Dipole Moment and Infrared Spectrum of 2, 3, 5, 6-Tetraisopropylnitrobenzene

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Dipole moment and infrared spectrum of 2, 3, 5, 6-tetraisopropylnitrobenzene were examined. The process of the dipole moment measurement is the same as that described in the articles[1].

The dipole moment of this compound is 3.57D (in benzene solution, at 25±0.01°C), and is actually less than that of nitrobenzene (3.97D)[2], but not so different from that of nitrodurene (3.60D)[3].

The small value of the dipole moment observed is attributed, as generally accepted, to the decrease of the resonance moment of the nitro-group due to steric hindrance.

The infrared spectra were measured with a Perkin-Elmer Model 21 spectrophotometer (with rock salt prism) in chloroform solution in the region from 1670 to 1250 cm^{-1}.

Fig. 1 shows the infrared spectra of nitrodurene and 2, 3, 5, 6-tetraisopropylnitrobenzene, and the data are shown in Table I.

TABLE I

Compound	N-O stretch. vib.		Diff. from C_6H_5-NO_2	
	Asym. cm^{-1}	Sym. cm^{-1}	ΔAs cm^{-1}	ΔS cm^{-1}
C_6H_5-NO_2	1527	1348	—	—
Nitrodurene	1526	1378	−1	30
Nitro-tetra-iso Pr-C_6H_5	1524	1389	−3	41

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[1] S. Mizushima and K. Higashi, *J. Chem. Soc. Japan (Nippon Kwagaku Kwaishi)*, 54, 226 (1933).

[2] Our observed data.

[3] L. E. Sutton et al., *Rec. trav. chim.*, 78, 790 (1959); In their paper, the dipole moment of nitrodurene was reported as 3.62 D, but they neglected P_A. So we recalculated their value in consideration of P_A (≈5% of P_E) to fit to our data.

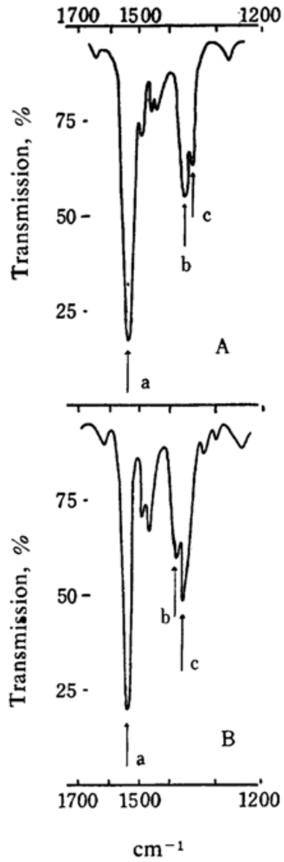

Fig. 1. Infrared spectra of nitrobenzenes (A: Nitrodurene, B: 2,3,5,6-tetra-isopropylnitrobenzene) in chloroform solution.

a: ν_{N-O} asym., b: ν_{N-O} sym., c: δ_{CH} in -CH_3

According to our previous observations on the general behavior of N–O sym. and asym. stretching vibrations of alkyl- and halogenonitrobenzenes[4], the N–O sym. was sensitive to the co-planarity of the nitro-group with the benzene plane, on the other hand, N–O asym. was affected by the polarity of substituents.

The infrared spectrum data obtained in the present investigation clearly reveal the general features mentioned above.

In comparing the value of ΔS, which seemed to represent the magnitude of steric hindrance, it may be suggested that a larger steric hindrance was in 2,3,5,6-tetraisopropylnitrobenzene than in nitrodurene.

There was a little discrepancy between the results obtained from the study with infrared spectrum and those from dipole moment.

A similar disagreement is found also in the series of the measurements of alkyl- and halogenonitrobenzenes, which will be discussed in elsewhere.

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[4] R. Nakashima et al., The 7th. IR and Raman Symposium at Osaka, Proceeding papers, p. 151 (1960).