolute enthalpy $H(T)$, whose reference point is unknown, is replaced (as is the case in thermochemical calculations) by the so-called total enthalpy

$$H_t^{(i)}(T) = \Delta_f H(T_0) + H(T) - H(T_0),$$

where $H(T) - H(T_0) = [H(T) - H(0)] - [H(T_0) - H(0)]$.

Carrying out summation over the mixture components, we obtain its specific enthalpy

$$H_t(T) = \frac{1}{\mu} \sum X_i H_t^{(i)}(T)$$

and pressure

$$P = \sum X_i NkT.$$

To determine the spectral absorption coefficients, it is necessary to sum up the contributions of the different types of radiative transitions: free–free, bound–free, and bound–bound. The types of dominating processes change substantially with temperature and depend on the spectral interval.

TABLE 2. Components Included in Thermochemical Calculations

1. Fe
2. O
3. Mg
4. Si
5. C
6. H
7. SiO
8. O_2
9. CO
10. H_2
11. C_2
12. C_3
13. CH
14. CH_2
15. CH_3
16. CH_4
17. CO_2
18. C_2O
19. C_3O_2
20. CHO
21. CH_2O
22. CHO_2
23. H_2CO
24. H_2CO_2
25. CH_3O
26. CH_2OH
27. CH_3OH
28. C_2H_5OH
29. C_4
30. FeO
31. $Fe(OH)_2$
32. H_2O
33. H_2O_2
34. OH
35. HO_2
36. MgH
37. MgOH
38.$Mg(OH)_2$
39. MgO
40. N
41. N^+
42. N_2
43. N_2^+
44. SN
45. NO
46. NO_2^-
47. Si_2
48. SiH
49. SiH_2
50. SiH_3
51. SiH_4
52. SiO_2
53. SiC
54. Si_2C
55. SiC_2
56. FeC
57. FeH
58. O_3
59. C_2H
60. C_2H_2
61. C_2H_3
62. C_2H_4
63. C_4H
64. C_3H
65. FeSi
66. Fe_2
67. C_2H_5
68. C_2H_6
69. S
70. MgS
71. SiS
72. SiS_2
73. CS
74. CS_2
75. COS
76. S_2
77. S_3
78. S_4
79. S_8
80. SO
81. SO_2
82. SO_3
83. S_2O
84. N_2O
85. NH
86. CN
87. HCN
88. N_3
89. N_2O_3
90. N_2O_4
91. N_2O_5
92. NH_2
93. SH
94. H_2S
95. Al
96. Al_2
97. AlO
98. AlO_2
99. Al_2O
100. Al_2O_2
101. Al_2O_3
102. AlH
103. AlH_2
104. AlH_3
105. AlOH
106. $Al(OH)_2$
107. $Al(OH)_3$
108. AlS
109. AlS_2
110. Al_2S
111. Al_2S_2
112. AlC
113. AlC_2
114. Al_2C_2
115. Ca
116. CaO
117. CaH
118. CaOH
119. $Ca(OH)_2$
120. CaS
121. Na
122. Na_2
123. NaO
124. Na_2O
125. Na_2O_2
126. NaH
127. NaOH
128. NH_3
129. NH_4^+
130. N_2H_2
131. N_2H_4
132. HN_3
133. HNO
134. HNO_2
135. HNO_3
136. NO^+
137. NH^+
138. CN^+
139. FeS
140. AlN
141. SiN
142. KO
143. K_2O
144. K_2
145. Ti
146. Cr
147. Mn
148 Ni
149. CrO
150. CrO_2
151. CrO_3
152. MnO
153. NiO
154. TiO
155. TiO_2
156. Fe^+
157. O^+
158. Mg^+
159. Si^+
160. C^+
161. H^+
162. Fe_2^+
163. Fe_2^-
164. Fe^-
165. O_2^+
166. O_2^-
167. O^-
168. Si_2^+
169. Si^-
170. C_2^-
171. C_2^+
172. C^-
173. H_2^+
174. H_3^+
175. H^-
176. NO_2^-
177. NO_3^-
178. Fe^{2+}
179. O^{2+}
180. Mg^{2+}
181. Si^{2+}
182. C^{2+}
183. S^{2+}
184. Al^{2+}
185. CH^+
186. CO^+
187. CO_2^+
188. OH^+
189. OH^-
190. H_2O^+
191. H_3O^+
192. HO_2^-
193. FeO^-
194. FeH^+
195. SiH^+
196. S^-
197. S_2^-
198. SO^-
199. SO_2^-
200. SH^-
201. AlO^-
202. AlO_2^-
203. CaO^+
204. $CaOH^+$
205. Na_2O
206. CrO_3^-
207. K_2^+
208. K_2O^+
209. K_2O_2
210. KH
211. KOH
212. TiO^+
213. S^+
214 Al^+
215. Ca^+
216. Na^+
217. K^+
218. Cr^+
219. Mn^+
220. Ti^+
221. Ni^+
222. Ca^{2+}
223. Na^{2+}
224. K^{2+}
225. Cr^{2+}
226. Mn^{2+}
227. Ti^{2+}
228. Ni^{2+}
229. e

Transitions in electron-vibrational bands, photodissociation and photoionization of molecules and molecular ions, photoabsorption of negative ions, and bremsstrahlung absorption in electron scattering on neutral and charged particles are the main mechanisms that determine molecular absorption.

Using the mean value of the rotational frequencies and the distance between the lines with account for the summation rule for rotational lines, for the value of the absorption cross section of the electron-vibrational band $mv'' - nv'$ averaged over the rotational structure it is possible to write [10-12] (the "just overlapping lines" model) in cm^2

$$\sigma(\nu) = 2.69 \cdot 10^{-18} \frac{\nu\,(2S_t + 1)\,(2 - \delta_{0,\Lambda' + \Lambda''})}{Q_\Sigma} \exp\left(-\frac{1.44 E_e''}{T}\right) \left[1 - \exp\left(-\frac{1.44\nu}{T}\right)\right] \times$$

$$\times \sum_{v''} \sum_{v'} q_{v'v''} \frac{(R_e^{v'v''})^2}{|\Delta B_v|} \exp\left\{-\frac{1.44}{T}\left[\frac{B_v''}{\Delta B_v}(\nu - \omega_{v''v'} - B_v') + E_v'\right]\right\}.$$

Here

$$B_v = B_e - \alpha_e (v + 1/2) + \gamma_e (v + 1/2)^2 + \ldots$$

$$E_v = \omega_e (v + 1/2) - \omega_e X_e (v + 1/2)^2 + \ldots\ .$$

In carrying out the summation, only terms that satisfy the condition of shading of bands are taken into account:

$$\begin{cases} \omega > \omega_{v'v''} & \text{for} \quad B_v'' < B_v' , \\ \omega < \omega_{v'v''} & \quad B_v'' > B_v' , \end{cases}$$

where $\omega_{v'v''} = \Delta E_e + \Delta E_v$.

For diatomic molecules, absorption in the following transitions was taken into account:

O_2 : $X^3\Sigma \longrightarrow B^3\Sigma$ (the Schumann–Runge system + photodissociation) ,

FeO : $X^5\Delta \longrightarrow a^5\Phi_i$, $X^5\Delta \longrightarrow a^5\Pi_i$, $X^5\Delta_i \longrightarrow {}^5\Delta_I$, ${}^5\Sigma^+ \longrightarrow a^5\Pi_i$,

MgO : $X^1\Sigma^+ \longrightarrow B^1\Sigma$, $A^1\Pi \longrightarrow B^1\Sigma^+$, $X^1\Sigma^+ \longrightarrow A^1\Pi$,

SiO : $X^1\Sigma \longrightarrow A^1\Pi$, $X^1\Sigma \longrightarrow E^1\Sigma$,

CO : $X^1\Sigma^+ \longrightarrow A^1\Pi$, $X^1\Sigma^+ \longrightarrow B^1\Sigma$, $X^1\Sigma \longrightarrow C^1\Sigma$,

$A^1\Pi \longrightarrow B^1\Sigma^+$, $A^1\Pi \longrightarrow C^1\Sigma$; $X^1\Sigma^+ \longrightarrow E^1\Pi$,

$a^3\Pi \longrightarrow b^3\Sigma$, $a^3\Pi \longrightarrow e^3\Sigma^-$, $a^3\Pi \longrightarrow a'^3\Sigma$,

$a^3\Pi \longrightarrow C^3\Pi$, $a^3\Pi \longrightarrow d^3\Delta$,

CO^+ : $X^2\Sigma^+ \longrightarrow B^2\Sigma^+$, $A^2\Pi \longrightarrow B^2\Sigma^+$, $X^2\Sigma \longrightarrow B^2\Sigma$,

H^2 : $X^1\Sigma_g^+ \longrightarrow B^1\Sigma_u^+$, $X^1\Sigma_g^+ \longrightarrow C^1\Pi_u$,

MgH : $X^2\Sigma^+ \longrightarrow A^2\Pi$, $X^2\Sigma \longrightarrow C^2\Pi$, $A^2\Pi \longrightarrow C^2\Pi$,

OH : $X^2\Pi \longrightarrow A^2\Sigma$, $A^2\Sigma^+ \longrightarrow B^2\Sigma^+$,

FeH : $X^4\Delta \longrightarrow F^4\Delta$, $X^4\Delta \longrightarrow H^4\Delta$, $A^4\Pi \longrightarrow E^4\Pi$,

$A^4\Pi \longrightarrow G^4\Pi$, $a^6\Delta \longrightarrow e^6\Pi$, $a^6\Delta \longrightarrow g^6\Phi$, SiH : $X^2\Pi \longrightarrow A^2\Delta$, $X^2\Pi \longrightarrow B^2\Sigma$, $X^2\Pi \longrightarrow C^2\Sigma$,

SiH$^+$: $X^1\Sigma \longrightarrow A^1\Pi$,

CS : $X^1\Sigma^+ \longrightarrow A^1\Pi$,

SiS : $X^1\Sigma \longrightarrow D^1\Pi$, $X^1\Sigma^+ \longrightarrow E^1\Sigma$,

S$_2$: $X^3\Sigma_g^- \longrightarrow B^3\Sigma_4^-$

SO : $X^3\Sigma^- \longrightarrow A^3\Pi$, $X^3\Sigma^- \longrightarrow B^3\Pi$,

SH : $X^2\Pi \longrightarrow A^2\Sigma^+$,

CrO : $X^5\Pi \longrightarrow B^5\Pi$,

MnO : $X^6\Sigma^+ \longrightarrow A^6\Sigma^+$,

TiO : $X^3\Delta \longrightarrow C^3\Delta$, $a^1\Delta \longrightarrow C^1\Phi$, $X^3\Delta \longrightarrow B^3\Pi$,
$X^3\Delta \longrightarrow A^3\Phi$, $X^3\Delta \longrightarrow E^3\Pi$, $a^1\Delta \longrightarrow b^1\Pi$, $d^1\Sigma \longrightarrow b^1\Pi$,

AlO : $X^2\Sigma^+ \longrightarrow B^2\Sigma^+$, $X^2\Sigma^+ \longrightarrow A^2\Pi$, $B^2\Sigma^+ \longrightarrow A^2\Pi$,

AlH : $X^1\Sigma \longrightarrow A^1\Pi$, $X^1\Sigma \longrightarrow C^1\Sigma$,

CaO : $X^1\Sigma \longrightarrow A^1\Sigma$, $X^1\Sigma \longrightarrow B^1\Pi$, $X^1\Sigma \longrightarrow C^1\Sigma$,

CaH : $X^2\Sigma \longrightarrow A^2\Pi$, $X^2\Sigma \longrightarrow B^2\Sigma$,

NaH : $X^1\Sigma^+ \longrightarrow A^1\Sigma^+$, $X^1\Sigma^+ \longrightarrow B^1\Pi$,

Na$_2$: $X^1\Sigma_g^+ \longrightarrow A^1\Sigma_4^+$, $X^1\Sigma_g^+ \longrightarrow B^1\Pi_4$.

The necessary spectroscopic constants, Franck–Condon factors, and strengths of electron transitions were taken from [7–13], and those for oxides of transition metals were taken from [14, 15]. In the absence of tables of Franck–Condon factors for some molecules, they were calculated on the basis of the Morse potential using existing spectroscopic constants.

Absorption in the processes of the photodissociation and photoionization of molecules was determined from approximation formulas given in [1, 12, 16].

Absorption in the fundamental bands and overtones of diatomic molecules was calculated in the approximation of total overlap of rotational lines [12, 16] with account for the data of [13].

A quantitative description of absorption in the bands of multiatomic molecules, such as water and carbon dioxide, is very important for calculation of radiative transfer in the infrared region of the spectrum, especially for ice bodies, comet matter, and carbonaceous chondrites, in which their content is quite high. Calculations of the absorption of water vapor and carbon dioxide are based on the use of parameters that have been found by now for the bands of these molecules [13]. The coefficient of absorption in a band in the approximation of total overlap of lines is

$$k_\nu(T) = \frac{\alpha(T)}{w(T)}\,\varphi(\nu, T).$$

For SO$_2$-type molecules, which are slightly asymmetric rotators, the following function was used as the shape of the contour [17]:

$$\varphi(\nu, T) = \frac{hc\nu}{kT}\sqrt{\left(\frac{AC}{B(A-B)}\right)}\;\Phi\left(\sqrt{\left(\frac{(A-B)\,hc}{kT}\,\frac{\nu}{2B}\right)}\right)\exp\left(-\frac{hc\nu^2}{4BkT}\right).$$

The photoabsorption cross sections for atoms and atomic ions of various multiplicities of ionization were calculated by means of wave functions of discrete and continuous spectra calculated by the Hartree–Fock method of a self-consistent field [18]. The photoionization cross sections of the shell $nl^{N\,2S+1}L$ were calculated according to [19, 20] (an atomic system of units is used):

$$\sigma_{nl}(\omega) = \frac{8\pi^2 N_{nl}}{3\omega c(2l+1)} \sum_{L'} \left(|D^{LL'}_{nl,\varepsilon l+1}|^2 + |D^{LL'}_{nl,\varepsilon l-1}|^2 \right).$$

To take account of correlations in calculations of the photoionization of multielectron shells the approximation of random phases with exchange [20] was used, in which the effective dipole moment D_{eff} is obtained by solving an integral equation that uses Hartree–Fock $D_{nl,\varepsilon l'}$ as a first approximation.

In the relativistic variant used to calculate the cross sections for continuous absorption in heavy elements the cross section of the shell nlj^N was determined from the formula (see, e.g., [20])

$$\sigma_{nlj}(\omega) = \frac{8\pi^2 N_{nlj}}{3\omega c(2j+1)} \left(|D_{jj+1}|^2 + |D_{jj}|^2 + |D_{jj-1}|^2 \right),$$

in which the dipole matrix elements D_{jj} were calculated using the large and small components of the relativistic wave function of an electron [18].

Radiation-gasdynamic calculations show that an appreciable portion of the radiated (or absorbed) energy is due to line radiation. Data on the strengths of the oscillators of the spectral lines were taken from [21, 22] or were calculated using wave functions [18]. Energy levels were taken from tables [23, 24] or, in their absence, were obtained by quantum-mechanical calculations.

The absorption cross section in a spectral line is determined by both the value of the corresponding strength of the oscillator and its contour, which depends on the mechanism of broadening due to the interaction of the radiating atom with the plasma particles surrounding it (the conventional notation will be followed here):

$$\sigma_{ll'}(\omega) = \frac{2\pi^2 e^2}{mc} f_{ll'}\, \varphi(\omega, T),$$

in which the contour of the line is a convolution of the electronic impact contour with the Doppler contour. For the case of high plasma densities the contour is supplemented with normalized additives due to the contribution of forbidden components [23]. For still higher densities the contour of the line becomes hydrogen-like.

Electron impact widths are calculated according to [25, 26]. In calculating the impact width of a line of an atom that is perturbed by neutral particles of plasma the interaction potential is assumed to be the van der Waals one. But in the case of broadening by hydrogen atoms, the dipole–dipole interaction was taken into consideration [25], and this increased the width of the line severalfold in comparison with the van der Waals mechanism of interaction. The corresponding width of the line is

$$\gamma = \alpha T^{\beta} n_{\text{H}}.$$

Inclusion of this mechanism of broadening increases the absorption in the lines at low temperatures, where the density of electrons is low and the density of hydrogen atoms is appreciable, for example, in comet matter and in C-chondrites.

The main influence of the plasma environment on the optical characteristics in the case of a slightly nonideal plasma amounted to deformation of the contour due to the appearance of forbidden components, a shift in the spectral lines, and a shift in the threshold of photoionization to the side of low energies [27]. For spectra of complex atoms a relation from [28] was used as a criterion for a confluence of lines.

To calculate statistical sums in the case of high densities of plasma and high nonideality of it, a form factor determined from the microfield model of plasma was introduced [29, 30].

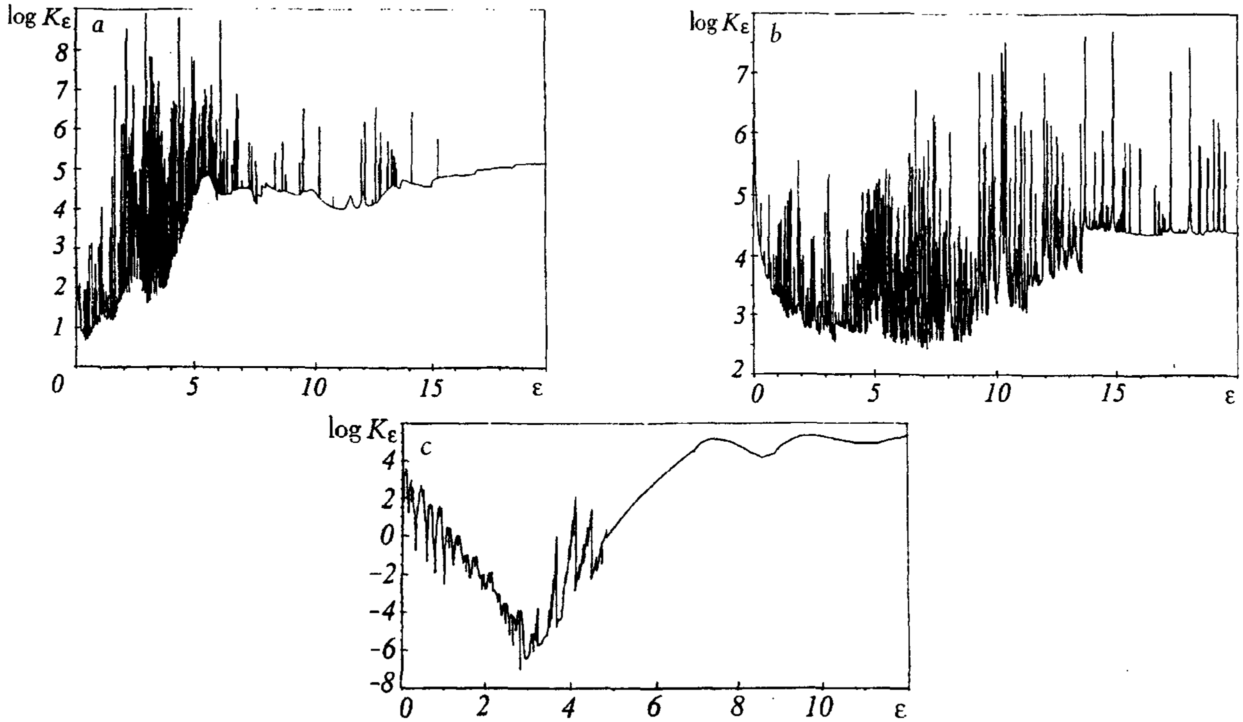

Fig. 1. Dependence of the spectral mass coefficient of absorption K_ε on the energy of the photons ε for the vapors of H-chondrite (a), comet matter (b), and water (c): a) $T = 4$ kK, $\rho = 1.09 \cdot 10^{-5}$ g/cm^3; b) 20 and $3.7 \cdot 10^{-6}$; c) 2 and $8 \cdot 10^{-6}$. K_ε, cm^2/g; ε, eV.

In the present work a model of effective populations of atomic levels in plasma microfields is used to describe the continuous spectrum in the near-threshold region [30]. A discrete level is realized with a certain probability W that depends on the plasma microfields, and the spectral lines emitted from this level are diminished in proportion to W. For each term of the spectral series that converges to the given threshold, the quantity $1 - W$ means the probability of the appearance of the state of the continuous spectrum instead of the upper state of the transition and, correspondingly, the probability of the appearance of the continuous spectrum instead of the line.

To approximate W, for example, in the case of atomic lines, the following empirical relation [31] was used:

$$W(\chi) = \begin{cases} 1.06 \exp(-4.26\chi), & 0.03 \le \chi \le 0.1, \\ 1.33 \exp(-6.56\chi), & 0.1 \le \chi \le 0.5, \end{cases}$$

where $\chi = 1.168 \cdot 10^{-15} n_e^{2/3} (nn^*)^2$. This relation is extrapolated to the region $0.01368 \le \chi \le 2$; $W = 1$ when $\chi < 0.01368$, and $W = 0$ when $\chi > 2$. The quantum numbers n and n^* are considered here as continuous functions of the energy $n^* = (\mathrm{Ry}/|E_{nl}|)^{1/2}$, $n = n^* + \kappa$.

Using the procedure described above, tables of optical and thermodynamic properties of the vapors of cosmic bodies of various chemical composition were calculated within the following range of change of the gasdynamic parameters: for the temperature $T = 2$–40 kK and for the relative density $\delta = 10^{-5}$–10.

The scale of energies of quanta contained about 22,000 points, the main portion of which fell in the optical range. Several thousand spectral lines were taken into account. Examples of calculations are given in Fig. 1 for the vapors of H-chondrite, comet matter, and water.

The tables obtained served as a basis for numerous calculations related to the passage of cosmic bodies through the atmosphere of the earth and other planets ([32, 33]; see also [34] and the references there) and radiation bursts caused by impacts of cosmic bodies on the moon's surface [35].

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NOTATION

N, total number of nuclei in the mixture; N_k, total number of nuclei of element k per unit volume; N_e, concentration of electrons; N_{nl}, number of electrons in the atomic shell with the quantum numbers nl; $b_{k,m}$, number of nuclei of the k-th element in a particle of species m; q, charge of a particle; $n_{m,q}$, number of particles of species m with the charge q; $K_{m,q}$, equilibrium constant; T, temperature; S, entropy; R, gas constant; $Q(T)$, statistical sum; N_A, Avogadro's number; $H(T)$, enthalpy of gas at the temperature T; $E(T)$, internal energy; $H_t^{(i)}$, total enthalpy of the i-th component of the mixture; $\Delta_f H(T_0)$, enthalpy of formation of the substance at the temperature T_0, K; here $T_0 = 0$ K; X_i, relative volume concentration of the i-th component of the mixture; μ, mean atomic weight; P, pressure; σ, absorption cross section; $q_{v'v''}$, Franck–Condon factor; Q_Σ, statistical sum of a molecule; $R_e^{v'v''} = R_e(\lambda_{v'v''})$, transition electron moment as a function of the transition wavelength $\lambda_{v'v''}$; $B_{v''}$, $B_{v'}$, rotational constants corresponding to the lower and upper rotational states; ΔE_e, difference of the electron energies of the upper and lower levels, $\Delta E_e = E_{e'} - E_{e''}$; ΔE_v, difference of the vibrational energies of the upper and lower levels, $\Delta E_v = E_{v'} - E_{v''}$; E_e', energy of the upper electron state; E_e'', energy of the lower electron state; S_t, quantum number of the total spin; Λ, quantum number corresponding to the eigenvalue of the operator of projection of the electron orbital moment onto the internuclear axis; $\alpha(T)$, total intensity of the band; $w(T)$, width of the band; $\varphi(\nu, T)$, absorption contour of the molecular band; $\varphi(\omega, T)$, contour of the spectral line of an atom; ν, wave number corresponding to the transition in molecules; A, B, C, rotational constants; Φ, probability function; n and n^*, principal and effective quantum numbers; α and β, tabulated parameters; n_H, density of atoms of hydrogen per unit volume; l, orbital quantum number of an electron; L, total orbital moment of the atomic state; L', total orbital moment of a state differing from L; ε, energy of a photoelectron; ω, energy of the transition; c, speed of light; k, Boltzmann constant, $1.38 \cdot 10^{-16}$ erg/deg; D, matrix element of the dipole moment of the transition; j, total angular momentum of an electron; e, charge of an electron; e, electronic component; m, mass of an electron; $f_{ll'}$, strength of the oscillator of the transition; γ, width of the line; W, probability of realization of a discrete atomic level; Ry = 13.6 eV; E_{nl}, energy of the atomic level; κ, quantum defect; v, vibrational quantum number. Subscripts: k, element; e, electronic; nl, nlj, quantum numbers; m, species of particle; q, charge of a particle; A, Avogadro; i, component; f, formation; ll', orbital quantum numbers of an electron; $v'v''$, vibrational numbers of molecular states; Σ, total statistical sum; ν, wave number; e″, e′, lower (e″) and upper (e′) electron states; t, total; H, hydrogen; N, number of electrons in the shell nlj; $2S+1$, multiplicity of the electron state; $\varepsilon l' - \varepsilon$, energy of an escaping photoelectron with the orbital momentum $l' = (l + 1)$ or $(l - 1)$.

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