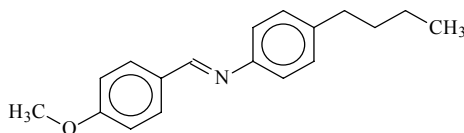


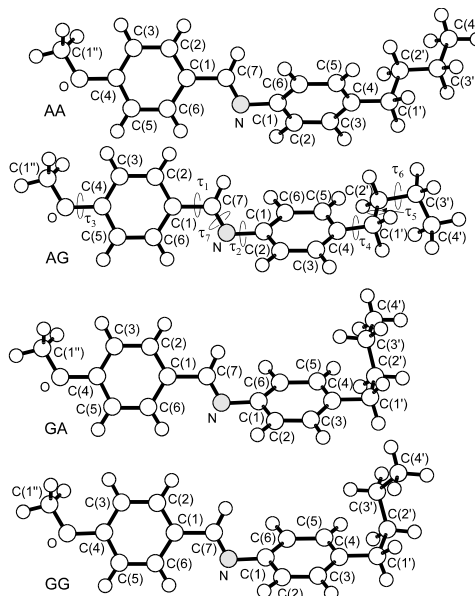
**938**    **C<sub>18</sub>H<sub>21</sub>NO**ED, *ab initio*  
calculations**4-Butyl-*N*-[(4-methoxyphenyl)methylene]benzenamine** C<sub>1</sub> (AA)4-Butyl-*N*-(*p*-methoxybenzylidene)anilineC<sub>1</sub> (AG)C<sub>1</sub> (GA)C<sub>1</sub> (GG)

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H (ring) <sup>b)</sup>	1.108(4)	C(1)–N=C(7)	119.0(18)
N=C(7)	1.290(12)	N=C(7)–C(1)	121.6(13)
C(1)–N	1.413(12)	N=C(7)–H	122.5 <sup>c)</sup>
C–C (ring) <sup>b)</sup>	1.400(6)	N–C(1)–C(6)	128.5(25)
C(1)–C(7)	1.467(3)	C(7)–C(1)–C(2)	121.2 <sup>c)</sup>
C(4)–C(1')	1.513(3)	C–C–C (ring) <sup>b)</sup>	120.0(3)
C(1')–C(2')	1.541(3)	C(4)–O–C(1'')	122.0 <sup>d)</sup>
C(2')–C(3')	1.534(3)	C(3)–C(4)–O	129.3(16)
C(3')–C(4')	1.533(3)	C(3)–C(4)–C(1')	121.1 <sup>c)</sup>
C(4)–O	1.364(3)	C–C–C (butyl) <sup>b)</sup>	116.2(11)
C(1'')–O	1.430(3)	$\tau_1$ <sup>c)</sup> <sup>f)</sup>	0(12)
		$\tau_2$ <sup>f)</sup> <sup>g)</sup>	48(9)
		$\tau_3$ <sup>f)</sup> <sup>h)</sup>	0 <sup>i)</sup>
		$\tau_4$ <sup>f)</sup> <sup>j)</sup>	88 <sup>i)</sup>
		$\tau_5$ <sup>f)</sup> <sup>k)</sup>	180 <sup>i)</sup>
		$\tau_6$ <sup>f)</sup> <sup>l)</sup>	180 <sup>i)</sup>
		$\tau_7$ <sup>f)</sup> <sup>m)</sup>	180 <sup>i)</sup>

It was assumed in the ED analysis that the four conformers with respect to the configurations of the *n*-butyl group, AA, AG, GA and GG, where  $\tau_5$  and  $\tau_6$  are equal to 180° for A (*anti*) or *ca.* 65° for the G (*gauche*) conformation, coexist in the gas phase with compositions of 43, 16, 30 and 11%, respectively.

These populations were estimated from the energy differences obtained by HF/4-21G\* calculations. The geometry of the core was assumed to be identical for all four conformers. Each of the two phenylene rings and C(1)–C(7)H=N–C(1) moiety were assumed to be planar. The differences between similar structural parameters were assumed to be equal to those from HF/4-31G\* calculations. The structural parameters are listed for the AA conformer.

The nozzle temperature was about 150 °C.



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

<sup>b)</sup> Average value.

<sup>c)</sup> Dependent parameter.

<sup>d)</sup> Assumed to be equal to the corresponding value of *p*-anisaldehyde from the literature.

- <sup>e)</sup> N=C(7)–C(1)–C(6) torsional angle.
- <sup>f)</sup> Zero degree for the *syn* position.
- <sup>g)</sup> C(7)=N–C(1)–C(6) torsional angle.
- <sup>h)</sup> C(3)–C(4)–O–C(1'') torsional angle.
- <sup>i)</sup> Assumed at the value from HF/4-21G\* calculations.
- <sup>j)</sup> C(3)–C(4)–C(1')–C(2') torsional angle.
- <sup>k)</sup> C(4)–C(1')–C(2')–C(3') torsional angle.
- <sup>l)</sup> C(1')–C(2')–C(3')–C(4') torsional angle.
- <sup>m)</sup> C(1)–N=C(7)–C(1) torsional angle.

Kuze, N., Fujiwara, H., Takeuchi, H., Egawa, T., Konaka, S., Fogarasi, G.: J. Phys. Chem. A **103** (1999) 3054.