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## Phosphorus, Sulfur, and Silicon and the Related Elements

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### Constitutionally Symmetric, Structurally Uneven Sulfuranes. A Theoretical Study

Michel Loos<sup>a</sup>; Jean-Louis Rivail<sup>a</sup>; Árpád Kucsman<sup>b</sup>; Imre G. Csizmadia<sup>c</sup>

<sup>a</sup> Laboratoire de Chimie Théorique, Université de Nancy I, Nancy, France <sup>b</sup> Department of Organic Chemistry, Eötvös University, Budapest, Hungary <sup>c</sup> Department of Chemistry, University of Toronto, Toronto, Canada

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## CONSTITUTIONALLY SYMMETRIC, STRUCTURALLY UNEVEN SULFURANES.

### A Theoretical Study

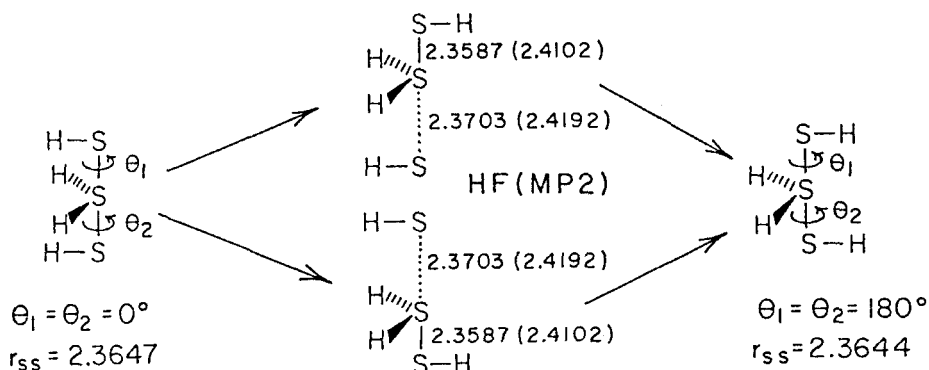
Michel LOOS<sup>a</sup>, Jean-Louis RIVAIL<sup>a</sup>, Árpád KUCSMAN<sup>b</sup> and Imre G. CSIZMADIA<sup>c</sup>

a) Laboratoire de Chimie Théorique, Université de Nancy I, Nancy, France

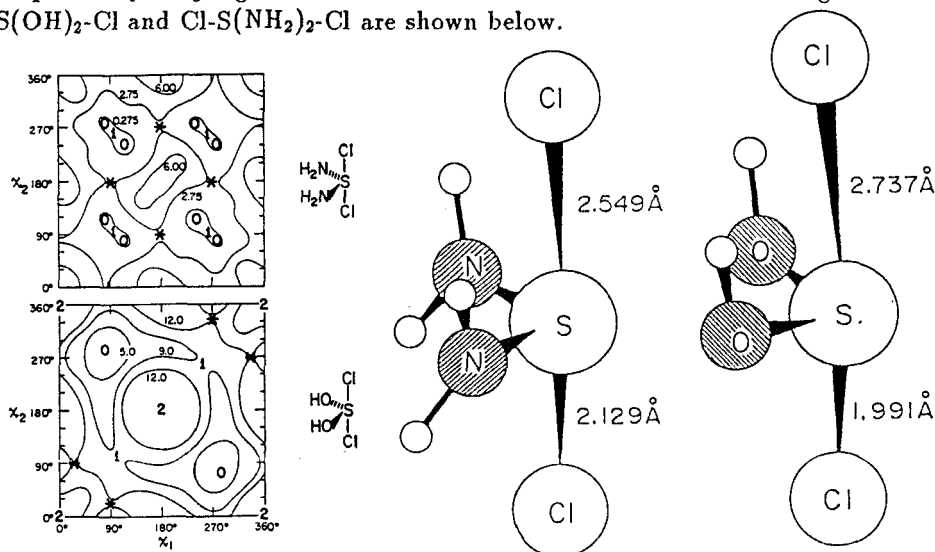
b) Department of Organic Chemistry, Eötvös University, Budapest, Hungary

c) Department of Chemistry, University of Toronto, Toronto, Canada

Uneven structures may be induced, conformationally, in constitutionally symmetric sulfuranes. In the case of  $\text{HS-S(H)}_2\text{-SH}$  the two different S-S bond lengths obtained [1] are shown below.



More recent investigations had demonstrated that in constitutionally symmetric sulfuranes, such as  $\text{Cl-S(OH)}_2\text{-Cl}$  or  $\text{Cl-S(NH}_2)_2\text{-Cl}$ , conformational induction is amplified by conjugative interaction. The resultant S-Cl bond lengths for  $\text{Cl-S(OH)}_2\text{-Cl}$  and  $\text{Cl-S(NH}_2)_2\text{-Cl}$  are shown below.



It is anticipated that  $2 \times 2 = 4$  minima will be found on the potential energy surface of the type  $E=E(\chi_1, \chi_2)$  where  $\chi_1$  and  $\chi_2$  are the torsional modes of motion about the S-N and S-O bonds. The 4 ideal geometries were to be the results of the combinations of  $90^\circ$  and  $270^\circ$ . Instead the oxygen containing compound had 2 equivalent minima and the nitrogen containing compound had 8 equivalent minima.

For the  $\text{Cl-S(OH)}_2\text{-Cl}$ , the two minima were located at the following two pairs of torsional angles.

$\chi_1$	$\chi_2$
$90^\circ + 6.23^\circ = 96.23^\circ$	$270^\circ - 6.23^\circ = 263.77^\circ$
$270^\circ - 6.23^\circ = 263.77^\circ$	$90^\circ + 6.23^\circ = 96.23^\circ$

For the  $\text{Cl-S(NH}_2)_2\text{-Cl}$ , the eight minima were located at the following eight pairs of torsional angles

$\chi_1$				$\chi_2$			
90.0	-	4.2	=	85.8	90.0	+	20.0 = 110.0
90.0	+	20.0	=	110.0	90.0	-	4.2 = 85.8
270.0	-	20.0	=	250.0	90.0	+	20.0 = 110.0
270.0	+	4.2	=	274.2	90.0	-	4.2 = 85.8
90.0	-	4.2	=	85.8	270.0	+	4.2 = 274.2
90.0	+	20.0	=	110.0	270.0	-	20.0 = 250.0
270.0	-	20.0	=	250.0	270.0	+	4.2 = 274.2
270.0	+	4.2	=	274.2	270.0	-	20.0 = 250.0

## Reference

- [1] M. Loos, J.-L. Rivail, A. Kucsman and I.G. Csizmadia  
J.Mol.Struct.(THEOCHEM) **230**, 143 (1991)