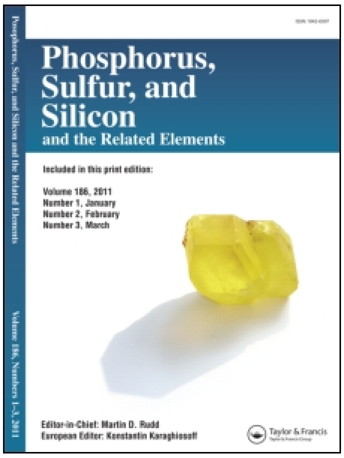

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Proton Acceptor Ability of the Compounds Containing SO and SO_2 Groups

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PROTON ACCEPTOR ABILITY OF THE COMPOUNDS CONTAINING SO AND SO_2 GROUPS

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Abstract. IR spectra, dipole moments and molar Kerr constants of complexes of phenols with the compounds containing SO and SO_2 groups are studied to establish correlation between proton acceptor capability and energies of the highest occupied molecular orbitals.

It is well known that compounds containing SO and SO_2 groups are able to form hydrogen bond with several proton donors (PD)[1,2]. The infrared studies of phenolic complexes ranked proton acceptors (PA) according to their proton affinity in the order: sulphoxides > sulphones > sulphites[3]. We have applied the IR spectroscopy, dipole moment (μ) and molar Kerr constants (mK) measurements to establish a relation between the structural features of sulphur compounds and their ability to act as PA in complex formation.

TABLE I. The shift $\Delta\nu$ (cm^{-1}) of OH stretching vibrations of phenols in their complexes[a].

p-X-C_6H_5OH	Me_2SO (**1a**)	$(MeO)_2SO$ (**2a**)	Sulpholan (**3a**)	$(MeO)_2SO_2$ (**4a**)
X = CH_3 (**1d**)	347	252	151	70
X = H (**2d**)	366	255	157	76
X = NO_2 (**3d**)	489	311	200	106

[a] Detailed data on the IR spectra (frequencies, absorption coefficients and bands contours) were published elsewhere[4]

The shift of OH groups stretching vibration due to the hydrogen bond formation of alkoxyl groups decreases in the order **1a** > **2a** > **3a** > **4a**. Inductive effect of alkoxyl groups decreases electron density on the oxygen atom (q_o) and consequently diminishes proton accept or ability of **2a** (**4a**) in comparison with **1a** (**3a**). For the same PA and variously substituted phenols, we have observed that electron demanding substitutents as the nitro group, increase, while electron releasing groups decrease $\Delta\nu$(OH).

Formation of hydrogen-bonded complexes can be easily detected by the IR spectroscopy but electrooptical methods provide more information on composition and structure.

TABLE 2. Dipole moments (μ) and molar Kerr constants (mK) of complexes (in CCl_4, at 25°C).

mK.10^{12}/μ,D	**1d** 27.7/1.65	**2d** 40.0/1.50	**3d** 2010/4.91
1a: 144/4.23	543/4.5	666/5.2	3886/8.6
2a: 22/3.15	315/4.0	334/4.5	3352/6.8
3a: 149/4.35	323/4.2	363/4.7	1908/6.3
4a: 101/4.31	230/4.1	246/4.3	2315/6.0

Examination of the μ and mK values allows to determine conformation of H-complexes and complex formation constants (K) as well as to compute the H-bond polarities (μ_H). The establish correlations of μ_H and logK with q_o conform with the modern theories on the nature of hydrogen bond.

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