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CHEMICAL SYSTEMS LABORATORY TECHNICAL REPORT

ARCSL-TR-81034

CALCULATED INFRARED EXTINCTION COEFFICIENTS
FOR GRAPHITE

by

Robert Frickel

Research Division

November 1981

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER ARCSL-TR-81034	2. GOVT ACCESSION NO. A108 051	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) CALCULATED INFRARED EXTINCTION COEFFICIENTS FOR GRAPHITE		5. TYPE OF REPORT & PERIOD COVERED Technical Report October 1979
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Robert Frickel		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Commander/Director, Chemical Systems Laboratory ATTN: DRDAR-CLB-PS Aberdeen Proving Ground, MD 21010		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Task 1T1611102A71A Scientific Area 5
11. CONTROLLING OFFICE NAME AND ADDRESS Commander/Director, Chemical Systems Laboratory ATTN: DRDAR-CLJ-R Aberdeen Proving Ground, MD 21010		12. REPORT DATE November 1981
		13. NUMBER OF PAGES 26
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE NA
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Aerosols Infrared spectra Extinction Mie theory Graphite Optical properties		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Calculations were made of the optical extinction for graphite using Mie theory, on assumption of spherical particles, and published complex index of refraction data for graphite and carbon. The results are presented in graph form showing extinction coefficient vs wavelength, displaying the scattering and absorption components of extinction. The results permit examination of the effect of particle size, particle distribution width, and complex index of refraction on calculated extinction.		

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PREFACE

The work described in this report was authorized under task IT1611102A71A, Scientific Area 5, Aerosol/Obscurant Research. The work was conducted in October 1979.

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CALCULATED INFRARED EXTINCTION COEFFICIENTS FOR GRAPHITE

1. INTRODUCTION

1.1. Objective. The objective of this work was to estimate the mass extinction coefficients of graphite smokes against visible and infrared radiation as a function of particle size distribution.

1.2. Background. This effort is part of a continuing study by Obscuration Sciences Section on extinction of visible infrared radiation by carbon and graphite smokes. An extensive collection of experimental data on extinction and particle size distribution for such smokes has been developed by Obscuration Sciences Section. This study was initiated to provide a better understanding of the behavior exhibited by these smokes and thus obtain some insight on how to optimize their performance as screening agents.

1.3. Theory. The estimates presented here are calculated using the theoretical solution presented by Gustave Mie in 1908 for the interaction between a plane electromagnetic wave and a homogeneous isotropic sphere of a given complex refractive index for a specified ratio of the circumference of the sphere to the wavelength of the radiation (size parameter). This calculation is an exact solution of Maxwell's equations in terms of spherical Bessel functions and Legendre polynomials.^{1,2} The extinction coefficients calculated directly via Mie theory are for monodisperse aerosols; for polydisperse aerosols these values are weighted according to the particle size distributions of the aerosol and integrated over particle size, viz,

$$\bar{\alpha} = \frac{\int \alpha(D) dm}{\int dm} \quad (1)$$

where $\alpha(D)$ is the mass extinction coefficient calculated for diameter D , dm is the mass concentration of particulate material in the aerosol whose diameter lies between D and $D + dD$, the integration is over the size distribution and $\bar{\alpha}$ is the mass extinction coefficient for this aerosol. In these calculations a log normal distribution was used so that

$$dm = \frac{M}{\sqrt{2\pi} \ln \sigma_0} \exp \left\{ -1/2 \left[\ln(D/D_0) / \ln \sigma_0 \right]^2 \right\} d \ln D \quad (2)$$

where D_0 is the mass median diameter of the aerosol, σ_0 is the logarithmic standard deviation of the distribution, and M is the total mass.

1.4. Approach. The distribution parameters used in these calculations are typical results of Andersen impactor measurements made during the extinction experiments. The calculations are based on index of refraction spectra presented by Foster and Haworth.^{3,4} It should be noted that graphite particles are not actually spherical, so that

- (a) Mie theory is not strictly applicable;

- (b) the aerodynamic diameters measured by the impactor are not necessarily the same as the corresponding optical diameter; and
- (c) the indices of refraction of graphite vary from sample to sample and the values here are, at best, typical.

Hence, the calculations presented here can be considered only as approximations. For comparison, extinction coefficient spectra were calculated using a typical infrared refractive index for carbon (1.55, 0.66).⁵

2. RESULTS

The results of the calculation for graphite are shown in figures 1 and 2. The abscissae are radiation wavelengths in micrometers; the ordinates are optical extinction coefficients in square meters/gram. The solid lines represent total extinction, the long-dashed lines adsorption, and the short-dashed lines scattering. The distribution parameters are shown on the figure and are defined by

$$\frac{dM}{d \ln D} = \frac{M}{\sqrt{2\pi} \ln \sigma_g} e^{-1/2} \left[\frac{\ln(D/D_0)}{\ln \sigma_g} \right]^2 \quad (3)$$

The MMD in the figures is the mass median diameter D_0 . The bulk density of the particle material is 2.25 g/cm³.

The results of the calculations for carbon are shown in figures 3 and 4.

Note that the values of σ_g used here are very large. Extinction coefficient spectra calculated for monodisperse graphite aerosols of the same MMD's are shown in figures 5 and 6.

The great difference between the spectra for the monodisperse and polydisperse aerosols is due to the presence of a large component of small (< 1 μ) particles in the broad distribution. Figures 7 - 11 illustrate this difference by exhibiting the extinction spectra for monodisperse graphite aerosols of various sizes.

3. CONCLUSIONS

3.1. Extinction coefficient spectra for graphite are calculated and may be used for comparison with measured spectra.

3.2. The calculated curves are approximations because of the uncertainty in the refractive index and the nonspherical shape of the particles.

3.3. Spectral shape appears to be dominated by the small particle component present in the very broad particle size distribution.

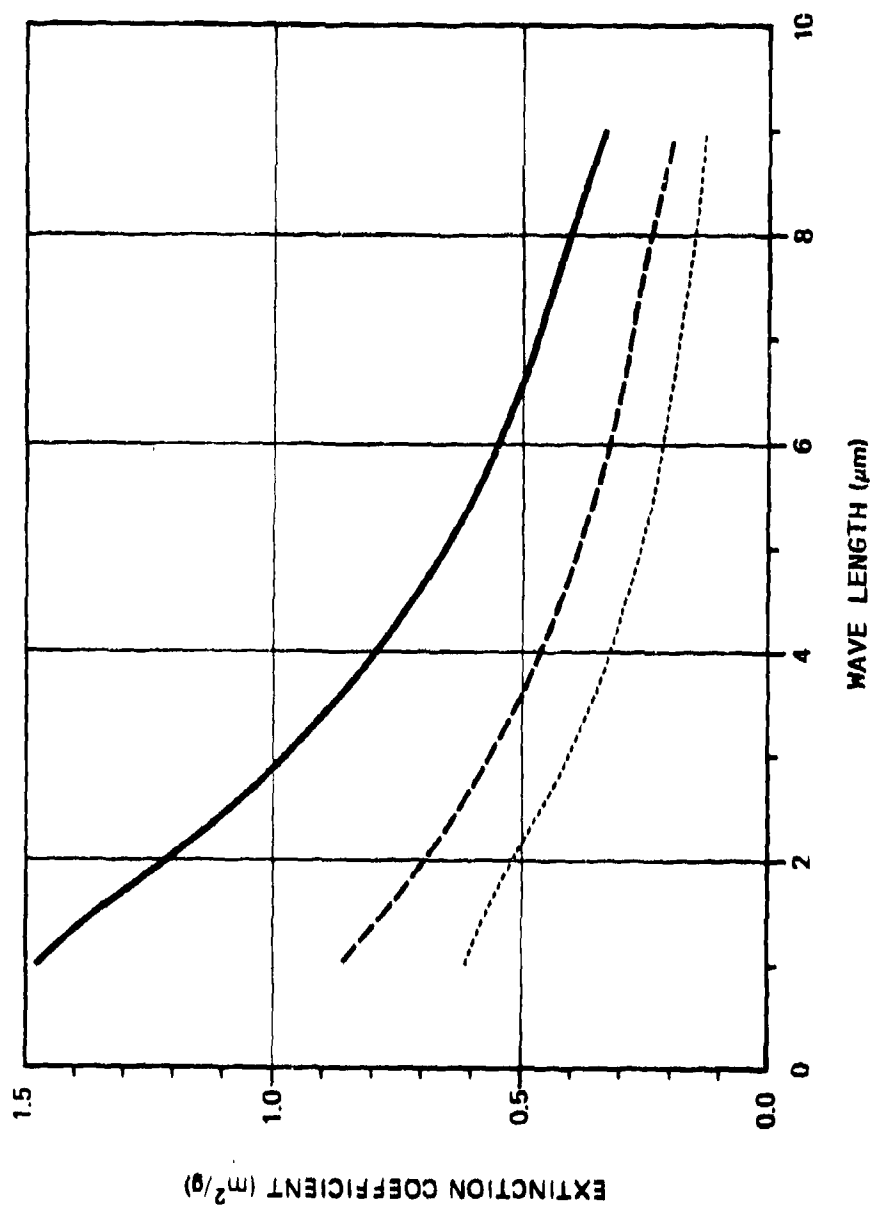


Figure 1. Extinction Coefficient for Graphite with Log Normal Particle Size Distribution
 $MWD = 1.85$ $\sigma_g = 3.18$

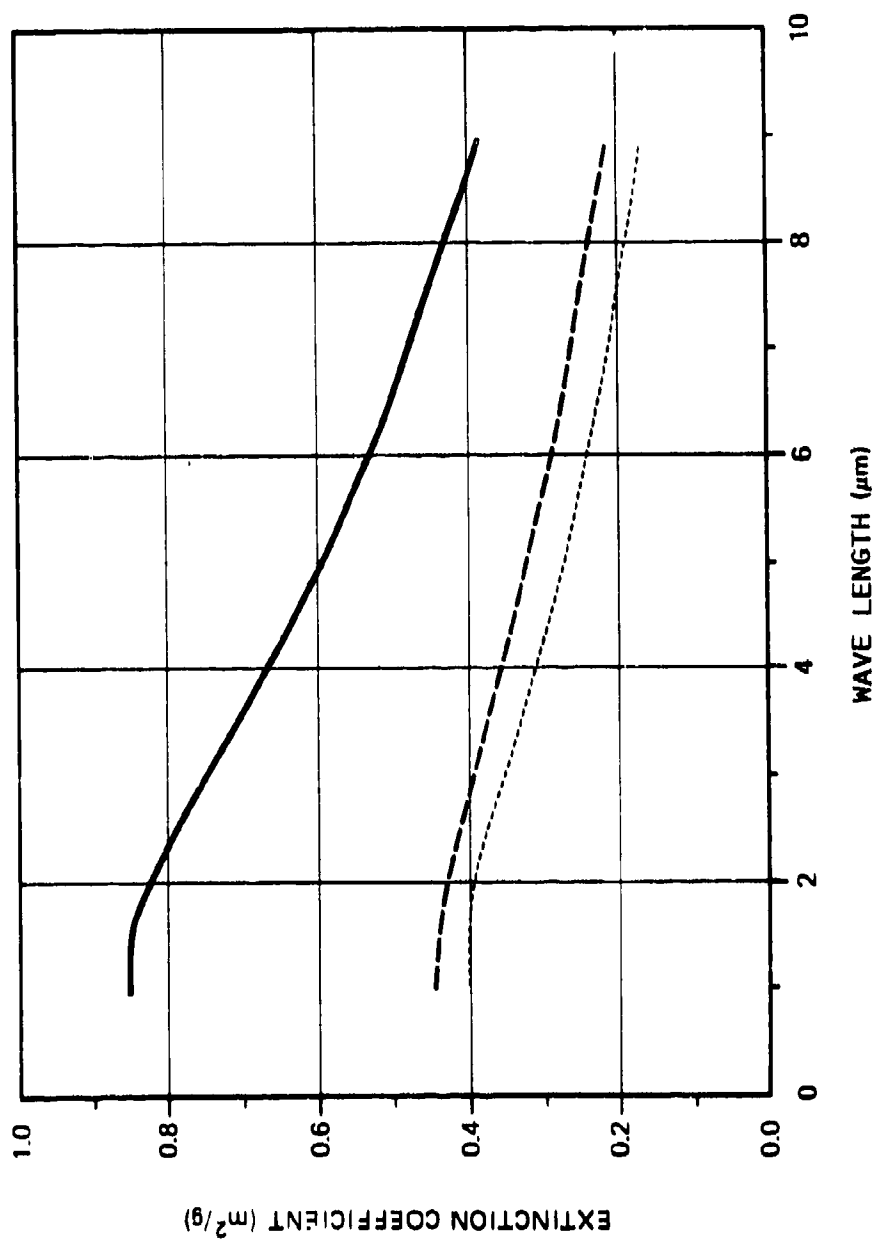


Figure 2. Extinction Coefficient for Graphite with Log Normal Particle Size Distribution
 $MWD = 3.32$ $\sigma_g = 2.80$

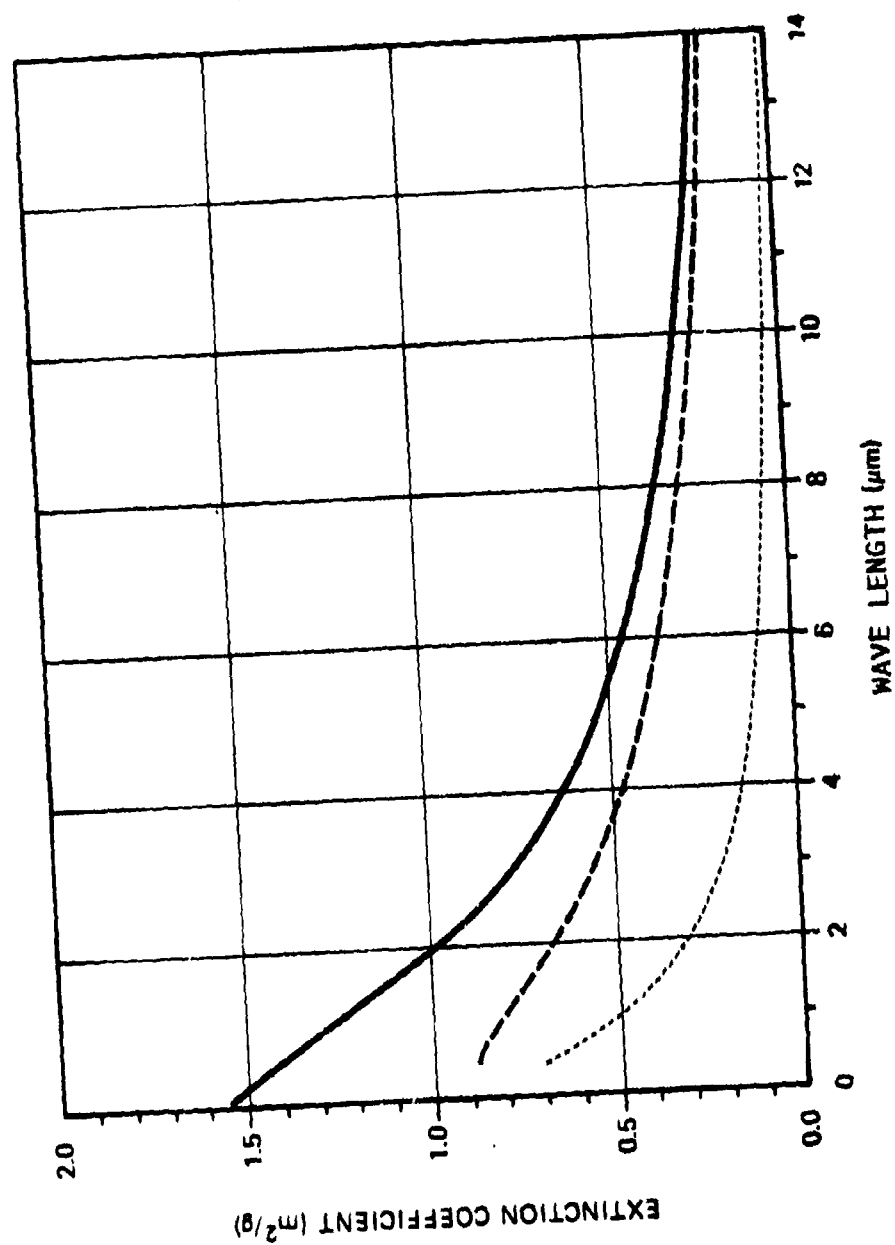


Figure 3. Extinction Coefficient for Carbon, $M = (1.55, .66)$ Log Normal Distribution
 $MMD = 1.85$ $\sigma_g = 3.18$

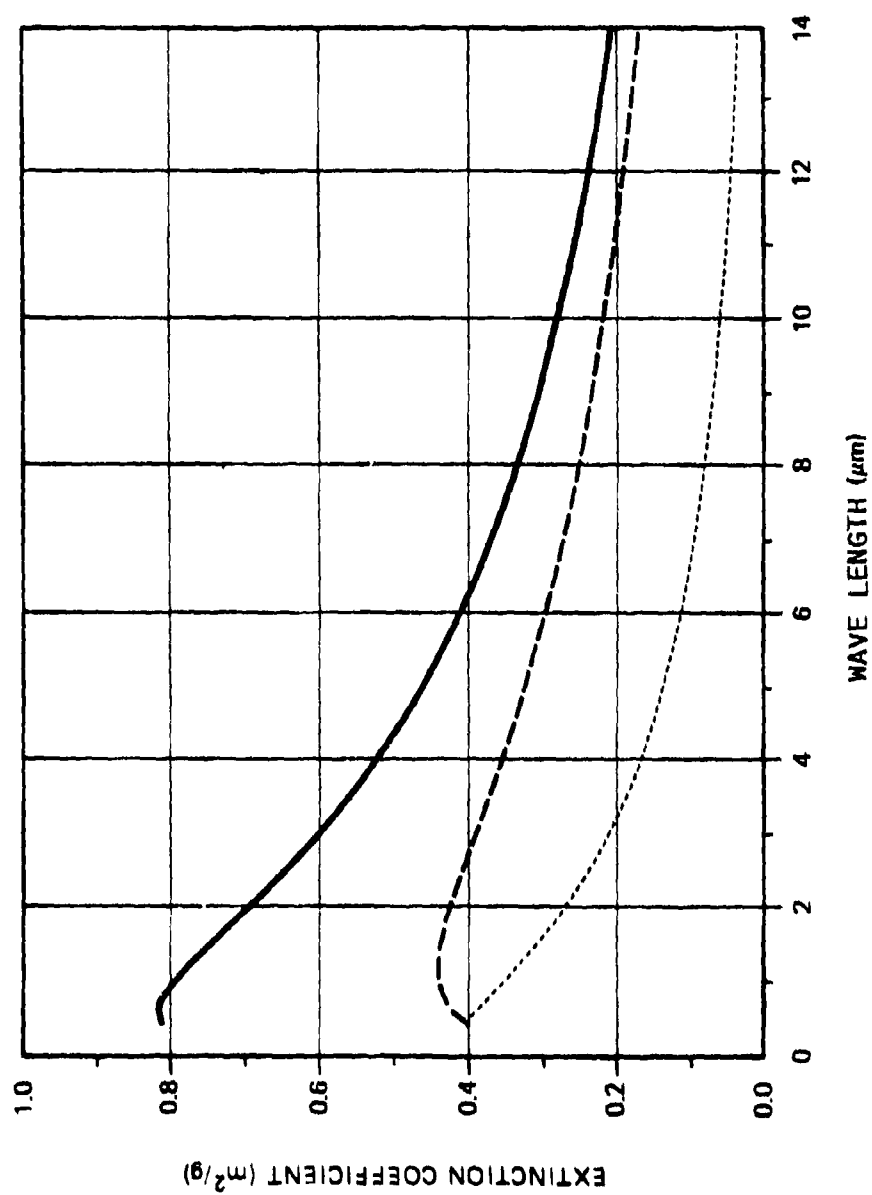


Figure 4. Extinction Coefficient for Carbon, $M = (1.55, .66)$ Log Normal Distribution
 $\text{MMD} = 3.32$ $\sigma_g = 2.80$

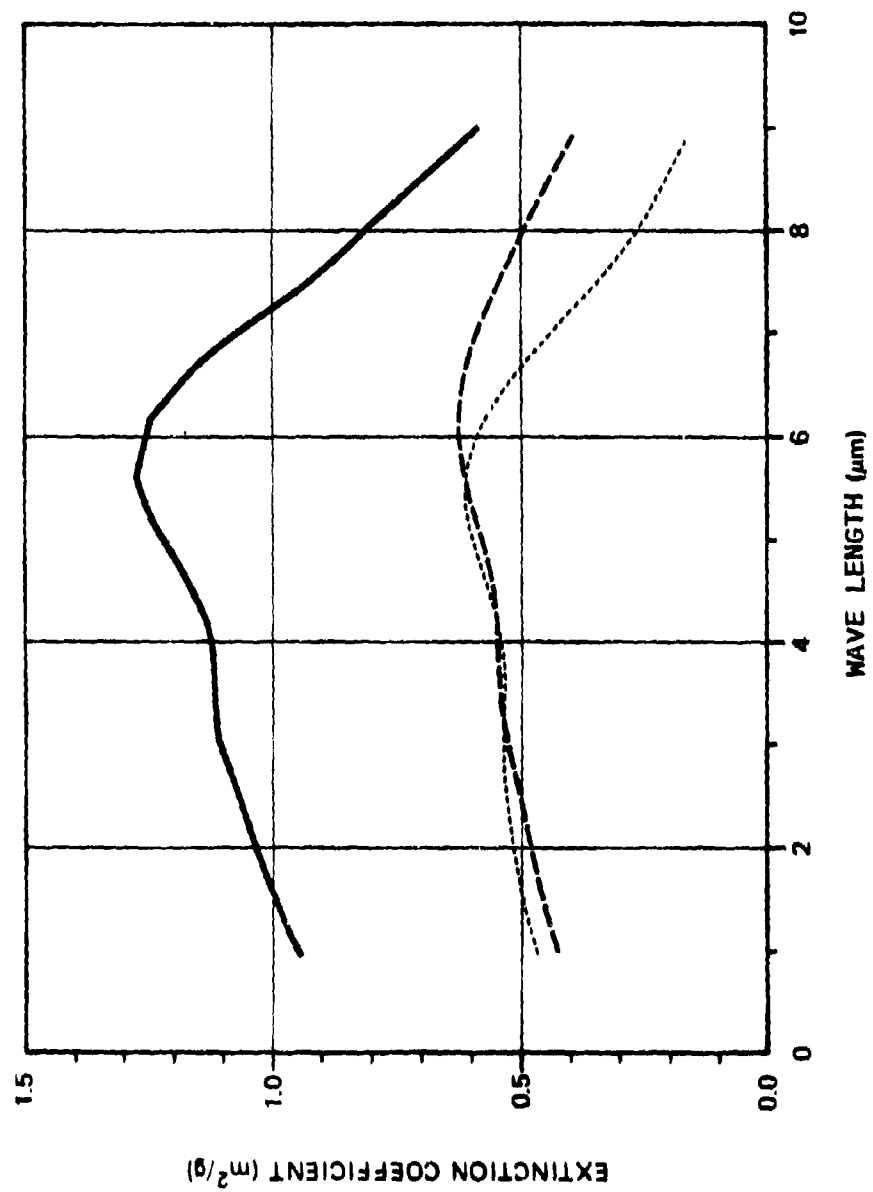


Figure 5. Extinction Coefficient for Graphite, Monodisperse
Diameter = 1.85

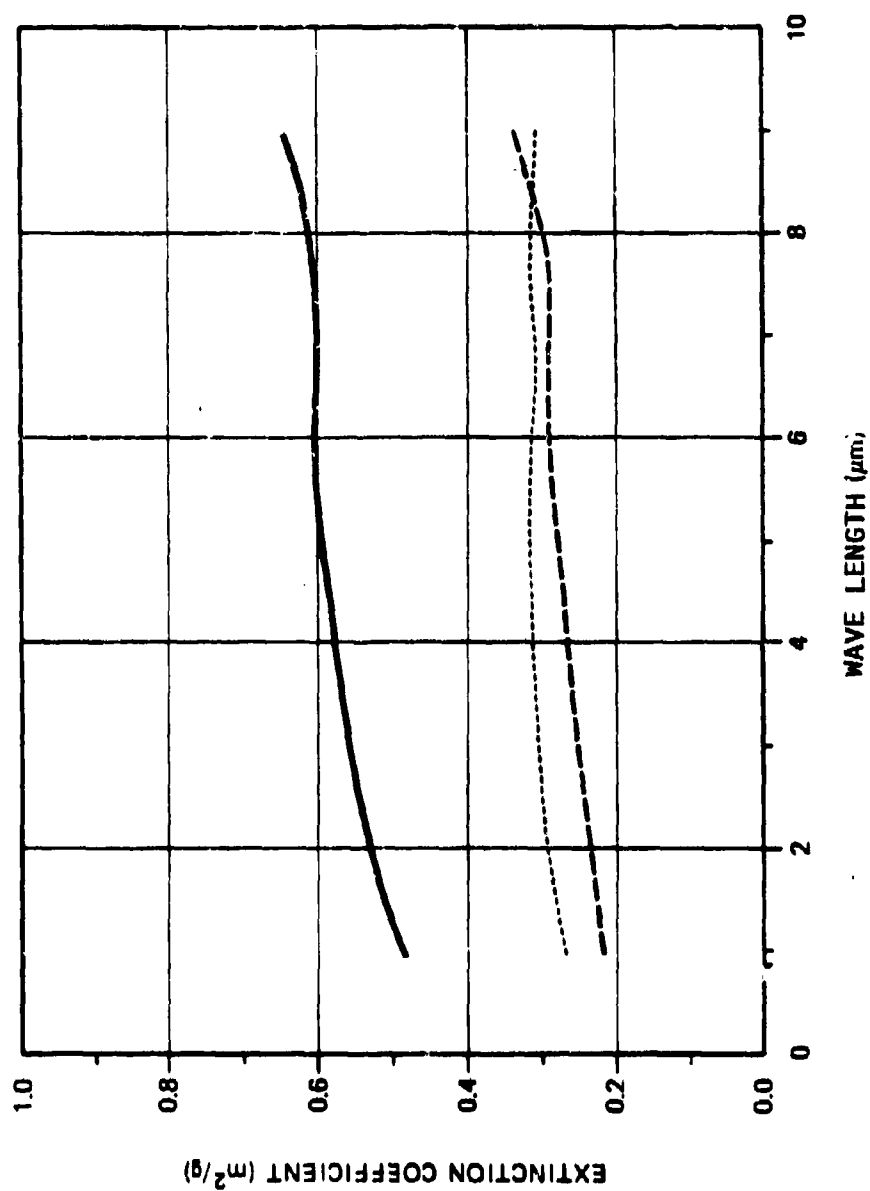


Figure 6. Extinction Coefficient for Graphite, Monodisperse
Diameter = 3.32

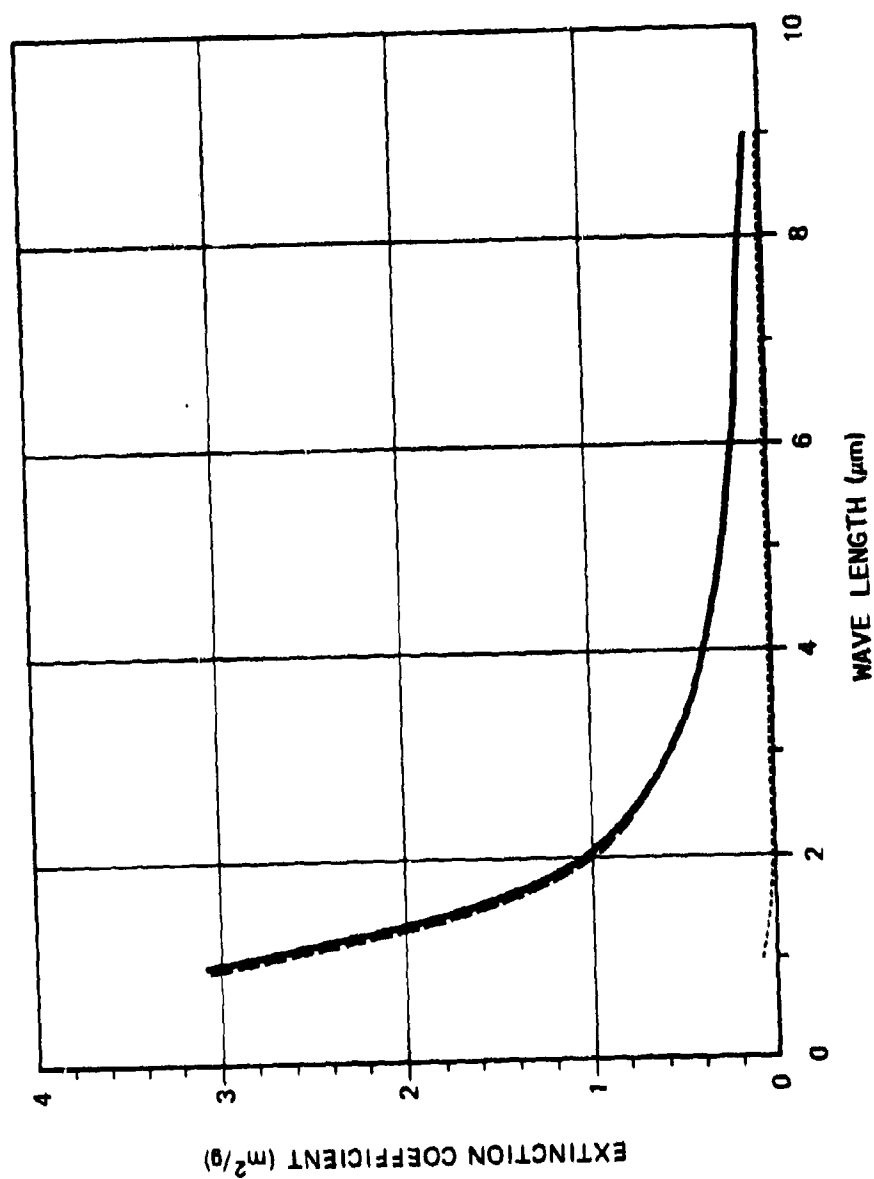


Figure 7. Extinction Coefficient for Graphite, Monodisperse
Diameter = .10

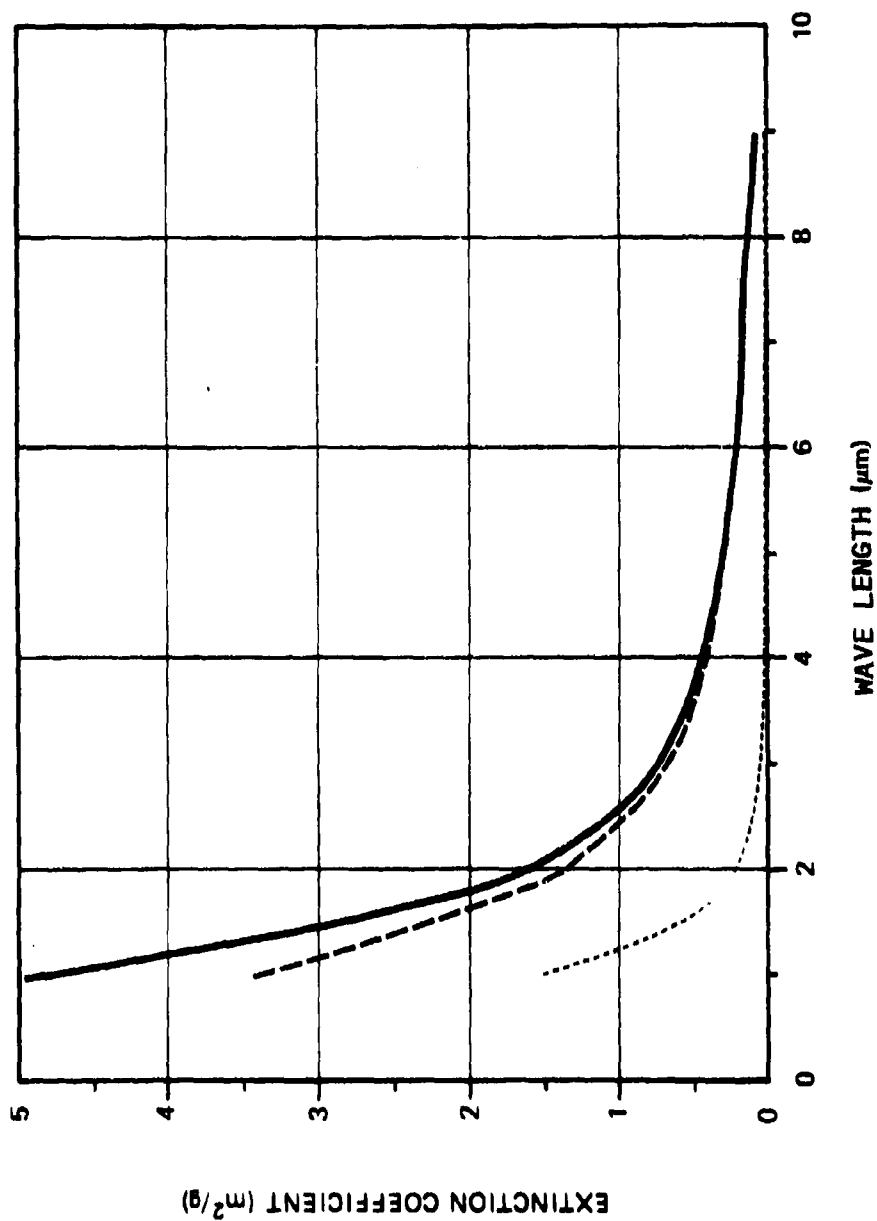


Figure 8. Extinction Coefficient for Graphite, Monodisperse
Diameter = .30

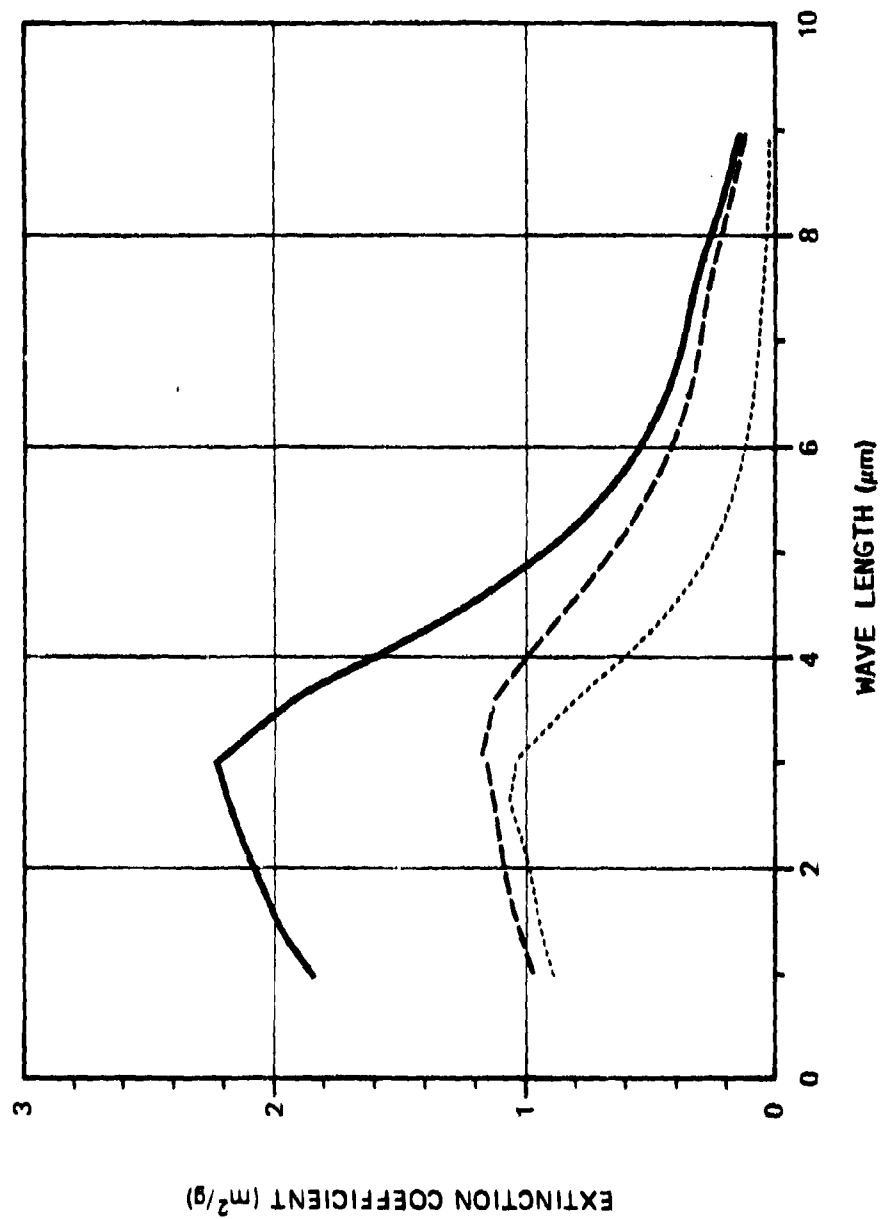


Figure 9. Extinction Coefficient for Graphite, Monodisperse
Diameter ≈ 1.00

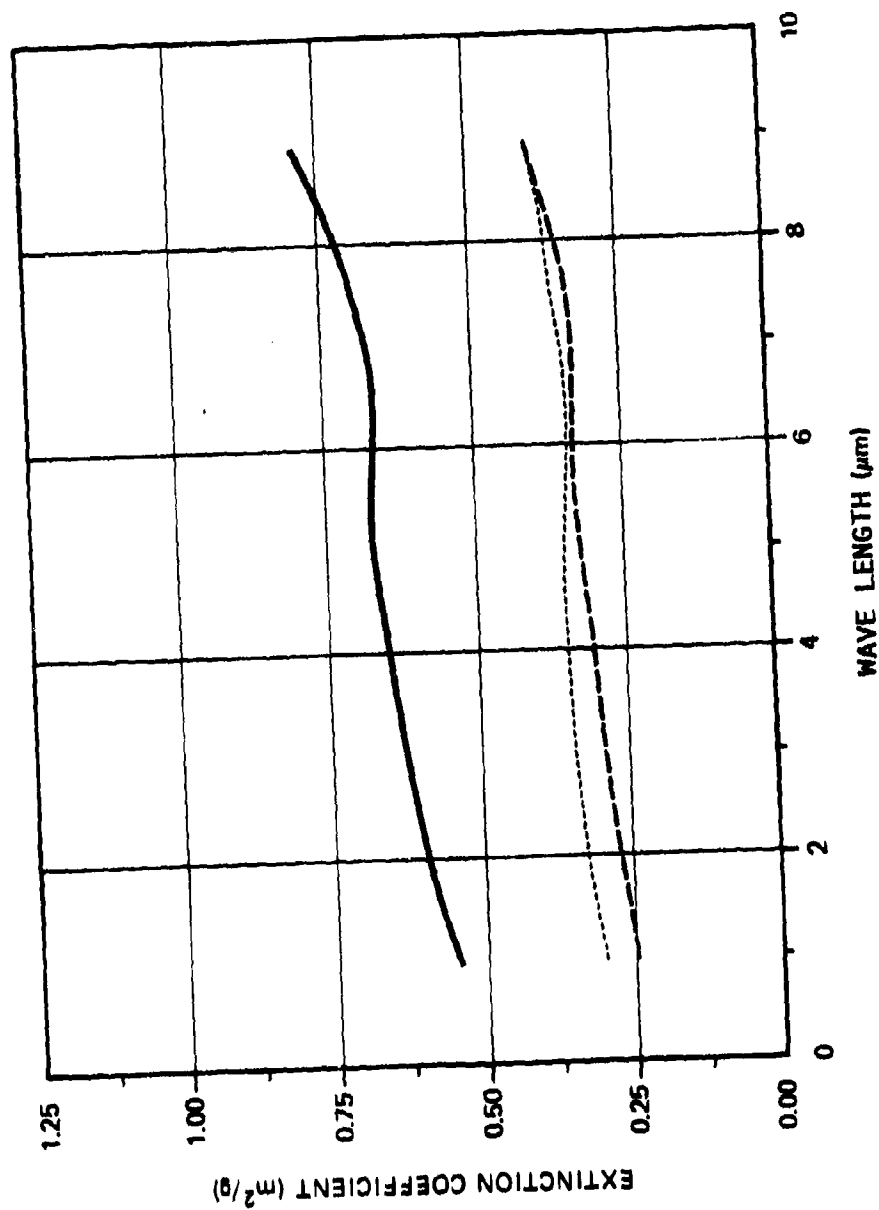


Figure 10. Extinction Coefficient for Graphite, Monodisperse
Diameter ≈ 3.00

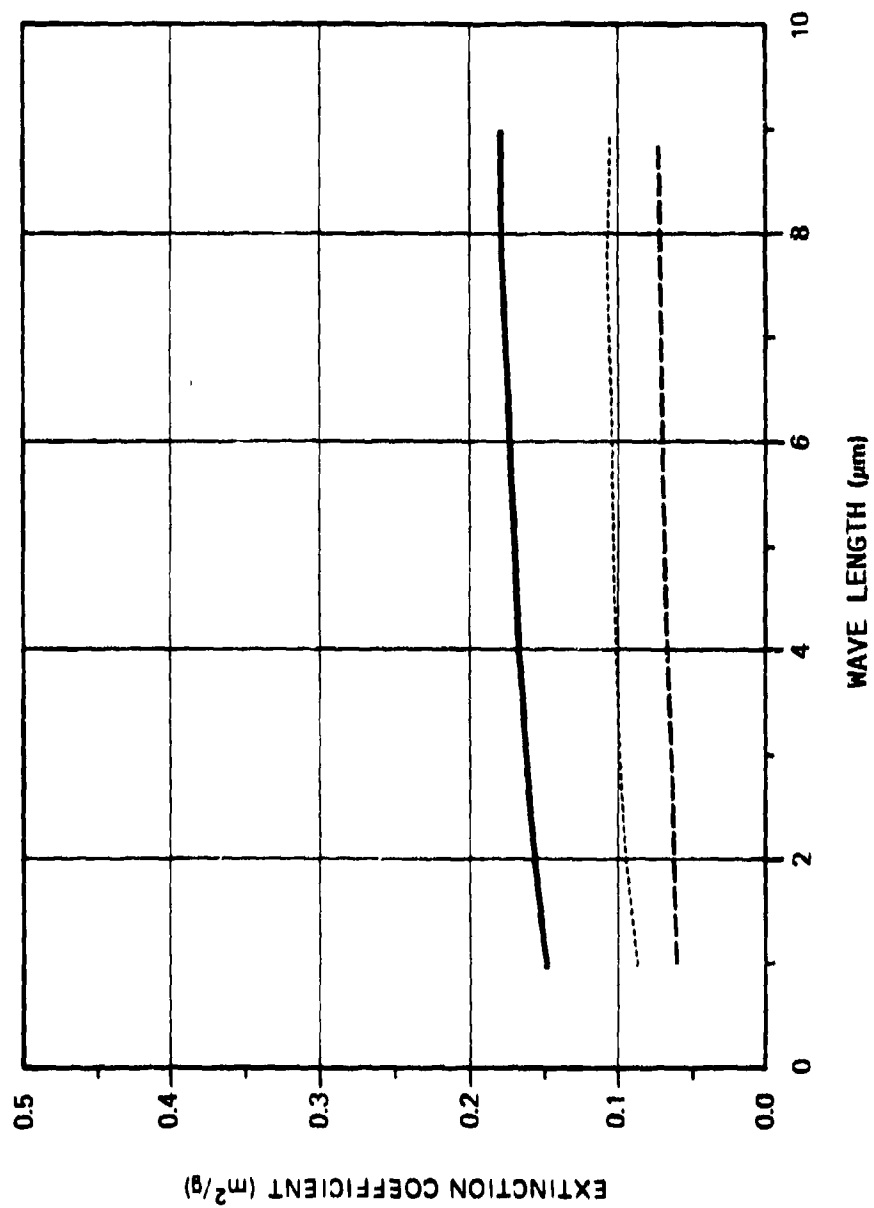


Figure 11. Extinction Coefficient for Graphite, Monodisperse
Diameter = 10.00

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