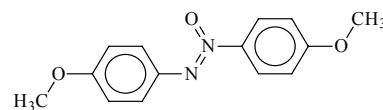


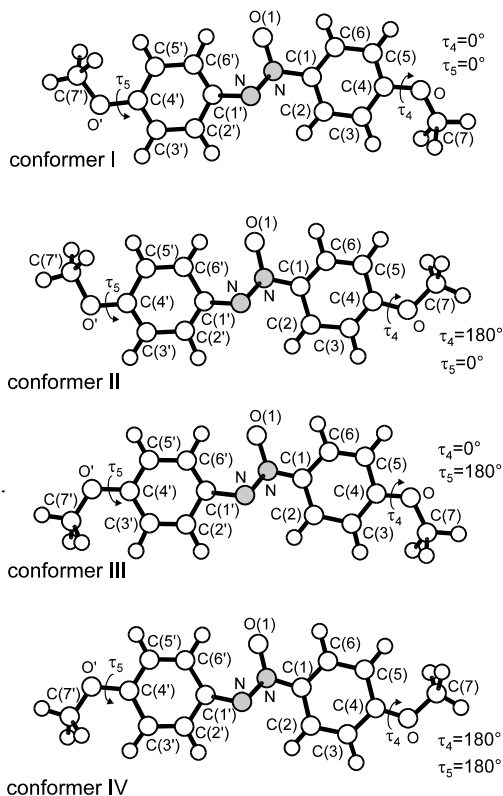
924 C₁₄H₁₄N₂O₃ED, *ab initio*
calculations**(Z)-Bis(4-methoxyphenyl)diazene 1-oxide**

(Z)-4,4'-Dimethoxyazoxybenzene

(Z)-*p*-Azoxyanisoleessentially C_s
(conformers I-IV)

r_g	Å ^{a)}	θ_α	deg ^{a)}
C-H ^{b)}	1.083(6)	N=N=O(1)	126.2(24)
C(methyl)-O ^{b)}	1.421(1)	N=N-C(1')	122.4(19)
C(ring)-O ^{b)}	1.350(1)	N=N-C(1)	115.8(21)
C-C (ring) ^{b)}	1.400(1)	N-C(1)-C(2)	122.2(10)
N=N	1.245(12)	N-C(1')-C(6')	130.0(10)
N=O(1)	1.303(12)	C-C-C (ring) ^{b)}	120.0(1)
C(1)-N	1.468(13)	C(3)-C(4)-O	124.8 ^{c)}
C(1')-N	1.429(13)	C(5')-C(4')-O'	124.8 ^{c)}
		C(4)-O-C(7)	122.7(17)
		C(4')-O'-C(7')	122.5(17)
		τ_1 ^{d)}	11(26)
		τ_2 ^{e)}	11(11)
		τ_3 ^{f)}	180 ^{g)}
		τ_4 ^{h)}	0 ^{g)}
		τ_5 ⁱ⁾	0 ^{g)}
		τ_6 ^{j)}	0 ^{g)}

According to the results of *ab initio* HF/4-21G(*) calculations, the following assumptions were made in the analysis of experimental data: four different conformers coexist in the gas phase with the mole fractions of 26.0, 33.0, 17.6 and 23.4%, respectively, and the azoxy group (C-N=N(=O)-C fragment) is planar. The differences between the similar parameters were assumed at the values from HF/4-21G(*) calculations. The parameters for conformer I are listed. The nozzle temperature was 170 °C.

^{a)} Three times the estimated standard errors.^{b)} Average value.^{c)} Dependent parameter.^{d)} Torsional angle C(2)-C(1)-N=N.^{e)} Torsional angle N=N-C(1')-C(6').^{f)} Torsional angle C(1)-N=N-C(1').^{g)} Assumed.^{h)} Torsional angle C(7)-O-C(4)-C(3).ⁱ⁾ Torsional angle C(5')-C(4')-O'-C(7').^{j)} Torsional angle C(1')-N=N=O(1).

Kuze, N., Ebizuka, M., Fujiwara, H., Takeuchi, H., Egawa, T., Konaka, S., Fogarasi, G.:
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