

## Structure Data of Free Polyatomic Molecules

 739  
MW

 $\text{C}_6\text{H}_7\text{NO}$ 
**Aniline – water (1/1)**

 Benzenamine – water (1/1)  
(weakly bound complex)

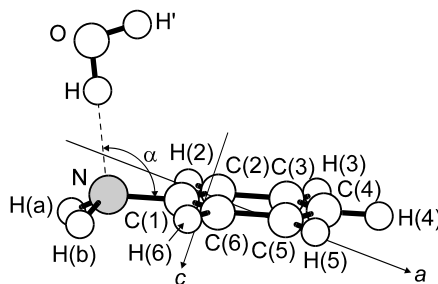
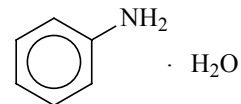
 $\text{C}_s$ 

 (effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}^a$	$\theta_0$	$\text{deg}^a$
N...O	3.03(1)	$\alpha^b$	101.31(50)

Atom	$ a_s  [\text{\AA}]$	$ b_s  [\text{\AA}]$	$ c_s  [\text{\AA}]$
O	3.3169	0.0	1.1366

Atom	$a_0 [\text{\AA}]$	$b_0 [\text{\AA}]$	$c_0 [\text{\AA}]$
C(1)	−0.211	0.0	0.628
C(2)	0.420	−1.206	0.313
C(3)	1.667	−1.202	−0.310
C(4)	2.302	0.0	−0.626
C(5)	1.667	1.202	−0.309
C(6)	0.420	1.206	0.313
H(2)	−0.070	−2.140	0.557
H(3)	2.145	−2.144	−0.548
H(4)	3.268	0.0	−1.108
H(5)	2.145	2.145	−0.548
H(6)	−0.070	2.140	0.557
N	−1.465	0.0	1.254
H(a)	−1.732	0.663	1.955
H(b)	−1.732	−0.663	1.955
H	−2.735	0.0	−0.382
O	−3.322	0.0	−1.138
H	−2.737	0.0	−1.896



Assuming a linear hydrogen N...H–O bond and that the water molecule was located in the symmetry plane of aniline, two structures were possible, but one of them is supported by *ab initio* calculations. The free water proton is directed toward the aniline ring.

<sup>a)</sup> Uncertainties were not estimated in the original paper.

<sup>b)</sup> See figure for the definition.

Spoerel, U., Stahl, W.: J. Mol. Spectrosc. **190** (1998) 278.