STANDARD ULTRA VIOLET Spectra

Vol. 92
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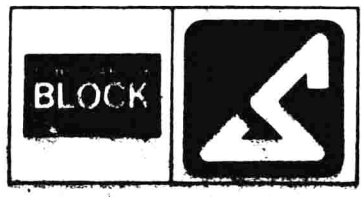

SADTLER RESEARCH LABORATORIES, INC.

ULTRA VIOLET SPECTRA

CREATIVE CHEMISTS SINCE 1874

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On the other hand every effort is made by Sadtler Research Laboratories, Inc. to assure the reliability of the published spectra. When improved data is available or errors are called to our attention we revise and reissue the proper replacement spectra.

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SADTLER STANDARD ULTRAVIOLET SPECTRA

VOLUMES 91 - 94

This 1977 supplement of 2,000 spectra to the Sadtler Standard Ultraviolet Spectra collection brings the total catalog to 40,000 ultraviolet and/or visible spectra representing 25,795 organic compounds. With the exception of colored compounds, spectra are determined in the ultraviolet region from 200 to 350 mμ. The spectra of colored compounds are extended to cover the visible region and are determined in the 200 to 500 mμ or 200 to 800 mμ regions.

The ultraviolet spectra of many compounds, especially those containing an ionizable group directly attached to a chromophore, are distinctly affected by the polarity of the solvent system in which they are determined. Therefore many of the compounds have been scanned in acidic and/or basic media to note the influence of pH on the spectrum.

I. Instrumentation:

All spectra in this supplement were prepared by Sadtler Research Laboratories on either a Cary 15 spectrophotometer or a Beckman Model 25 spectrophotometer.

II. Experimental:

The first spectrum of a compound, in neutral medium, was run on a solution of the compound in methanol. If the nature of the compound indicated that a change in pH would alter the neutral spectrum, the pH was adjusted to 1 or 11 by the addition of aqueous 2NHCl or 2NKOH respectively and the "acid" and/or "base" spectra prepared. If the spectra did not alter after pH adjustment or precipitation occurred, these spectra were not included in the publication. Thus a single compound may be represented by one, two or three spectra depending upon the results obtained.

Generally, when more than one concentration was required to bring the absorbance maxima within the absorbancy range of the instrument it was preferrable to alter the cell thickness rather than the concentration.

III. Chart Legend:

In order to make both qualitative and quantitative aspects of the curves more evident, each chart is provided with a legend tabulating the following information.

1. λ max. – the wavelength of maximum absorption, indicated to the closest 0.5 mμ.

2. Concentration, in grams/liter; g/l

3. a_m – molar absorptivity (also known as ϵ, the molecular extinction coefficient). This term is calculated from the equation,

$$a_m = \frac{A}{b.c_m}$$

, where A = observed absorbancy
c_m = conc. in mol/l
b = cell thickness in cm.

4. Cell thickness

5. Solvent

NOTE: 1. a_m has been calculated to three significant figures, the limit of accuracy attainable in reading A.

2. The position of λ max. and the values of A were determined from the chart paper, which in turn was calibrated using a standard, not from the instrument dials. For reasons of available space, up to six maxima are indicated (if more than six maxima are exhibited by a compound, only six are shown). A maximum is interpreted as the point at which the slope of the curve changes sign (+ to - or vice versa). Therefore, a shoulder, although quite pronounced, is not recorded. Also, as solvent cutoff, atmospheric absorption and widening slits influence the shape of the curve at shorter wavelength, no maximum is reported for a wavelength below 210 mμ unless it is a pronounced peak.

3. a_m does not appear for many of the earlier run spectra

IV. Compound Data:

Each substance is listed by its Chemical Abstracts name, molecular formula, molecular weight, melting point and other physical data, when available, and source. Commencing with this issue of publication, all ultraviolet spectra are numbered consecutively by a UV number and a notation is also made of the corresponding infrared (IR) number. This practice will be continued so that interleaving of subsequent spectra is no longer required, as was the case when the spectra were numbered only with IR numbers.

V. Indices:

The chemical compounds scanned for the Sadtler Ultraviolet Spectra collection were selected from the compounds listed in the Sadtler Standard Infrared collection. Compounds can be searched for using an Alphabetical Index, by name; a Molecular Formula Index, Numerical Index, Chemical Classes Index, according to functional group and a Locator, according to maxima and absorbance.

24815 UV

Sadtler Research Laboratories, Inc.,

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IR 48806

5-(α-HYDROXY-p-NITROBENZYL)HYDANTOIN

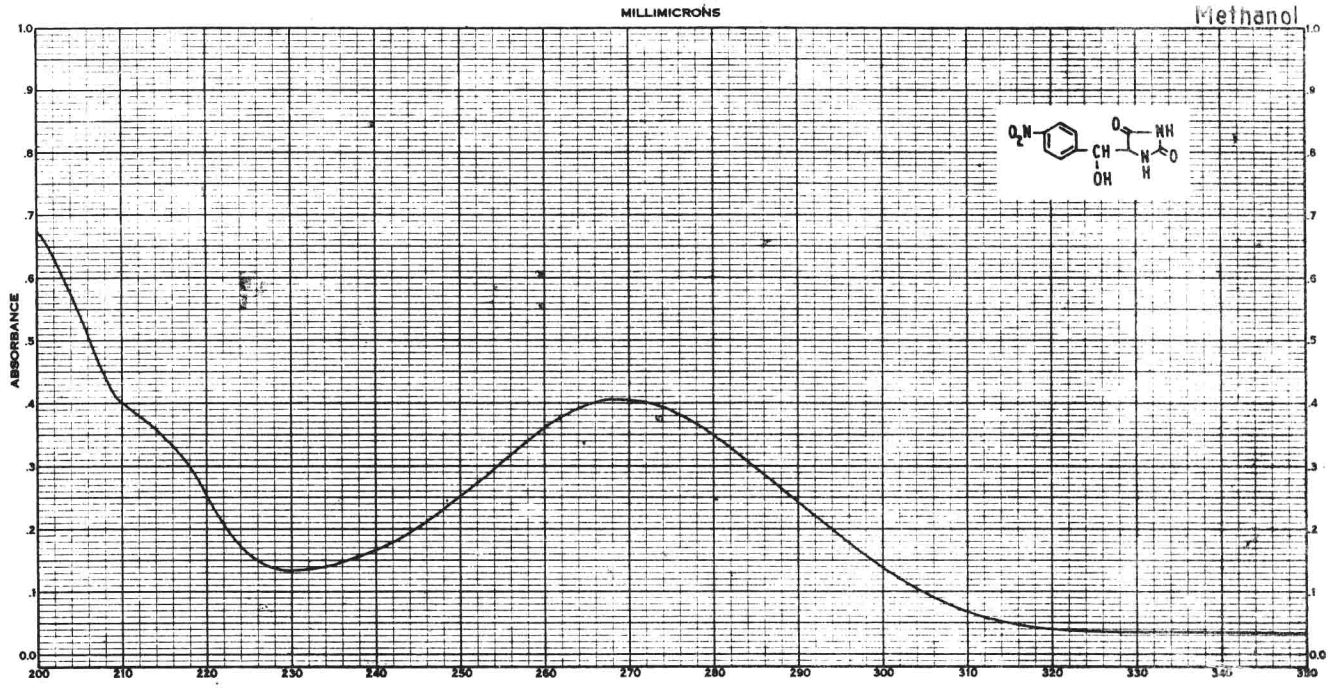
$C_{10}H_9N_3O_5$ Mol. Wt. 251.20 M.P. 241°C

Source of Sample: Maybridge Chemical Company Ltd., North Cornwall, England

		A	B	C	D	E
Methanol	Conc. g/L	0.100				
	Cell mm	1				
	^{a}m	10200				
	λ Max. mμ	268				

	Conc. g/L					
	Cell mm					
	^{a}m					
	λ Max. mμ					

	Conc. g/L					
	Cell mm					
	^{a}m					
	λ Max. mμ					



24816 UV

Sadtler Research Laboratories, Inc.,
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IR 48809

3-[(4-PYRIDYL)METHYL]RHODANINE

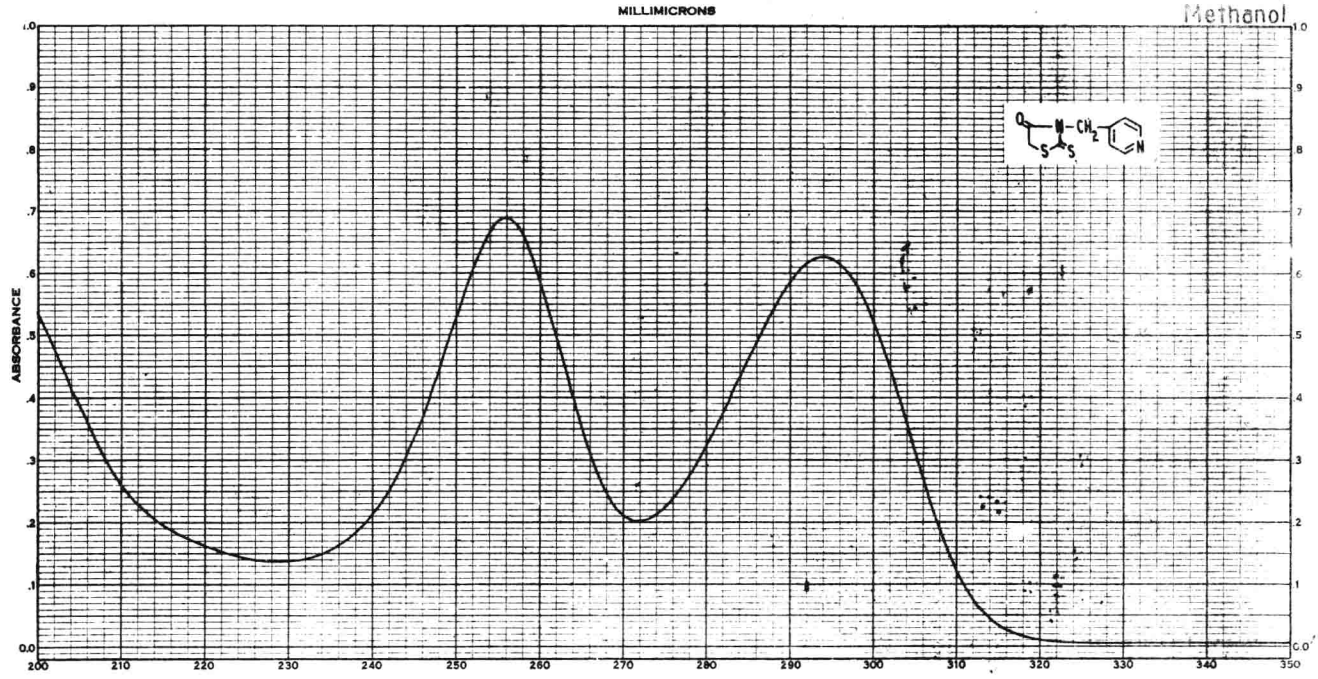
$C_9H_8N_2OS_2$ Mol. Wt. 224.30 M.P. 149°C

Source of Sample: Maybridge Chemical Company Ltd.,
North Cornwall, England

		A	B	C	D	E
Methanol	Conc. g/L	0.100	0.100			
	Cell mm	1	1			
	a_m	14000	15500			
	λ Max. mμ	294	256			

	Conc. g/L					
	Cell mm					
	a_m					
	λ Max. mμ					

	Conc. g/L					
	Cell mm					
	a_m					
	λ Max. mμ					



Sadtler Research Laboratories, Inc.,
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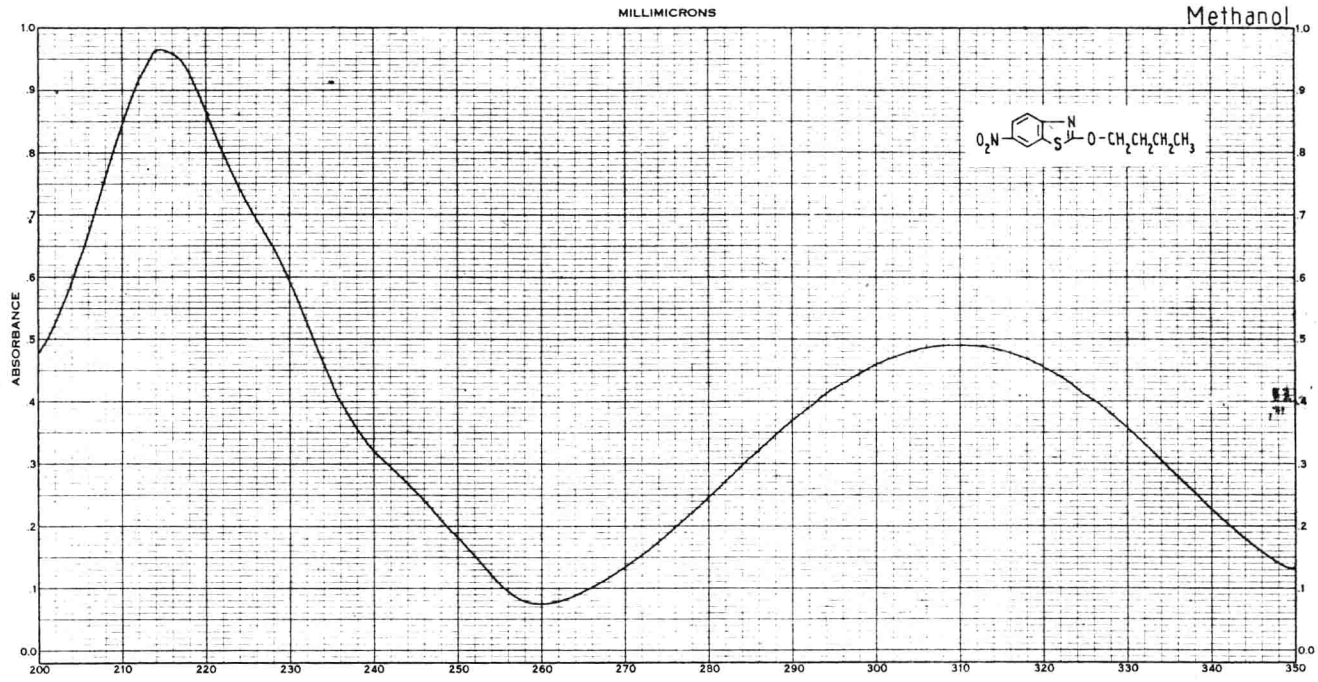
IR 48810

2-BUTOXY-6-NITROBENZOTHIAZOLE

$C_{11}H_{12}N_2O_3S$ Mol. Wt. 252.29 M.P. 57-58°C

Source of Sample: Maybridge Chemical Company Ltd.,
North Cornwall, England

		A	B	C	D	E
Methanol	Conc. g/L	0.100	0.100			
	Cell mm	1	1			
	^{a}m	12400	24600			
	λ Max. mμ	310	215			
	Conc. g/L					
	Cell mm					
	^{a}m					
	λ Max. mμ					
	Conc. g/L					
	Cell mm					
	^{a}m					
	λ Max. mμ					



24818 UV

Sadtler Research Laboratories, Inc.,
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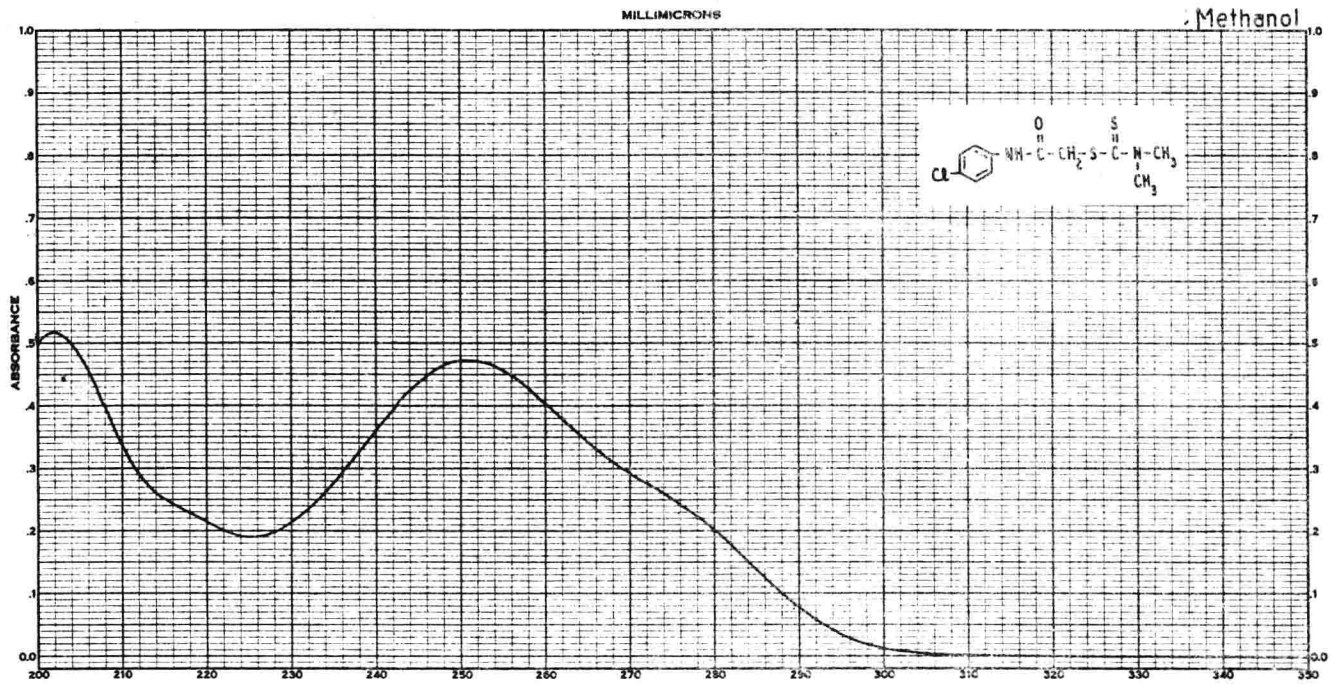
IR 48811

DIMETHYLDITHIOCARBAMIC ACID, ESTER WITH 4'-CHLORO-2-MERCAPTOACETANILIDE

$C_{11}H_{13}ClN_2OS_2$ Mol. Wt. 288.82

Source of Sample: Maybridge Chemical Company Ltd.,
North Cornwall, England

		A	B	C	D	E
Methanol	Conc. g/L	0.100				
	Cell mm	0.5				
	^{a}m	27300				
	λ Max. mμ	250.5				
	Conc. g/L					
	Cell mm					
	^{a}m					
	λ Max. mμ					
	Conc. g/L					
	Cell mm					
	^{a}m					
	λ Max. mμ					



24819 UV

Sadtler Research Laboratories, Inc.,

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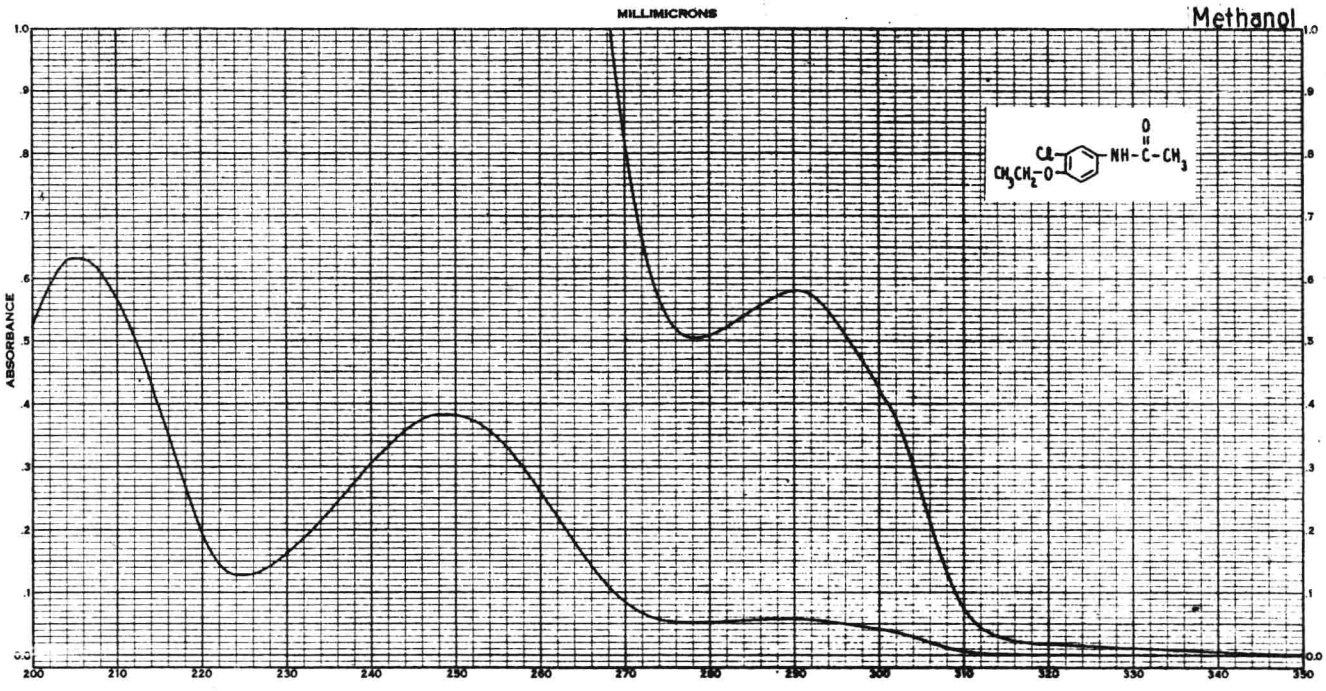
IR 48812

3'-CHLORO-p-ACETOPHENETIDIDE

$C_{10}H_{12}ClNO_2$ Mol. Wt. 213.67

Source of Sample: Maybridge Chemical Company Ltd., North Cornwall, England

		A	B	C	D	E
Methanol	Conc. g/L	0.100	0.100	0.100		
	Cell mm	5	0.5	0.5		
	a_m	2480	16400	27100		
	λ Max. mμ	290	249	205		
	Conc. g/L					
	Cell mm					
	a_m					
	λ Max. mμ					
	Conc. g/L					
	Cell mm					
	a_m					
	λ Max. mμ					



24820 UV

Sadtler Research Laboratories, Inc.,
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IR 48813

2-[(4-CHLORO-3,5-XYLYL)OXY]PROPIONIC ACID

$C_{11}H_{13}ClO_3$ Mol. Wt. 228.68

Source of Sample: Maybridge Chemical Company Ltd.,
North Cornwall, England

		A	B	C	D	E
Methanol	Conc. g/L	0.100	0.100	0.100	0.100	0.100
	Cell mm	10	10	2.5	2.5	0.5
	$^{a}_{m}$	1220	1270	8870	8900	x
	λ Max. mμ	284	277	226	220	x
	Conc. g/L					
	Cell mm					
	$^{a}_{m}$					
	λ Max. mμ					
	Conc. g/L					
	Cell mm					
	$^{a}_{m}$					
	λ Max. mμ