This article was downloaded by:

On: 29 January 2011

Access details: Access Details: Free Access

Publisher Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Phosphorus, Sulfur, and Silicon and the Related Elements

Publication details, including instructions for authors and subscription information: http://www.informaworld.com/smpp/title~content=t713618290

Proton Acceptor Ability of the Compounds Containing SO and SO₂ Groups

Victor Prezhdo^a; Oleg Prezhdo^b; Elena Vaschenko^c

^a Institute of Chemistry, University of Opole, Poland ^b Chemistry Department, University of Texas, Austin, USA ^c Politechnical University, Kharkov, Ukraine

To cite this Article Prezhdo, Victor , Prezhdo, Oleg and Vaschenko, Elena(1994) 'Proton Acceptor Ability of the Compounds Containing SO and SO_2 Groups', Phosphorus, Sulfur, and Silicon and the Related Elements, 95: 1, 417 - 418 To link to this Article: DOI: 10.1080/10426509408034258

URL: http://dx.doi.org/10.1080/10426509408034258

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

PROTON ACCEPTOR ABILITY OF THE COMPOUNDS CONTAINING SO AND SO_2 GROUPS

VICTOR PREZHDO
Institute of Chemistry, University of Opole, Poland
OLEG PREZHDO
Chemistry Department, University of Texas, Austin, USA
ELENA VASCHENKO
Politechnical University, Kharkov, Ukraine

Abstract. IR spectra, dipole moments and molar Kerr constants of complexes of phenols with the compounds containing SO and SO 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 SO₂ 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 > sulphites³. 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.

р-Х-С ₆ Н ₅ ОН	Me ₂ SO (1a)	(MeO) ₂ SO (2a)	Sulpholan (3a)	(MeO) ₂ SO 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

^aDetailed data on the IR spectra (frequencies, absorption coefficients and bands contours) were published elsewhere

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_0) 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 comple	exes	(in	CCl,	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.

REFERENCES

- M. D. Joster and Z. J. Schaad. <u>Hydrogen bonding</u> (M. Dekker, New York, 1974), p. 350.
- 2. V.A.Terent'ev. <u>Termodinamika donorno-akceptornoj swiazi.</u>
 (Universitet, Saratov, 1981), p.277.3. T.Gramstad,
- P. Bescarini, G. Galloni and F. Chersetti, <u>Spectrochim. Acta</u>
 20, 267 (1964).
- 4. V. V. Prezhdo, V. A. Vetrov and V. V. Bocharova, Ukrain. chim. zhurnal, 55, 1022 (1989).