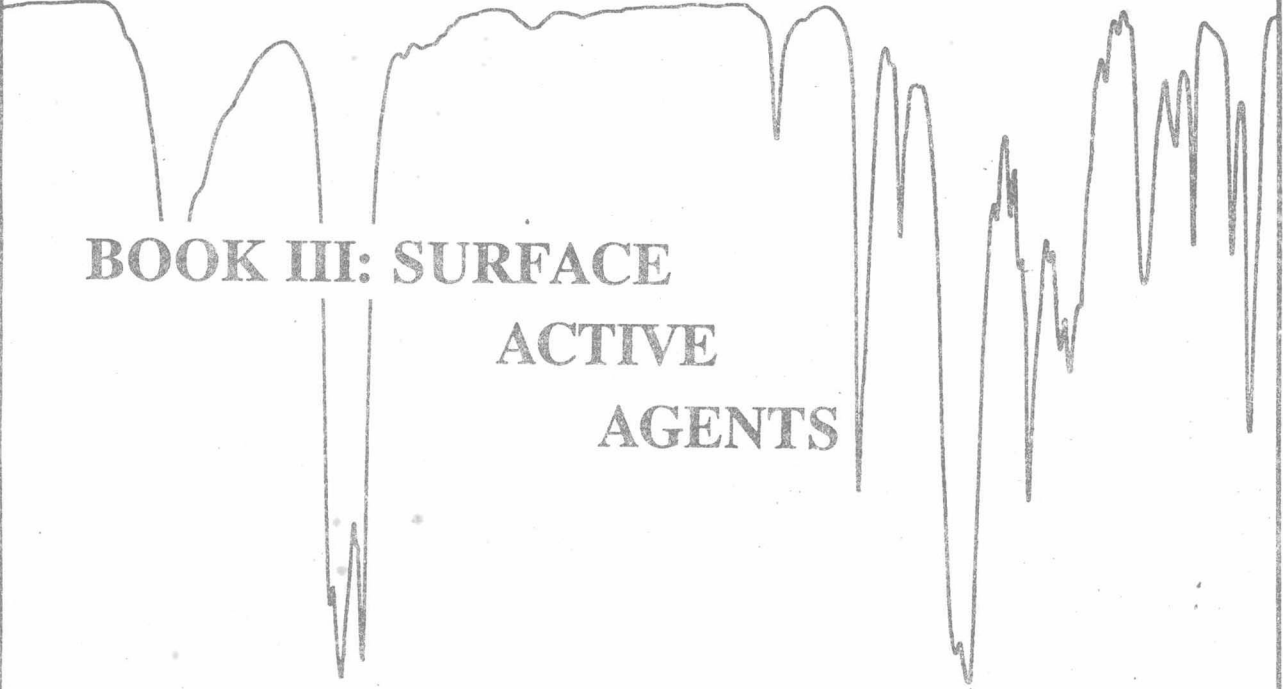


**SPROUSE
COLLECTION
OF
INFRARED SPECTRA**

An infrared spectrum line graph showing transmittance versus wavenumber. The graph features several prominent absorption bands, including a broad peak around 3400 cm⁻¹, sharp peaks in the 1600-1800 cm⁻¹ region, and a complex series of peaks in the fingerprint region below 1500 cm⁻¹.

**BOOK III: SURFACE
ACTIVE
AGENTS**

Sprouse Scientific Systems, Inc.

Distributors

USA and Canada

Elsevier Science Publishers
Journal Information Centre
655 Avenue of the Americas
New York, NY 10010

Rest of World

Elsevier Science Publishers
P.O. Box 211
1000 AE Amsterdam
The Netherlands

Copyright ©1988 Sprouse Scientific Systems, Inc.

All rights reserved.

No part of the material protected by this copyright notice may be reproduced or reprinted by optical, digital, electronic, mechanical or other means, including photocopying and recording, or by any information storage and retrieval system, without prior written permission from the copyright owner.

Library of Congress Catalog Card Number: 88-60429

ISBN 0-942595-03-3

Printed in the United States of America

**SPROUSE COLLECTION
OF
INFRARED SPECTRA**

**BOOK III: SURFACE ACTIVE
AGENTS**

Diana L. Hansen

EDITOR

Published by:

Sprouse Scientific Systems, Inc.
19 East Central Avenue
Paoli, Pennsylvania 19301 USA

PREFACE

TABLE OF CONTENTS

INTRODUCTION

SPECTRAL COLLECTION

NUMERICAL INDEX

ALPHABETICAL INDEX

CHEMICAL ABSTRACTS SERVICE
REGISTRY NUMBER INDEX

PREFACE

When Jim Sprouse and Diana Hansen asked me to write this preface, I felt honored, and also excited by the chance to say a few things about which I feel strongly concerning surfactants and surfactant chemistry.

Surfactants are among the most vital ingredients of many of the products we use, both industrially and on an everyday personal basis. In many instances, the surfactant is one of the small percentage "inactive" ingredients that doesn't show up on the label list until the very last. BUT almost every compounded product includes a surfactant, needs one, or could use a change in one. The use of surfactants makes possible the development of products in uniform stable emulsions which increase functionality, shelf life and attractiveness.

In the simplest sense, surfactants form the bridges that join oil to water, making it possible to disperse oil in water, or vice versa, which negates the old saying that oil and water don't mix. An emulsion, is of course, the oil-surfactant-water complex, a complex whose exact structure and behavior is dependent on the order in which the components contact one another, their concentrations, temperature and a number of other factors.

In working with surfactants, no course or training program takes the place of the old "on-the-job" method. A surfactant is a molecule that has an oil-like or lipid-soluble portion AND a waterlike or water-soluble portion. In other words, it doesn't know its head from its tail! A surfactant designed for an aqueous environment reacts in an altogether different way than in an oil environment. This alone makes predictability difficult -- not to mention the effects of surfactant-surfactant interactions! The first rule I learned on dealing with surfactants is -- throw away all the rules I already knew! Like dissolves like -- OUT! Heat it up and it dissolves faster--OUT! Add more and it thickens linearly -- OUT! All the rules I had already learned were no good anymore. In one of my first jobs, to my dismay, I found that because I knew how each surfactant from drums A, B, and C would behave in water, it did not mean that I could make predictions on how mixtures of A, B, and C would behave. Not only that, change the percentages of A, B, and C, and behavior took on a whole new direction. Change the order of addition -- put in B before A and C -- and a whole new product emerged.

Of course, there are some rules -- there always are -- but the polarity of the surfactant molecule makes those rules considerably different from the salt-in-water solution.

In considering analysis of surfactants which are emulsified, we have to consider that the surfactant is in close association with the two (or more) phases of the emulsion. In some types of analysis the emulsion must be broken in order

PREFACE

to identify the surfactant component. This emulsion-breaking can be difficult or impossible -- or the presence of the surfactant can completely skew the results. However, with FTIR, spectral subtraction, and spectral stripping, it becomes possible to identify components without emulsion-breaking, and to detect the extremely low levels of surfactant without "breaking" or extraction (remember, it is the "minor" component).

From a philosophical point of view, I would comment that the consideration of "organized solutions" is, for me, one of the most purely beautiful concepts in chemistry. We are accustomed to a sense of order in solids -- we can see that they are ordered -- a block sits there, does not change shape, evaporate or puddle out. Liquids are homogenous but chaotic. Surfactants, dispersed in a pure liquid, migrate to the surface and arrange themselves in uniform layers, in a manner dictated by their own structure and the character of the liquid. When no more surface area is available, micelles form, roughly spherical shapes which optimize the space available and set lipophilic tail-to-tail or hydrophilic head-to-head. At higher concentrations, where even micellar arrangements do not afford room, liquid crystals form slab-like structures that, again, use the space available to the fullest extent possible. The dictionary defines crystal as "a three-dimensional atomic, molecular, or ionic structure consisting of periodically repeated, identically constituted, congruent unit cells." The term "liquid crystal" appears to be an oxymoron, a combination of contradictory terms, but the surfactant molecules, in the move to optimize free energies, are arranged in "congruent unit cells" within an environment otherwise characterized by random movement and low interactions. It is this same phenomenon which forms membranes -- the "lipid bilayer" of phospholipids in our bodies, allowing the compartmentalization that allows us to exist. At 90+ % water, we are "organized solutions" made possible by surfactant arrangement.

When we encounter membranes, paints, adhesives, shampoos, resins, lotions, creams, squeezable ketchup, fire-fighting foams, bubble soap, surfactants, - those "minor" ingredients - are a vital, if not obvious, part of our way of life.

Connie M. Hendrickson, Ph.D.
Director
Ar'kon Consultants
Dallas, Texas

ACKNOWLEDGEMENTS

We would like to thank the following people whose efforts have been instrumental in the publication of this third book of the SPROUSE COLLECTION OF INFRARED SPECTRA.

A special thanks goes to Dr. Connie Hendrickson of Ar'kon Consultants, Dallas, Texas, for her assistance and support during the preparation of this collection of Infrared spectra. Her first hand knowledge of surfactants and the surfactant industry has given her an invaluable role in the production of this book.

We would also like to thank the personnel at Sprouse Scientific Systems, Inc. for their continued efforts in preparing both the spectra and the final copy for the book.

Sprouse Scientific Systems, Inc.

INTRODUCTION

HANDBOOK ORGANIZATION

The surface active agents in this handbook are grouped into four categories with ionic nature as the classification criterion. These categories - Anionic, Cationic, Nonionic and Amphoteric - are further subdivided and arranged by functional classification. This type of classification allows the user to easily compare absorption characteristics of compounds with similar functionality. Each compound in this collection is presented in a single page format, comprised of the infrared reference spectrum and pertinent chemical and physical property information. A spectrum number is located at the top or bottom center of each page and is used as a reference for all indices presented, as well as in conjunction with software programs offered along with the book. Primary names, located in the upper left-hand corner, are those generally accepted in the current body of literature. In some of the cases the Cosmetic, Toilet and Fragrance Association (CTFA) recommended name is used and a few entries follow the Chemical Abstract Service (CAS) naming conventions. Surface active agent manufacturers do not follow a specific naming convention, therefore, we have included available synonyms for each compound along with the primary name. These synonyms are also listed in the alphabetical index, so that a reference spectrum for a particular compound can be easily located by any of the names. Since all surfactants in this book were obtained directly from commercial manufacturers, the source and its patented tradename are listed separately from the other synonyms. It is important to note that samples from different manufacturers will have slight spectroscopic variances due to the type of raw materials used in the synthetic process. Also listed along with the tradename and source are the percent activity and the diluent associated with that commercial product. The physical properties selected for Book III, include specific gravity, viscosity, cloud point, pH and physical form. Additional information such as sample preparation technique, formula weight and general formula (based on chemical name) is also provided. All temperatures are given in degrees Celsius at standard temperature and pressure unless otherwise noted.

Wherever possible, the Hydrophile-Lipophile Balance (HLB) value is given. The HLB System, introduced by ICI Americas Inc. in the late 1940's, aids in the selection of an emulsifying agent for a given compound or mixture. The system allows the assignment of a "number" to the ingredient or combination of ingredients to be emulsified, which can then be matched to an emulsifier with the same number. An emulsifier that is lipophilic in character is assigned a low HLB number (below 9.0) and one that is hydrophilic is assigned a high HLB number (above 11.0). In general, the HLB is an accurate indicator of what the emulsifier system will do, that is, whether it will make a water-in-oil (W/O) emulsion, an oil-in-water (O/W) emulsion or act as a solubilizer for an oil.

Three indices are included in this handbook. The first is a numerical index of the compounds, listing the primary name given for each compound. An alphabetical index is second, inclusive of the many synonyms, acronyms and common manufacturer tradenames associated with each of the primary names. The Chemical Abstracts Service registry number index is presented last, and lists each compound by increasing CAS number. All information listed in these indices is represented by spectral number. All samples were obtained directly from commercial manufacturers and are readily available from these sources.

INTRODUCTION

SAMPLE PREPARATION

Surfactant samples were received from suppliers as solids, liquids and solutions. The solid samples were dissolved in an appropriate solvent and a thin film was cast onto potassium bromide (KBr) salt plates. Liquid organic samples were measured neat between two KBr salt plates. Samples obtained in solution were cast directly onto KBr salt plates and the solvent was evaporated. Extreme care was taken to avoid residual solvent band contamination in the spectra. The following is an explanation of the abbreviations used in this book for sample preparation techniques:

Neat - A liquid sample was prepared as a thin film between two KBr salt plates.

Solvent/Cast - A solid sample was dissolved in an organic solvent. Then a film of the solute was cast onto a KBr plate by evaporating the solvent. The actual name of the solvent is given, e.g. Chloroform/Cast.

Melt - The sample was melted and spread into a film between two KBr salt plates. It was then allowed to recrystallize at room temperature before the spectrum was measured.

KBr - A hygroscopic sample was ground into a powder using a mortar and pestle and then pressed into a KBr matrix using 6.8 metric tons of pressure.

INSTRUMENTATION

All Infrared spectra presented in this book were measured on either a Digilab FTS-40 or a Perkin-Elmer 1710 Fourier Transform Infrared (FTIR) Spectrometer, measured with an optical retardation of 0.125 equivalent to 2 cm^{-1} nominal resolution over the mid-IR spectral range (4400-400 cm^{-1}). Data were collected with sufficient signal averaging to provide signal-to-noise ratio greater than 5,000 to 1 over the entire spectral region. Fast Fourier Transform (FFT) processing was completed using triangular apodization with a zero filling factor of two. These spectrometers are equipped with laser guided interferometers which ensure wavenumber accuracy better than $\pm 0.01 \text{ cm}^{-1}$. Samples were carefully prepared in order to provide strongest band absorbance in the range between 0.5 and 1.5 absorbance units. All spectra in the book are presented in a %Transmission format and were plotted directly to the graphs from the digital reference spectrum. Sprouse Scientific's standards require that all hard copy spectra have a flat baseline, set as close to 100%T as possible. A low level of digital smoothing was performed for appearance sake.

INTRODUCTION

INSTRUMENT QUALITY CONTROL

The infrared spectrometer was tested for frequency calibration, photometric accuracy and baseline stability on a routine basis throughout data measurement. In addition, all spectra were carefully checked for residual solvent bands and sample contamination. The following quality control methods are used as standard operating procedure in the Sprouse Scientific laboratories:

1) Wavenumber Calibration

The IUPAC (International Union of Pure and Applied Chemistry) recommended wavenumber standard material was used for the spectrometer wavenumber calibration. Two mixtures were used:

- a) A solution of 98.4 parts Indene, 0.8 parts Camphor and 0.8 parts Cyclohexanone (wt/wt) was used to calibrate the spectral range between 4400-600 cm^{-1} .
- b) A solution containing equal parts (wt/wt) of Indene, Camphor and Cyclohexanone was used to calibrate the spectral range between 600-400 cm^{-1} .

Infrared spectra of the two calibration mixtures were obtained using a 0.25mm fixed path length liquid cell. The peak positions of 50 bands were located and confirmed to the IUPAC assigned band locations. This performance check was run approximately every 30 days. Carbon dioxide reference bands were used for daily wavenumber calibration checks. Peak positions were measured at 2361.6 ± 0.2 , 2336.6 ± 0.2 and 668.5 ± 0.2 cm^{-1} .

2) Instrument Performance and Stability

The performance and stability of the instrument was monitored on a daily basis by measuring the RMS noise in a 100%T baseline at selected frequencies across the spectral range. The 100%T line was measured each day by taking the ratio of one single beam spectrum to another. The 100% line was plotted between 98 and 102%T and the RMS noise level was calculated in the spectral regions of 3950-4050, 1950-2050, 950-1050 and 450-550 cm^{-1} . A baseline with a maximum of 2% RMS peak-to-peak noise within these regions was used as the criterion for acceptable performance for this instrument.

3) Atmospheric Contaminants

The presence of water vapor, carbon dioxide and hydrocarbons were strictly monitored during sample scanning. The optical head was purged continuously with $\text{N}_2(\text{g})$ boiled off from liquid nitrogen in order to minimize background contamination. Repeated scanning of the background and sample were made for total compensation of these contaminants. For spectra measured as KBr pellets, spectra containing water absorption bands were not accepted if their intensity exceeded 2%T peak-to-peak. Some water vapor bands are evident in the spectra despite thorough purging of the optical head with dry nitrogen. However, these background bands are generally obvious and do not interfere with the important spectral bands in the sample.

SPECTRAL
COLLECTION

TABLE OF CONTENTS

<u>Name</u>	<u>Page No.</u>
INTRODUCTION	ix-xi
SPECTRAL COLLECTION (Indexed by Spectrum #)	1-700
ANIONICS	1-184
Carboxylic Acid Salts	1-57
Sulfonic Acid Salts	58-121
Alkylbenzene Sulfonates	58-63
Toluene-, Xylene-, and Cumene Sulfonates	64-68
Lignosulfonates	69-75
Petroleum Sulfonates	76-80
N-Acyl-n-alkyltaurates	81-84
Sulfosuccinate Esters	85-101
Naphthalene Sulfonates	102-109
Misc. Sulfonates	110-121
Sulfuric Acid Ester Salts	122-170
Sulfated Linear Alcohols	122-136
Sulfated POE Alcohols	137-148
Misc. Sulfated Linear Alcohols	149-160
Glutamates	161-165
Sarcosines and Sarcosinates	166-170
Fluorinated Anionics	171-174
Phosphoric and Polyphosphoric Acid Esters	175-184
CATIONICS	185-328
Long-Chain Amines	185-209
Cyclic Amines	210-217
Long-Chain Amine Esters	218-225
Diamines and Their Salts	226-240
Triethanolamine Salts	241-251

TABLE OF CONTENTS

<u>Name</u>	<u>Page No.</u>
Morpholine Salts	252-261
Quarternary Ammonium Salts	262-291
Fluorinated Cationics	292-293
POE Long-Chain Amines	294-319
Amine Oxides	320-328
NONIONICS	329-659
Long-Chain Fatty Acids	329-356
Long-Chain Oils and Fats	357-367
Long-Chain Alcohols	368-380
POE Alkylphenols	381-406
POE Alkyl Ethers (Alcohols)	407-438
POE and POP Glycols	439-455
POE Mercaptans	456-460
Long-Chain Carboxylic Acid Esters	461-624
Alkyl Carboxylic Acid Esters	461-477
Glycerol and Polyglycerol Esters	478-494
Trimethylolpropane and Pentaerythritol Esters	495-503
POE Fatty Acid Esters	504-574
Sorbitan and Sorbitol Esters	575-599
Sucrose Esters	600-605
Glutamates	606-609
Misc. Amine Derivatives	610-611
Amides	612-624
Amine Alcohols	625-627
Alkanolamides	628-648
Siloxanes	649-652
Fluorinated Nonionics	653-657
POE Phosphates	658-659

<u>Name</u>	<u>Page No.</u>
AMPHOTERICS (ZWITTERIONICS)	660-700
N-Alkyl-beta-Aminoalkyl Acids	660-661
N-Alkyl-beta-Iminodipropionates	662-664
Oxazoline Derivatives	665-666
Alkyl Esters	667-677
n-Alkyl Betaines	678-691
Misc. Betaines	692-694
Sultaine and Sulfonate Derivatives	695-700
NUMERICAL INDEX	702-722
ALPHABETICAL INDEX	724-794
CHEMICAL ABSTRACTS REGISTRY NUMBER INDEX	796-808

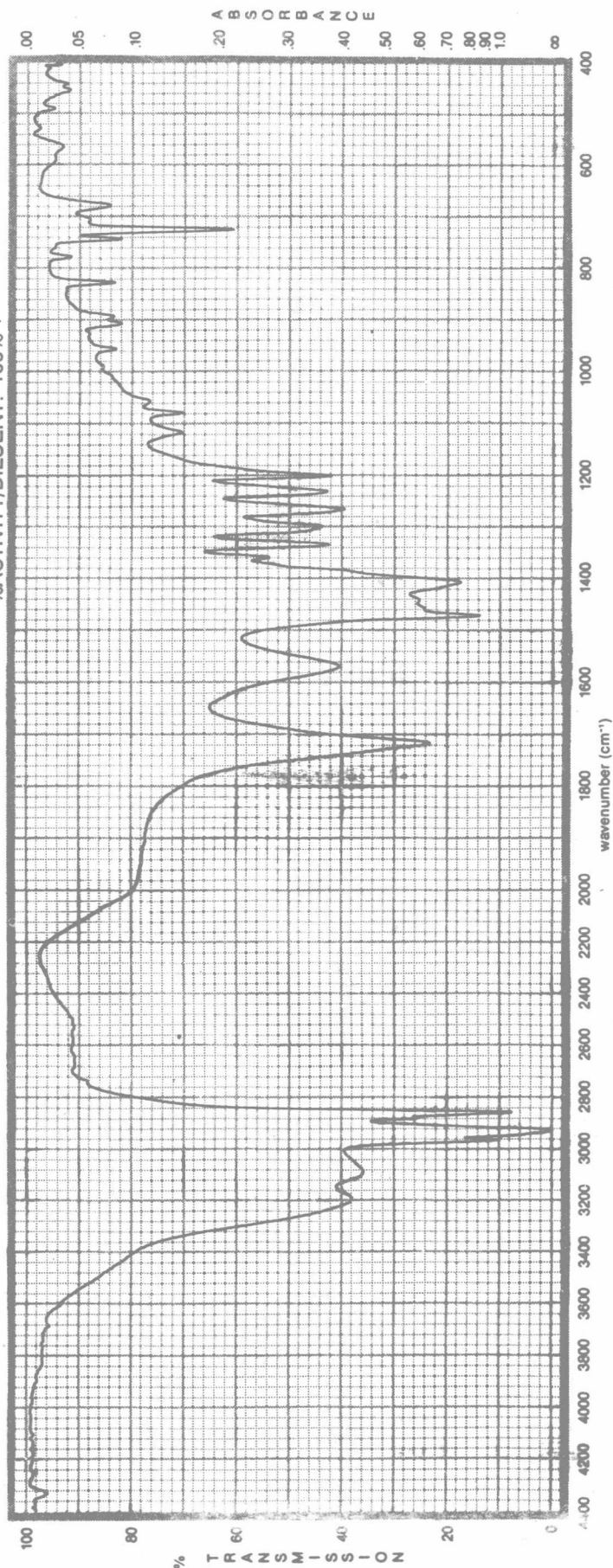
spectrum

1

AMMONIUM CAPRATE

SYNONYMS: AMMONIUM DECANOATE
CAPRIC ACID, AMMONIUM SALT
DECANOIC ACID, AMMONIUM SALT

CAS #: —
SOURCE: Sprouse Scientific Systems, Inc.
TRADENAME:
%ACTIVITY/DILUENT: 100%



Perkin-Elmer 1710

TECHNIQUE: KBr

PHYSICAL PROPERTIES

PHYSICAL FORM: Colorless solid crystals

FORMULA WEIGHT: 189.30

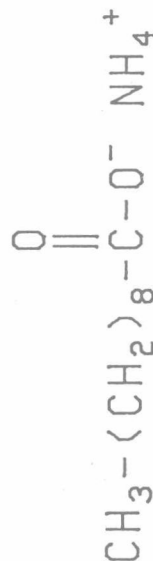
SPECIFIC GRAVITY: —

VISCOSITY: —

CLOUD POINT: —

pH: —

HLB: —



GENERAL FORMULA: C₁₀H₂₃N₁O₂

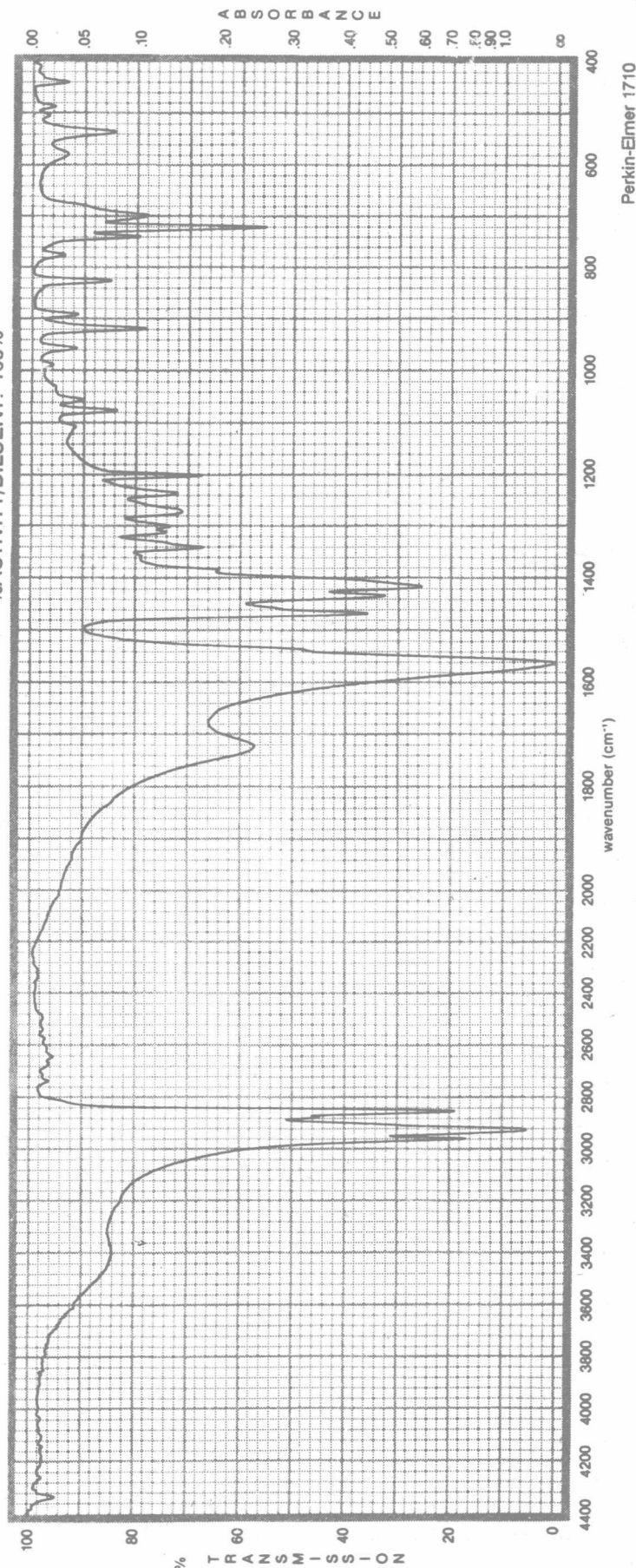
© 1988 Sprouse Scientific Systems, Inc.



POTASSIUM CAPRATE

SYNONYMS: POTASSIUM DECANOATE
CAPRIC ACID, POTASSIUM SALT
DECANOIC ACID, POTASSIUM SALT

CAS #: —
SOURCE: Chem Service
TRADENAME:
%ACTIVITY/DILUENT: 100%



TECHNIQUE: KBr

PHYSICAL PROPERTIES

PHYSICAL FORM: Off-white solids

FORMULA WEIGHT: 210.36

SPECIFIC GRAVITY: —

VISCOSITY: —

CLOUD POINT: —

pH: —

HLB: —



GENERAL FORMULA: C₁₀H₁₉O₂K₁

2
spectrum

© 1988 Sproule Scientific Systems, Inc.

