

1666  
ED

**C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>S**

**Divinyl sulfone**

**C<sub>1</sub> (conformer I)**  
**C<sub>2</sub> (conformer II)**  
**H<sub>2</sub>C=CH-SO<sub>2</sub>-CH=CH<sub>2</sub>**

<i>r<sub>a</sub></i>	Å <sup>a)</sup>	<i>θ<sub>a</sub></i>	deg <sup>a)</sup>	
S=O	1.438(3)	O=S=O	119.5(12)	
S-C	1.769(4)	S-C=C	121.5(3)	
C=C	1.332(4)	C-S-C	107.7(6)	
C-H	1.118(6)	C=C-H	124.2(12)	
			conformer I	conformer II
		<i>τ</i> <sub>1</sub> <sup>b)</sup>	272(9)	76(9)
		<i>τ</i> <sub>2</sub> <sup>b)</sup>	48(9)	= <i>τ</i> <sub>1</sub>

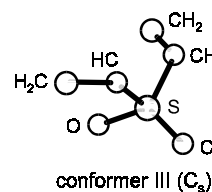
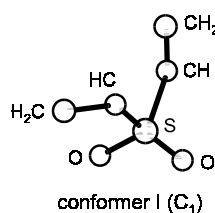
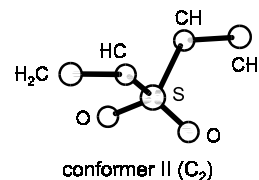
CNDO/2 molecular-orbital calculations indicate the coexistence of three conformers.

Set A (conformer I (69%), conformer II (31%)) is preferred to set B (conformer I (20%), conformer II (40%) and conformer III (40%)) in the analysis of the ED data.

The nozzle temperature was 100...108 °C.

<sup>a)</sup> Estimated total errors. Some of the estimates are larger than those listed in the original paper.

<sup>b)</sup> Dihedral angle C-S-C=C, defined as zero when the C=C bond is *anti* to the S-C bond.



Hargittai, I., Rozsondai, B., Nagel, B., Bulcke, P., Robinet, G., Labarre, J.-F.: J. Chem. Soc., Dalton Trans. (1978) 861.