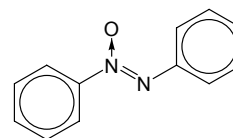


**905**      **C<sub>12</sub>H<sub>10</sub>N<sub>2</sub>O**ED, *ab initio* and  
DFT calculations**(Z)-Diphenyldiazene 1-oxide***trans*-Azoxybenzene**C<sub>s</sub>**

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
O–N(1)	1.271(3) <sup>b)</sup>	O–N(1)=N(2)	127.7(16)
N(1)=N(2)	1.271(3) <sup>b)</sup>	O–N(1)–C(1)	119.0(13)
N(1)–C(1)	1.464(7) <sup>c)</sup>	N(1)=N(2)–C(1')	121.3(13)
N(2)–C(1')	1.414(7) <sup>c)</sup>	tilt(C(1')) <sup>d)</sup>	9.0(14)
C–C (average) <sup>c)</sup>	1.400(1)	tilt(C(1)) <sup>f)</sup>	2.6(23)
C–H (average)	1.100(6)		

Each phenyl ring and the C(1)N(O)NC(1') moiety were assumed to be planar. All C–C–C bond angles were assumed at the values from RHF/6-31G\*\* calculations. The torsion of the phenyl rings around the N–C bonds was treated as a large-amplitude motion using the pseudoconformers method. The potential constants were determined to be  $V_{12} = 1.7(10)$  kcal mol<sup>−1</sup>,  $V_{14} = -0.1(13)$  kcal mol<sup>−1</sup> and  $V_{22} = 3.5(16)$  kcal mol<sup>−1</sup>. Both torsional angles were found to be zero, *i.e.*, the molecule was found to be planar.

The nozzle temperature was about 160 °C.

<sup>a)</sup> Three times the estimated standard errors.

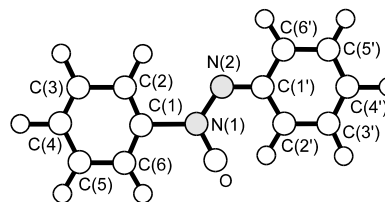
<sup>b)</sup> The O–N and N=N bond lengths were assumed to be equal.

<sup>c)</sup> Difference between the  $r_a$ [N(1)–C] and  $r_a$ [N(2)–C] parameters was assumed at the value from RHF/6-31G\*\* calculations.

<sup>d)</sup> Tilt angle defined as  $\{[N(2)–C(1')–C(2')] - [N(2)–C(1')–C(6')]\}/2$ .

<sup>e)</sup> Differences between the C–C bond lengths in the rings were assumed at the values from RHF/6-31G\*\* calculations.

<sup>f)</sup> Tilt angle defined as  $\{[N(1)–C(1)–C(2)] - [N(1)–C(1)–C(6)]\}/2$ .



Tsuji, T., Takashima, H., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **554** (2000) 203.