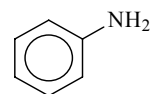


**727**      **C<sub>6</sub>H<sub>7</sub>N**  
ED, *ab initio*  
calculations

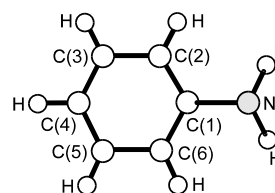
**Benzenamine**  
Aniline

**C<sub>s</sub> assumed**



$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–C(mean)	1.398(3)	C(2)–C(1)–C(6)	119.0(2)
C(1)–C(2)	1.403(3)	C(1)–C(2)–C(3)	120.3(1)
C(2)–C(3)	1.395 <sup>b)</sup>	C(2)–C(3)–C(4)	120.7(1)
C(3)–C(4)	1.397 <sup>b)</sup>	C(3)–C(4)–C(5)	119.0(3)
C–N	1.407(3) <sup>b)</sup>	H–N–H	109.8 <sup>c)</sup>
C–H(mean)	1.099(3)	$\varphi$ <sup>d)</sup>	44(4)
N–H	1.026 <sup>b)</sup>		
$\Delta N$ <sup>e)</sup>	0.072 <sup>c)</sup>		

Local C<sub>2v</sub> symmetry was assumed for the benzene ring.  
The nozzle was at *ca.* 334 K.



<sup>a)</sup> Estimated total errors.

<sup>b)</sup> Differences [C(1)–C(2)] – [C(2)–C(3)],  
[C(2)–C(3)] – [C(3)–C(4)], [C(1)–N] – [C(3)–C(4)] and [C–H(mean)] – [N–H(mean)]  
were assumed at the values from MP2/6-31G\*(6D) calculations.

<sup>c)</sup> Assumed at the value from MP2/6-31G\*(6D) calculations.

<sup>d)</sup> Dihedral angle between the H–N–H and ring planes.

<sup>e)</sup> Displacement of the nitrogen atom from the ring plane, on the side opposite to the amino hydrogen atoms.

Schultz, G., Portalone, G., Ramondo, F., Domenicano, A., Hargittai, I.: Struct. Chem. 7 (1996) 59.

[II/25D \(3, 2260\)](#)