

ULTRAVIOLET STUDY OF SOME NEW N,N -  
DISUBSTITUTED THIOUREA COMPOUNDS OF POTEN-  
TIAL BIOLOGICAL INTEREST

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تم دراسة امتصاص الأشعة فوق البنفسجية لمجموعة من مركبات الثيوريوريا  
الناتجة التتويج. ولقد وجد بأن الامتصاص في الموضع 361-312 نانوميتر يعزى إلى انتقال  
الشحنة التجمعية.

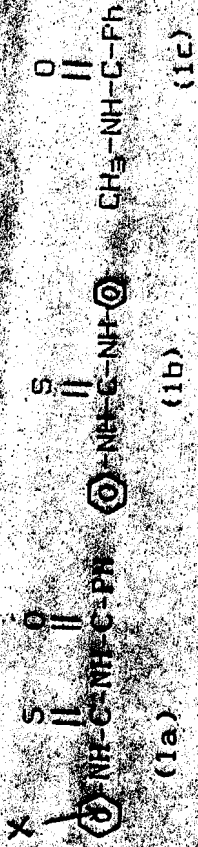
The Ultraviolet absorption spectra of fourteen compounds of N,N-  
disubstituted thioureas have been investigated. The band at 312-361 nm was assigned to  
an intramolecular charge transfer transition.

INTRODUCTION

Previous work on N,N- disubstituted thioureas had been  
concentrated on the synthesis [1,2] and infrared studies  
[3-5]. the present work deals with the interpretation of the  
UV absorption bands of N,N-disubstituted thioureas (Scheme  
1), a work which has not been attempted previously. The UV  
data of the fourteen compounds are interpreted in terms of  
two chromophores, the N,N-diphenyl thiourea (Scheme 1b) and  
the substituted anilide (Scheme 1c).

4 Free

Substitution of unsaturated chromophore to a benzene ring  
produces a strong effect on the 203 and 256 nm band [6,7].  
In substituted anilide (1c) the 'B<sub>1u</sub>' ← 'A<sub>1g</sub>' transition  
occur at 238 nm [8] while in compound 1 (1b) (Table 1) the



(Scheme 1)

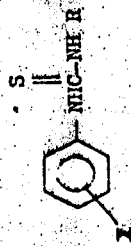
'A<sub>1g</sub>' transition of the phenyl moiety is  
shifted to 276 nm (logε = 4.462). No absorption in both  
(1b) and (1c) exist at wavelength higher than 276 nm.  
The n → π\* transition of the C = S moiety appears at  
longer wavelength to that of the carbonyl group (9-11). The  
intensity of the n → π\* transition is quite small and  
embodied under the intense π → π\* band.  
The aim of this work is to gain further insight into  
the UV spectra of N,N-disubstituted thioureas.

EXPERIMENTAL

The method of preparation of the N,N-disubstituted  
thiourea is given elsewhere [2]. All solvents used in  
UV measurements were of spectroscopic grade (Fluka Ltd) and  
were used without further purification. The UV spectra were  
recorded on Pye-Unicam SP 800B and Pye-Unicam SP 8-100.

Table 1

UV absorption of N,N-disubstituted thiourea.



Compd No.	X	Solvent	band I	log ε	band II	log ε	H
1	H	CHCl <sub>3</sub>	276	4.462	-	-	Phenyl
2	H	CHCl <sub>3</sub>	266	4.380	314	4.000	benzoyl
		ethanol	265	4.312	306	3.929	benzoyl
		E.G	264	4.097	304	3.699	benzoyl
3	p-NO <sub>2</sub>	CHCl <sub>3</sub>	282	4.347	344	4.114	benzoyl
		ethanol	284	3.600	345	4.146	benzoyl
		E.G	280	4.243	340	3.954	benzoyl
4	p-OC <sub>2</sub> H <sub>5</sub>	CHCl <sub>3</sub>	279	4.342	324	3.837	benzoyl
5	p-N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	CHCl <sub>3</sub>	285	4.347	390	3.796	benzoyl
6	p-EtN-N-	CHCl <sub>3</sub>	296	4.264	356	4.332	benzoyl
7	p-CH <sub>3</sub> CONH	CHCl <sub>3</sub>	276	4.366	328	3.889	benzoyl
8	p-Cl	CHCl <sub>3</sub>	270	4.284	318	3.860	benzoyl
9	m-NO <sub>2</sub>	CHCl <sub>3</sub>	264	4.505	313	4.044	benzoyl
10	m-Cl	CHCl <sub>3</sub>	267	4.312	314	3.942	benzoyl
11	o-OC <sub>2</sub> H <sub>5</sub>	CHCl <sub>3</sub>	272	4.301	326	4.021	benzoyl
12	o-Cl	CHCl <sub>3</sub>	270	4.279	316	3.903	benzoyl
13	o-NO <sub>2</sub>	CHCl <sub>3</sub>	255	4.439	360	3.477	benzoyl
14	o-OC <sub>2</sub> H <sub>5</sub>	CHCl <sub>3</sub>	286	3.613	370	3.470	benzoyl
14	p-NO <sub>2</sub>	ethanol	284	3.646	361	3.415	benzoyl

E.G = ethylene glycol.

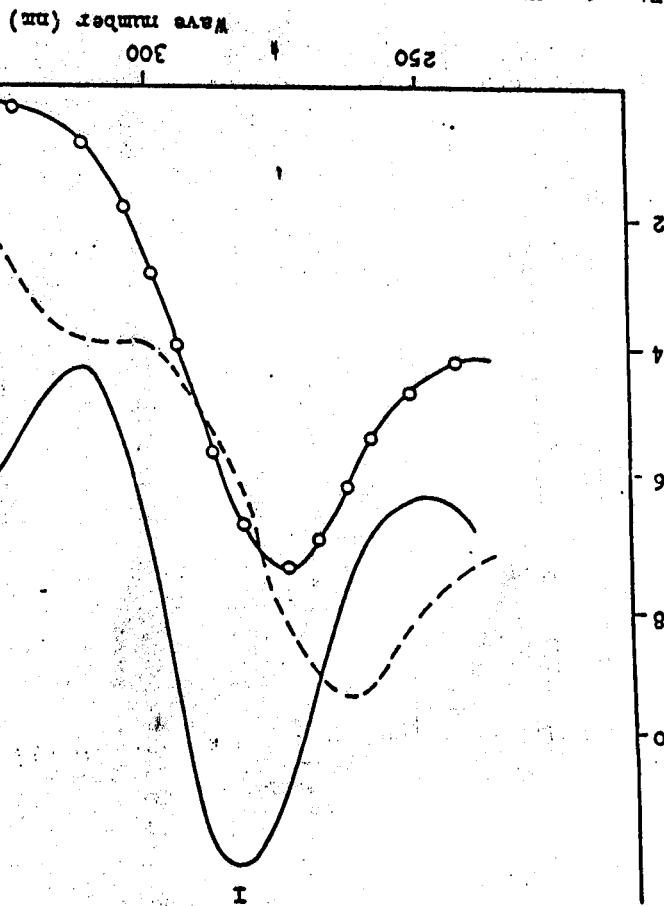


FIG. 1: UV spectra of compounds (1)

## RESULTS AND DISCUSSION

The 'B<sub>2u</sub> ← A<sub>1g</sub> transition of the phenyl moiety in our thioureas is shifted to 266 nm (compound 2, Table 1). This absorption is sensitive toward substitution, thus it undergoes a red shift when there is a para substituent on the phenyl ring (Table 1). The absorption at 314 nm in compound 2 is a II → II\* transition which originates from the PhCo ring and extended over the whole molecule. This band is not present in the two molecules (1b and 1c), which form compound 2 (Table 1). Thus it could be assigned to intramolecular charge transfer transition [12,13]. Substitution in the PhN ring cause a red shift to the band at 314 nm (band II Fig 1). Changing the solvent from chloroform to ethanol or to ethylene glycol causes a blue shift of the bands I and II. Also the intensity of bands I and II decreases solvents. This might be due to hydrogen bond formation between the alcohol and the studied compounds [6].

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