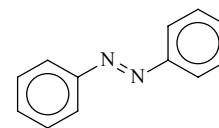


**904**      **C<sub>12</sub>H<sub>10</sub>N<sub>2</sub>**ED, *ab initio*  
calculations***trans*-Azobenzene**  
(*E*)-Diphenyldiazene**C<sub>2h</sub>**

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
N=N	1.260(8)	N=N-C	113.6(8)
N-C	1.427(8)	N-C(1)-C(2)	124.7(9)
C-C (average)	1.399(1)	C(2)-C(1)-C(6)	120.5 <sup>b)</sup>
C(1)-C(2)	1.405 <sup>c)</sup>	C(1)-C(2)-C(3)	119.1 <sup>b)</sup>
C(2)-C(3)	1.393 <sup>c)</sup>	C(1)-C(6)-C(5)	119.9 <sup>b)</sup>
C(3)-C(4)	1.402 <sup>c)</sup>	C(2)-C(3)-C(4)	120.6 <sup>b)</sup>
C(4)-C(5)	1.397 <sup>c)</sup>	C(3)-C(4)-C(5)	120.0 <sup>b)</sup>
C(5)-C(6)	1.396 <sup>c)</sup>	C(4)-C(5)-C(6)	119.9 <sup>b)</sup>
C(1)-C(6)	1.401 <sup>c)</sup>	$\tau^d)$	0 <sup>e)</sup>
C-H	1.102(7)		

The CNNC fragment was found to be planar with equivalent phenyl rings. The torsion of each phenyl ring around the N-C bond was treated as a large-amplitude vibration. Contrary to the previous ED study [1], the stable form of this molecule was found to be planar. The potential constants for the torsion,  $V_2$  and  $V_4$ , were determined to be 1.7(6) and 0.6(13) kcal mol<sup>-1</sup>, respectively.

The nozzle temperature was *ca.* 407 K.

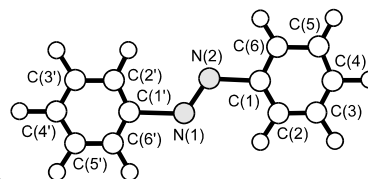
<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Assumed at the value from MP2/6-31+G\* calculations.

<sup>c)</sup> Differences between the C-C bond lengths were assumed at the values from MP2/6-31+G\* calculations.

<sup>d)</sup> Torsional angle C-N=N-C.

<sup>e)</sup> Uncertainty is not given in the original paper.



Tsuji, T., Takashima, H., Takeuchi, H., Egawa, T., Konaka, S.: J. Phys. Chem. A **105** (2001) 9347.

[1] Trøttemberg, M., Hilmo, I., Hagen, K.: J. Mol. Struct. **39** (1977) 231.

Replaces [II/25D \(3, 2802\)](#)