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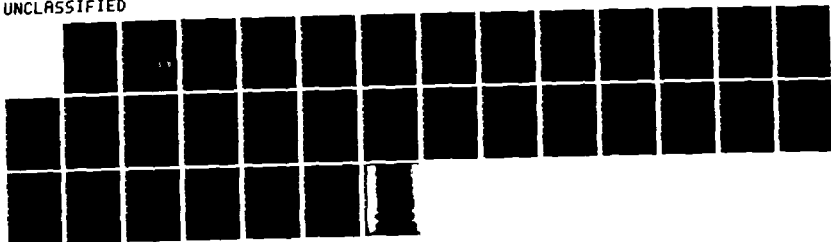
SCATTERING PROPERTIES OF A MOVING DIELECTRIC OBJECT(S)
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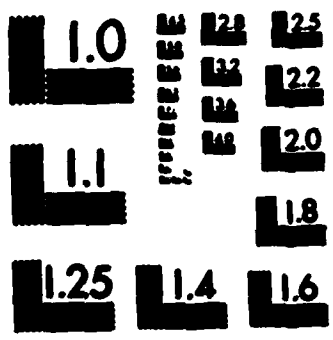
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Scattering Properties of a Moving Dielectric Object

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Istituto di Struttura della Materia
Università di Messina

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Second Periodic Report

January 1984-June 1984

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There are two aspects of electromagnetic scattering from moving object that attracted my attention during the last five months. The first aspect is the possibility of collisions between the scatterers with consequent change of shape; the second aspect is the possibility that a moving scatterer appears to an observer in the laboratory as an object of rather high refractive index. Let us discuss in turn these two facts.

The phenomenon of aggregation of more than one object as a consequence of collisions is the mechanism usually assumed by the chemists to describe the occurrence of chemical reactions. Therefore, if the objects are assumed to be clusters of spheres, it is reasonable that, as a consequence of the collision, the spheres rearrange to give origin to clusters of different geometry and composition. As a consequence the optical spectrum of an aerosol in which such phenomena occur should undergo detectable changes. This mechanism has been thoroughly investigated in collaboration with proff. Borghese, Denti and Toscano and the result of the calculations, through limited to rather simple cases, show that the change in the optical spectra are actually well visible and could thus be used to detect the occurrence of chemical reactions within real aerosols.

This research gave rise to the enclosed paper which has already been submitted for publication. A word of caution should be added. In the above described research no attempt has been made to take account either of the frequency dependence dependence of the refractive indexes of the spheres or of the changes of the refractive indexes as a consequence of

the reactions. In other words no dispersion or changes of valence or bonds has been accounted for although improvements to this effect can be easily included in the theory.

The second aspect I examined with profound interest is the possibility that moving scatterers appears as objects of high refractive index. In fact as a consequence of the general covariance of Maxwell equations under olonomic transformations it turns out that in certain states of motion the refractive index as observed in the laboratory may appear very high.

Now it is well known that in this case resonances of the scattering cross section may occur with an increase of scattering power of a factor of 10 to 100.

Note that resonance scattering has been widely studied with in the framework of Mie theory as an attempt to explain the absorption spectrum e.g. of water droplets.

The procedure I used is rather different. I considered a cluster and searched for the condition of resonance of its constituent spheres. The resulting refractive indexes were then introduced into the program for the cross section of the cluster in order to see the effects of the resonance on the behaviour of the cluster as a whole. Although the results I got till now are only preliminary ones, it is apparent that the scattering cross section shows peaks at frequencies different from those expected from Mie theory. The consequence for this behaviour are at present under further investigation.

Effect of the "chemical reactions" on the absorption

coefficient of a polydisperse model aerosol^(*)

by

R. Saija⁽⁺⁾, O.I. Sindoni^(§), G. Toscano⁽⁺⁾, F. Borghese⁽⁺⁾,
and P. Dentì⁽⁺⁾

Summary.

In a preceding paper the absorption coefficient for the propagation of the electromagnetic field through a low-density dispersion of nonspherical scatterers of random orientation was calculated by modelling them as clusters of spheres. In this paper the spheres are allowed to rearrange among the clusters to simulate chemical reactions and the changes induced on the absorption coefficient of the dispersion are discussed in a few significant cases.

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1. INTRODUCTION.

It is well established through experimental measurements that the refractive index and the absorption coefficient of a dispersion of identical scatterers sensibly depend on their shape⁽¹⁻⁴⁾. On the side of the theoretical investigations several authors dealt in different ways with the scattering by nonspherical objects⁽⁵⁻⁷⁾. The present authors⁽⁸⁾ as well as Gerardy and Ausloos^(9,10) proposed independently to model some kind of nonspherical scatterers as clusters of spheres. The individual optical response of these model scatterers can be effectively calculated as a function of their orientation with respect to the incident field; furthermore, we recently devised an original formalism to calculate the optical constants for the propagation through a low-density random dispersion of identical clusters⁽¹¹⁾. In spite of the prevalent interest in nondielectric scatterers⁽¹²⁻¹⁵⁾, we resolved to include into the clusters only dielectric spheres with frequency-independent refractive index; in this way the effects of the nonspherical shape of the individual clusters are not masked at all and prove to be quite important.

Since our formalism of ref.(11) also applies to di-

persions containing more than one kind of identical scatterers (e.g. polydisperse aerosols) the cluster model is very suitable to describe the effects induced on the scattered field by modifications of the individual scatterers. Such modifications can in turn be described in the framework of the model by rearrangements of the spheres either within the same cluster or among different clusters. This mechanism could be identified with that of the chemical reactions as long as a cluster of spheres can represent a molecule from the point of view of classical optics.

In this paper we intend to show the effects of the above mentioned "chemical reactions" on the absorption coefficient of the dispersion of scatterers. Therefore, in the following section, we concisely report our formalism for the absorption coefficient of a low-density random dispersion of clusters. In the last section we apply the formalism to the dispersions of the clusters modelling the "reagents" and the "products" of a few sample "reactions"; then we collect the results of the calculations so that the effects of the "reactions" are profitably displayed.

We conclude these introductory remarks by observing

that even in this paper we consider only clusters of dielectric spheres whose refractive indices are frequency-independent because we want to single out the influence of the structural modifications of the scatterers; in any case our formalism can be extended to the clusters of nondielectric spheres with refractive indices obeying some dispersion relations.

2. THE CONSTANTS OF COHERENT PROPAGATION THROUGH A DISPERSION OF CLUSTERS.

Referring elsewhere for further details⁽¹¹⁾, here we concisely recall how the refractive index and the absorption coefficient of a dispersion of identical clusters within a matrix can be calculated. In the formalism reported below the dispersion of clusters is assumed to be random and its number density low enough to allow us to disregard the multiple-scattering effects among different clusters. We also assume that the spheres in the clusters as well as the matrix including them are made of isotropic, homogeneous dielectric materials.

Let us consider a low-density dispersion of scatterers whatever and send through it the circularly-polarized plane-

wave field

$$\underline{E}_\eta = \sqrt{\epsilon} \underline{E}_0 \underline{u}_\eta \exp(i \underline{k} \cdot \underline{r}) ,$$

$$i \underline{B}_\eta = \eta \underline{E}_\eta ,$$

where

$$\underline{u}_\eta = (\underline{E}_1 + i \eta \underline{E}_2) / \sqrt{\epsilon} ,$$

with

$$\underline{E}_m \cdot \underline{E}_n = \delta_{mn}$$

and $\eta = \pm 1$ according to the helicity⁽¹⁶⁾. The (complex) refractive index matrix of the dispersion is consequently given by⁽¹⁷⁾

$$\mathcal{N}_{\eta'\eta} = \delta_{\eta'\eta} + \frac{2\pi}{V k^2} \sum_{\nu} f_{\nu, \eta'\eta} ,$$

where the index ν numbers the scatterers in the volume V and

$f_{\nu, \eta'\eta}$ is related to the forward-scattering amplitude of the ν -th scatterer, through

$$f_{\nu, \eta'\eta} = \underline{u}_{\eta'}^* \cdot \underline{f}_{\nu, \eta} .$$

The absorption coefficient and the customary refractive index of the dispersion are given by⁽¹⁷⁾

$$\gamma_{\eta} = 2k \operatorname{Im}(\mathcal{A}_{\eta\eta}^0) \quad , \quad n_{\eta} = \operatorname{Re}(\mathcal{A}_{\eta\eta}^0) \quad ,$$

respectively.

Now we recall that $\mathcal{L}_{\eta\eta}$ is independent of the location of the η -th scatterer but does depend on its orientation with respect to the incident field. Therefore, if the low density of the dispersion is not too low we can substitute $f_{\eta\eta}(\Theta)$ for $\mathcal{L}_{\eta\eta}$ and write

$$\mathcal{A}_{\eta\eta}^0 = \delta_{\eta\eta} + \frac{2\pi}{k^2} \int N(\Theta) f_{\eta\eta}(\Theta) d\Theta \quad ,$$

where the argument Θ is a collective symbol for the Euler angles that individuate the orientation of the scatterers and $N(\Theta)$ is the number density of the scatterers with orientation Θ . At this stage we specify the scatterers in the dispersion as clusters of spheres and assume that their orientation is random. Then we express $f_{\eta\eta}(\Theta)$ in terms of the amplitudes of the multipole fields scattered by a cluster whatever with orientation Θ and, making full use of the features of the cluster model, we succeed in factorizing this quantity into a part depending

only on the structure and a part depending only on the orientation. This allows us to perform the integration over the orientations analytically with the result

$$A_{\eta\eta}^0 = \delta_{\eta\eta} + \frac{N}{4k^2} \sum_{LM} \frac{1}{2L+1} W_{\eta LM}^* W_{\eta LM} \sum_{\mu} (\bar{U}_{\eta, LM, \mu}^{(A)} + \eta' \bar{U}_{\eta, LM, \mu}^{(B)}). \quad (1)$$

For later purposes we rewrite

$$A_{\eta\eta}^0 = \delta_{\eta\eta} + N \sum_L \xi_{\eta\eta L} S_{\eta\eta L} \quad (2)$$

where we define

$$\xi_{\eta\eta L} = \frac{1}{4\pi^2} \frac{1}{2L+1} \sum_{\mu} W_{\eta LM}^* W_{\eta LM},$$

$$S_{\eta\eta L} = \frac{1}{k^2} \sum_{\mu} (\bar{U}_{\eta, LM, \mu}^{(A)} + \eta' \bar{U}_{\eta, LM, \mu}^{(B)}).$$

In the equations above N is the number density of the clusters; the quantities

$$W_{\eta LM} = 4\pi i^L \sqrt{L} \underline{u}_{\eta} \cdot \underline{X}_{LM}^* (\hat{k}) ,$$

where the \underline{X}_{LM} 's are vector spherical harmonics⁽¹⁶⁾, are proportional to the multipolar amplitudes of the incident plane-wave field; the matrices $\bar{U}_{\eta}^{(A)}$ and $\bar{U}_{\eta}^{(B)}$, whose meaning will be discussed below, have a rather complicated expression for which we

explicitly rely upon ref.(11).

By their very definition the W 's and consequently the \mathbf{g} 's depend only on the direction of the wavevector of the incoming field. The \bar{U} 's as well as the S 's depend on the magnitude of the wavevector of the plane wave and on the refractive indices of the spheres constituting the (identical) clusters in the dispersion. The \bar{U} 's account also for the structure of the clusters and need to be calculated once for all referring to a cluster whatever with arbitrary orientation. As a matter of fact, the \bar{U} 's are responsible for almost all of the amount of computations required by eq.(1) because their calculation implies the inversion of a matrix of order $2N_s L_M(L_M+2)$, where N_s is the number of spheres in a cluster and L_M is the least value to which the sum over L must be extended to obtain well converged results. The convergence of the multipolar expansion on which eq.(1) is grounded has been discussed elsewhere^(8,10); of course we shall return to this subject when considering the specific computations reported in the next section. Finally it is useful to recall that, if the clusters possess symmetry elements, such as reflection planes and/or symmetry axes, Group theory can substantially help to compute the \bar{U} 's

for it implies the inversion of matrices of smaller order than otherwise^(18,19).

3. CHANGES IN THE ABSORPTION COEFFICIENT CAUSED BY "CHEMICAL REACTIONS".

In the case of a low-density dispersion containing more than one kind of clusters eq.(2) becomes⁽¹⁷⁾

$$\mathcal{N}_{\eta'\eta} = \delta_{\eta'\eta} + N \sum_{\alpha, L} c_{\alpha} \mathcal{E}_{\eta'\eta L} S_{\alpha\eta'\eta L},$$

where the index α refers to the α -th kind of clusters with number density $N_{\alpha} = N c_{\alpha}$.

Now, it is well understood that, if a "chemical reaction" rearranges the spheres among the clusters, it determines, starting with the relative concentrations c_{α} of the "reagents", the relative concentrations d_{β} of the "reaction products" as well as those of the "residues of the reaction", c'_{α} (one at least of these latter is zero when the reaction is over). Therefore we can calculate the absorption coefficients before and after the "reaction", and denote them by

$$\gamma_{\eta}^{(i)} = N \sum_{\alpha} c_{\alpha} Z_{\alpha\eta}$$

and

$$\gamma_{\eta}^{(f)} = N \left[\sum_a c'_a Z_{a\eta} + \sum_{\beta} d_{\beta} Z_{\beta\eta} \right] ,$$

respectively, where

$$Z_{a\eta} = 2k \mathcal{G}_m \left[\sum_L \xi_{\eta\eta_L} S_{a\eta\eta_L} \right] .$$

Clearly, a very useful quantity in detecting the structural effects on the absorption is

$$\Gamma = \frac{p \gamma^{(f)} + (1-p) \gamma^{(i)}}{\gamma^{(i)}} = p\Delta + 1 ,$$

where we dropped the label η , p is the completion index of the "reaction" ($0 \leq p \leq 1$), and

$$\Delta = \gamma^{(f)} / \gamma^{(i)} - 1 .$$

In the following part of this section we present the results for a few "chemical reactions". Before any explanation and comment, however, we want to stress a point to avoid any substantial misunderstanding of the purposes of the present work. Our results refer to sample calculations, indeed, and do not pretend to give a realistic description of actual optical

phenomena: too many details should be added to the very schematic cluster model. Consequently one should not bother neither about the choice of the parameters defining the structure of the clusters nor about the possibility of the "reactions" in the assumed low-density limit of the dispersion. We confirm that our question is: if the structure of the cluster changes, how much is the absorption coefficient affected? The results we are going to discuss make we answer that in general these structural changes modify to a significant extent the coherent propagation of the field through the dispersion.

The "reactions" for which Γ was actually computed are listed in Table I. A,B and C label the spheres with the refractive indices $n_A=1.30$, $n_B=1.50$ and $n_C=1.40$, and the radii $r_A=1.0 u_1$, $r_B=0.50 u_1$ and $r_C=0.75 u_1$, respectively, where u_1 is an arbitrary unit. The clusters are individuated by their "chemical formulae" in terms of the "elements" A,B and C, and their structures are built so as to match those of the chemical compounds listed under the heading "EXAMPLE". Since the radii and the refractive indices of the spheres are assumed not to change due to the "reactions", changes of "valence" or "bonds" are not accounted for. In Table I the "reactions" are partitioned into three groups: the first group, "reactions"

1-4, where only the spheres A and B are implied; the second group, "reactions" 5 and 6, where also the spheres C are implied; the third group, that includes the family of "reactions" 7-10.

In table II we list the clusters as well as the "reactions" in which they are involved according to Table I. We also report the co-ordinates of the centres of the spheres to complete the definition of the structures; in this respect one can observe that the neighbouring spheres touch each other.

Figures 2, 4 and 6 show Γ with $p=1$ versus k for the "reactions" included into each of the above mentioned three groups, respectively. Figures 1,3 and 5 show in turn $g_\alpha = Z_\alpha / Z_\alpha^{(0)}$ versus k . $N_\alpha Z_\alpha$ is the absorption coefficient of a dispersion containing only the α -th kind of clusters. $N_\alpha Z_\alpha^{(0)}$ is the same, save that it is obtained by the Mie theory⁽¹⁷⁾ after substituting for the dispersion of the clusters the dispersion of their constituent spheres with no mutual presence effect allowed. Figures 1,3 and 5 are not immediately comparable with figs. 2, 4 and 6, respectively, on account of the different normalization; on the other hand, the chosen normalizations render Γ independent of N and g_α independent of N_α , although it should

be borne in mind that our results are valid only for low-density dispersions.

All our calculations were actually performed for k ranging from $0.002 u_1^{-1}$ to $2.0 u_1^{-1}$, so that the wavelength of the incident field is allowed to decrease to about the overall dimension of the clusters. However, in all the figures, k ranges from $0.2 u_1^{-1}$ to $2.0 u_1^{-1}$, the interval in which the results show a more striking k -dependence. Since all the results refer to $\eta=1$ the index η has been everywhere dropped.

Before discussing the results we premise a few words about their convergence. It is well known that the multiple scattering processes among the spheres of each cluster enhance the strength of multipole fields of higher order^(8-11,18,19), so that the L -expansions cannot be truncated to too low a value, whereas too high values imply time-consuming computations and enormous memory requirements. As a matter of fact, we found that a quite reasonable $L_M=4$ ensures converged results for all the clusters considered here with k ranging from $0.002 u_1^{-1}$ to $2.0 u_1^{-1}$.

From a general point of view, figs. 1,3 and 5 show clearly that the multiple-scattering processes among the spheres of a cluster cannot be disregarded without affecting dra

matically the correctness of the results. Therefore, it is a very reasonable prediction that structural modifications of the clusters cause appreciable variations of the absorption of the dispersion. As we anticipated, this actually occurs: the Γ -ratios are significantly different from unity for k in the range from $0.002 u_1^{-1}$ to $0.2 u_1^{-1}$. In figs. 2, 4 and 6, however, we see that when k increases the effect of the "reaction" becomes smaller and smaller, although for almost all the "reactions"

Γ is significantly different from unity at least up to $k \approx 1.0 u_1^{-1}$. In this respect we remark that in general the more the structure of the clusters is modified the more Γ remains different from unity. Even the curves of g_α in figs. 1, 3 and 5 the less differ from each other the more similar are the structures. As an example, in fig. 1 the curves for CO_2 and SC_2 are indistinguishable from each other. The component spheres are identical for the two clusters AB_2 , indeed, and the structural differences are too small to give appreciably different spectra also on account of the randomness of the orientations.

In conclusion, the cluster model accounts for the nonspherical shape of the scatterers so effectively that it renders the structural modifications quite detectable. In this

sense, and on account of the possible improvements, the cluster model should be suitable for approaching the experimentally measured properties of real aerosols.

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TABLE I

REACTION	EXAMPLE
1) $3B_2 \rightarrow 2B_3$	$3O_2 \rightarrow 2O_3$
2) $2AB + B_2 \rightarrow 2AB_2$	$2CO + O_2 \rightarrow 2CO_2$
3) $2AB_2 + B_2 \rightarrow 2AB_3$	$2SO_2 + O_2 \rightarrow 2SO_3$
4) $A_2 + 3B_2 \rightarrow 2AB_3$	$N_2 + 3H_2 \rightarrow 2NH_3$
5) $AC + 3B_2 \rightarrow AB_4 + B_2C$	$CO + 3H_2 \rightarrow CH_4 + H_2O$
6) $2AB_3 + C_2 \rightarrow 2ACB_3$	$2PH_3 + O_2 \rightarrow 2POH_3$
7) $C_2 + AB_4 \rightarrow AB_3C + BC$	$Cl_2 + CH_4 \rightarrow CH_3Cl + HCl$
8) $2C_2 + AB_4 \rightarrow AB_2C_2 + 2BC$	$2Cl_2 + CH_4 \rightarrow CH_2Cl_2 + 2HCl$
9) $3C_2 + AB_4 \rightarrow ABC_3 + 3BC$	$3Cl_2 + CH_4 \rightarrow CHCl_3 + 3HCl$
10) $4C_2 + AB_4 \rightarrow AC_4 + 4BC$	$4Cl_2 + CH_4 \rightarrow CCl_4 + 4HCl$

TABLE I - List of the "reactions" considered in this paper.

The refractive indices and radii of the elements A,B and C are:

$n_A=1.30$, $n_B=1.50$, $n_C=1.40$, and $r_A=1.0 u_1$, $r_B=0.50 u_1$, $r_C=0.75 u_1$, where u_1 is an arbitrary unit.

TABLE II

CLUSTER	CO-ORDINATES	REACTIONS
E_2	(-0.5,0,0) (0.5,0,0)	1,2,3,4,5
A_2	(-1.0,0,0) (1.0,0,0)	4
C_2	(-0.75,0,0) (0.75,0,0)	6,7,8,9,10
AB	(-1.0,0,0) (0.5,0,0)	2
AC	(-1.0,0,0) (0.75,0,0)	5
BC	(-0.5,0,0) (0.75,0,0)	7,8,9,10
B_3	(0, 0.57735,0) (0.5,-0.28867,0) (-0.5,-0.28867,0)	1
AB_2	(0,0,0) (-1.5,0,0) (1.5,0,0)	2
AB_2	(0,0,0) (1.22873,-0.86036,0) (-1.22873,-0.86036,0)	3
B_2C	(1.02394,-0.71697,0) (-1.02394,-0.71697,0) (0,0,0)	5
AB_3	(0,0,0) (0,1.5,0) (1.29904,-0.75,0) (-1.29904,-0.75,0)	4,6
AB_3	(0,0,1.38444) (0.5,-0.28867,0) (-0.5,-0.28867,0) (0,0.57735,0)	3
AB_4	(0,0,0) (-0.86602,-0.86602,0.86602) (-0.86602,0.86602,-0.86602) (0.86602, -0.86602,-0.86602) (0.86602,0.86602,0.86602)	5,7,8,9,10
ACB_3	(0,0,1.38444) (0,0,3.13444) (0,0.57735,0) (0.5,-0.28867,0) (-0.5,0.28867,0)	6
AB_3C	(0,0,1.38444) (0,0.57735,0) (0.5,-0.28867,0) (-0.5,-0.28867,0) (0,0,3.13444)	7

TABLE II (continued)

CLUSTER	CO-ORDINATES	REACTIONS
AF_2C_2	(0,-0.375,1.45237) (0,0,0) (0,-0.375,2.95237) (0.75,-1.0,0) (-0.75,-1.0,0)	8
ABC_3	(0,1.52069,0) (0,3.02069,0) (0,0.84602,0) (0.75,-0.43301,0) (-0.75,-0.43301,0)	9
AC_4	(0,0,0) (-1.01036,-1.01036,1.01036) (-1.01036,1.01036,-1.01036) (1.01036,-1.01036, -1.01036) (1.01036,1.01036,1.01036)	10

Table II

Co-ordinates of the centres of the spheres constituting the clusters implied in the "reactions" of Table I.

The co-ordinates refer to each sphere in the same order in which it appears in the name of the cluster. The "reactions" in which each cluster is implied according to Table I, are also listed.

Riassunto.

In un articolo precedente è stato calcolato il coefficiente di assorbimento per la propagazione del campo elettromagnetico attraverso una dispersione a bassa densità di diffusori non sferici, modellizzandoli come "cluster" di sfere. In questo articolo si permette ai "cluster" di variare la loro struttura in maniera da simulare delle reazioni chimiche e le conseguenti variazioni del coefficiente di assorbimento della dispersione vengono calcolate in alcuni casi significativi.

FIGURE CAPTIONS

Figure 1.

Plot of g_{α} vs k for the clusters implied in the "reactions" 1-4 of Table I. The dashed curves refer to the "reagents" and the solid curves to the "reaction products".

Figure 2.

Plot of Γ vs k for $p=1$ for the "reactions" 1-4 of Table I.

Figure 3.

Plot of g_{α} vs k for the clusters implied in the "reactions" 5-6 of Table I. The dashed curves refer to the "reagents" and the solid curves to the "reaction products".

Figure 4.

Plot of Γ vs k for $p=1$ for the "reactions" 5-6 of Table I.

Figure 5.

Plot of g_{α} vs k for the clusters implied in the "reactions" 7-8 of Table I. The dashed curves refer to the "reagents" and the solid curves to the "reaction products".

Figure 6.

Plot of Γ vs k for $p=1$ for the "reactions" 7-10 of Table I.

FIG. 1

g_a

O_3

3.0

2.5

NH_3

SO_3

$H_2=O_2$

2.0

N_2

$SO_2=CO_2$

1.5

CO

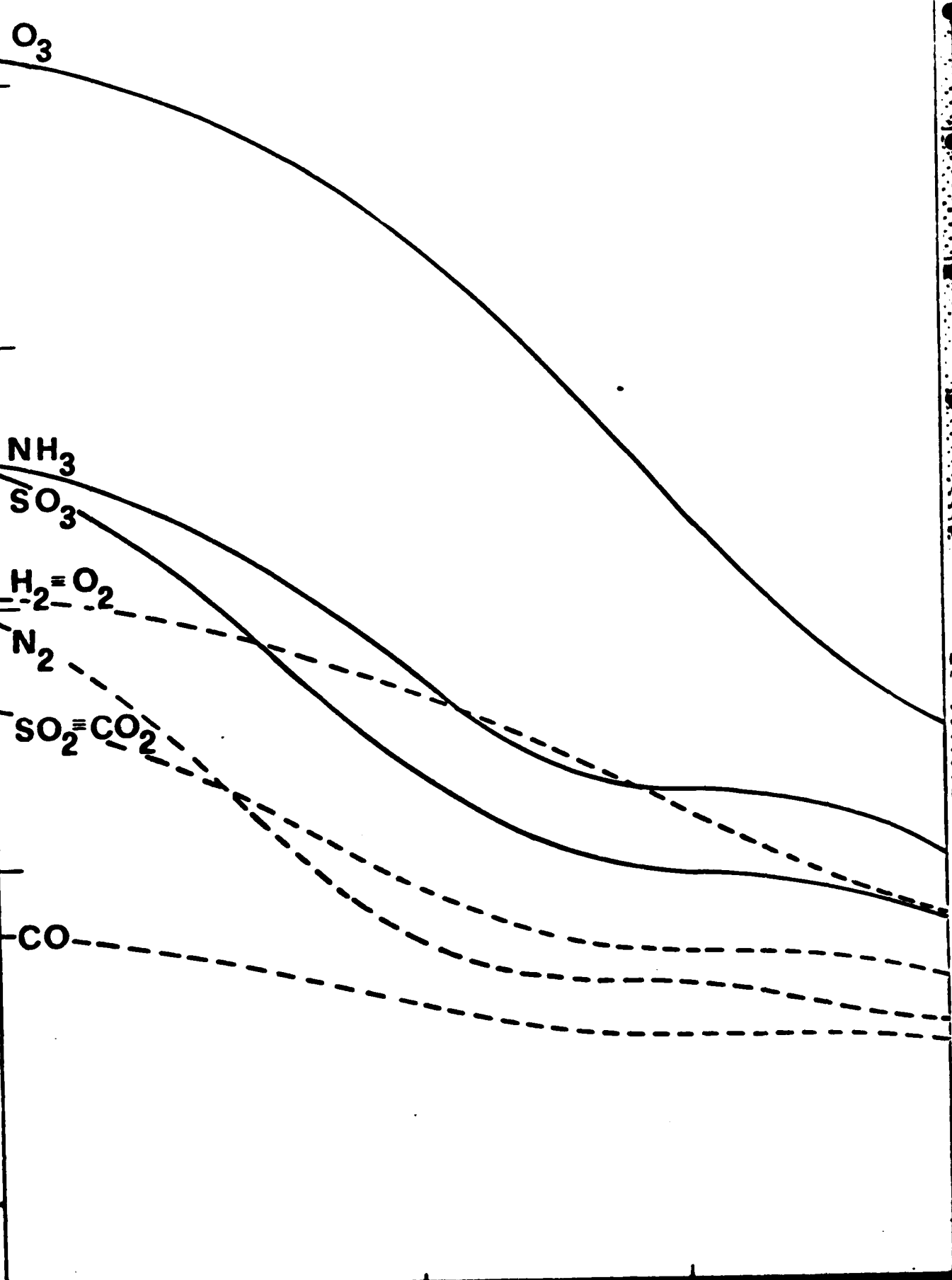


FIG. 2

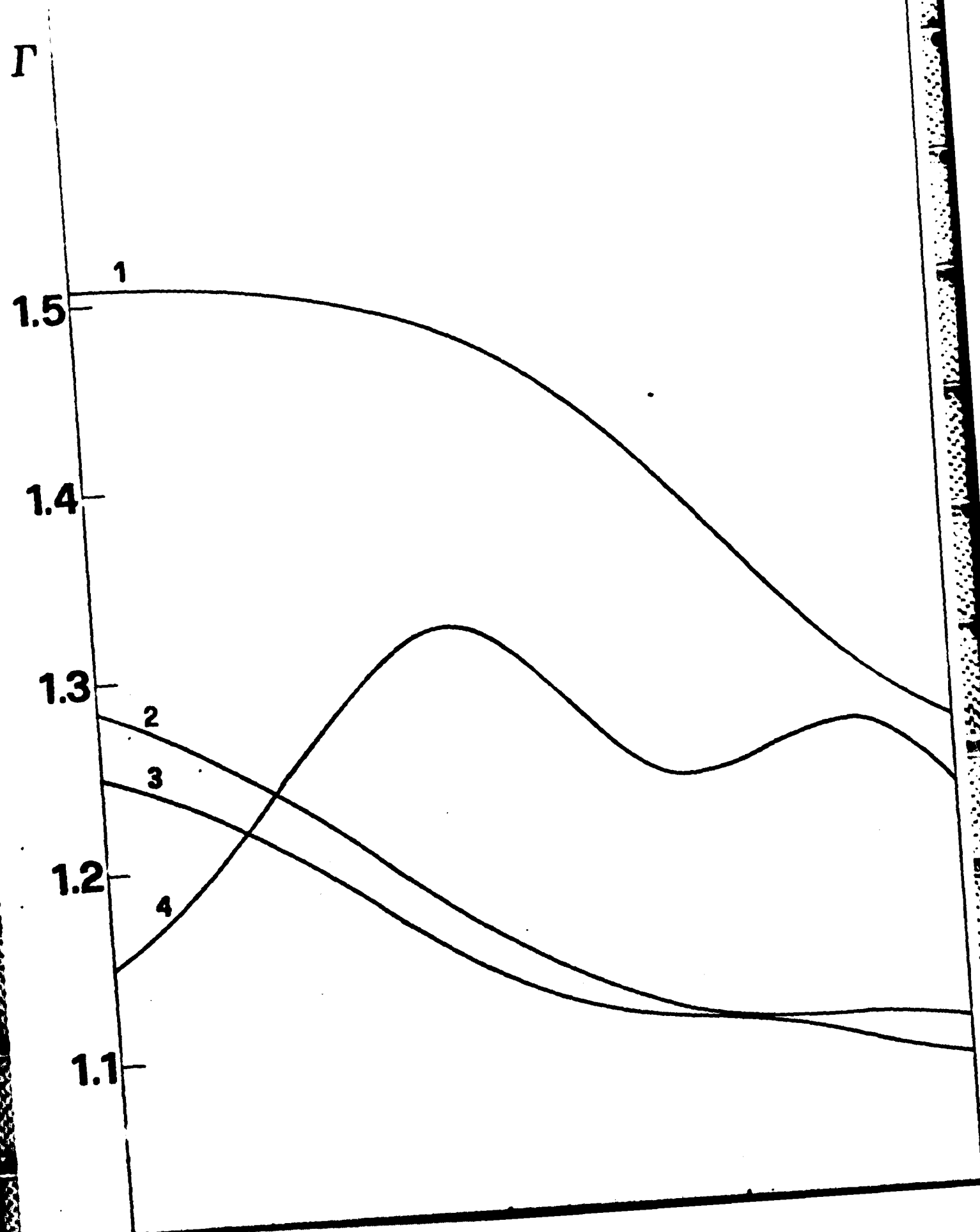


FIG. 3

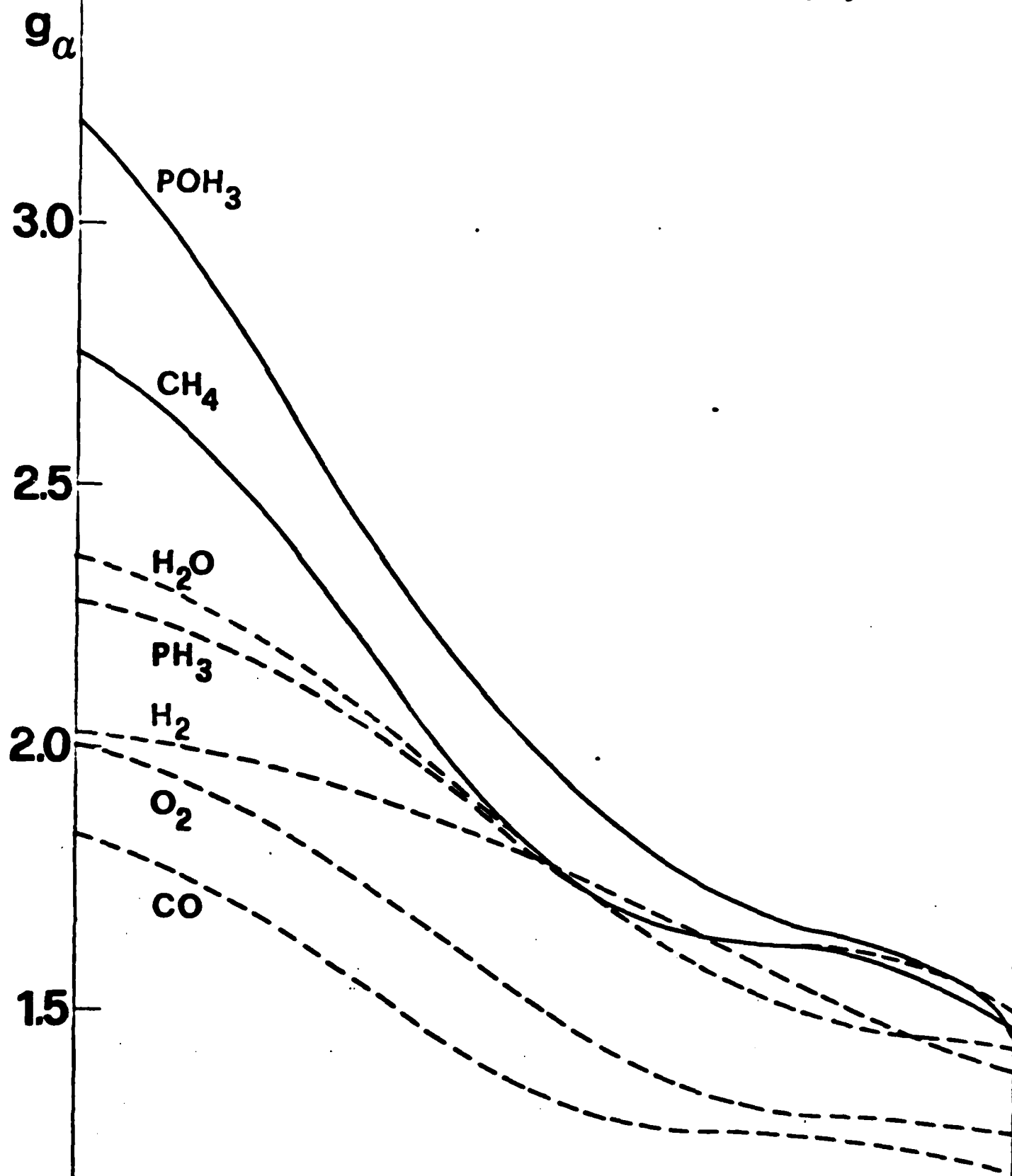
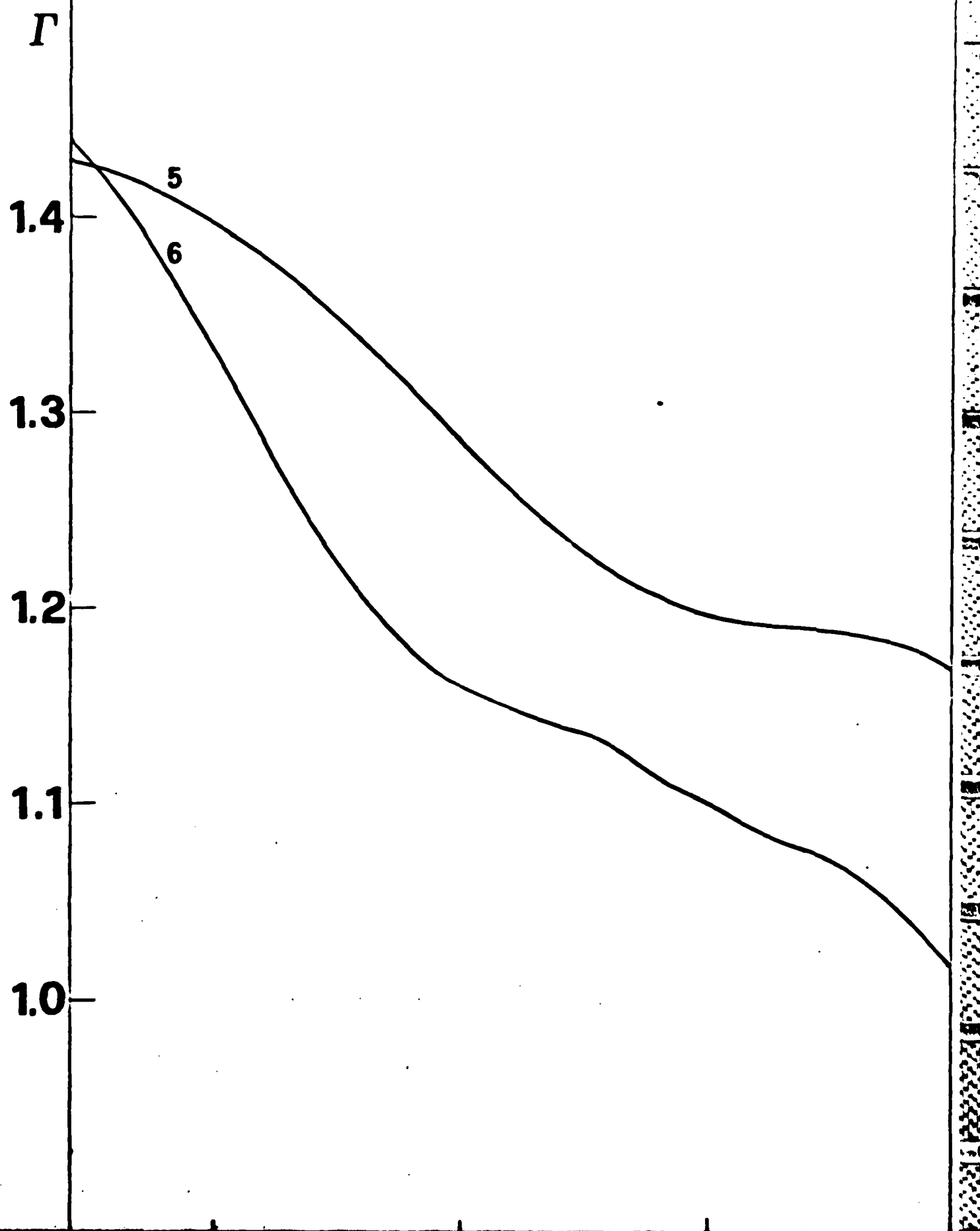


FIG. 4



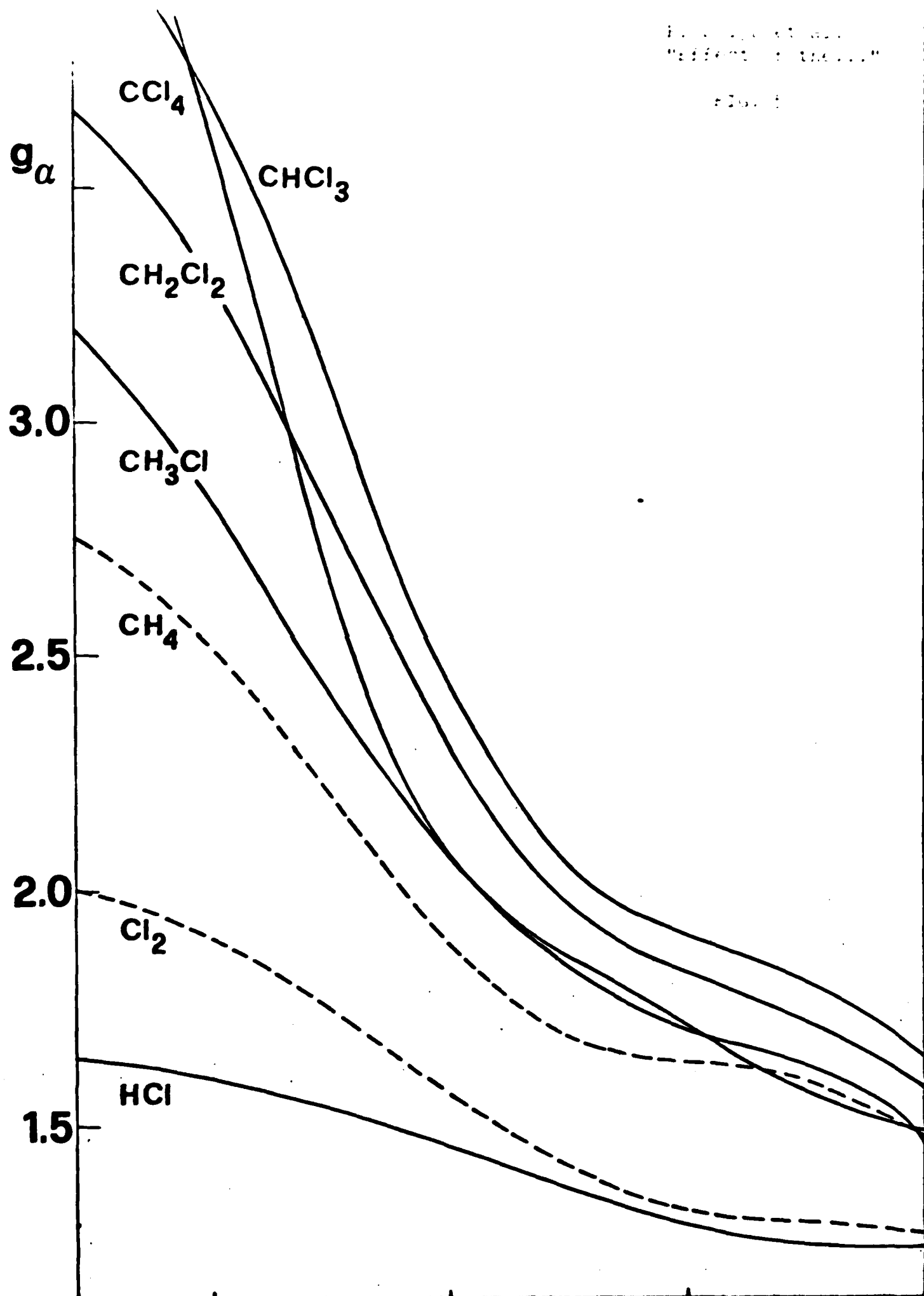


FIG. 6

Γ

1.5

1.4

1.3

1.2

1.1

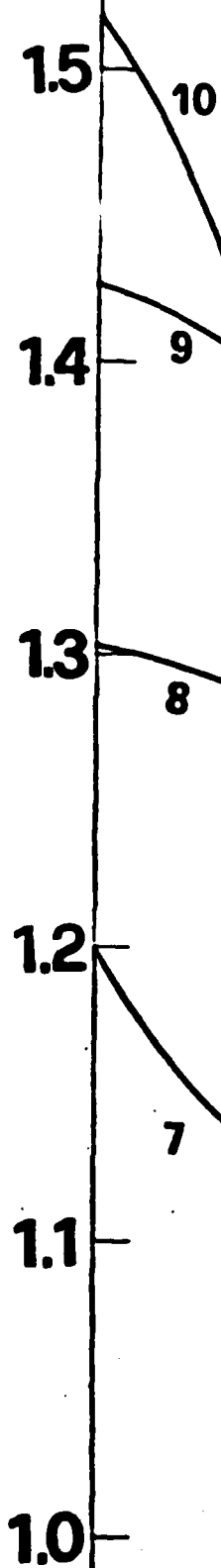
1.0

10

9

8

7



END

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8

DNIC