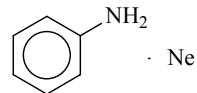


729  
MW

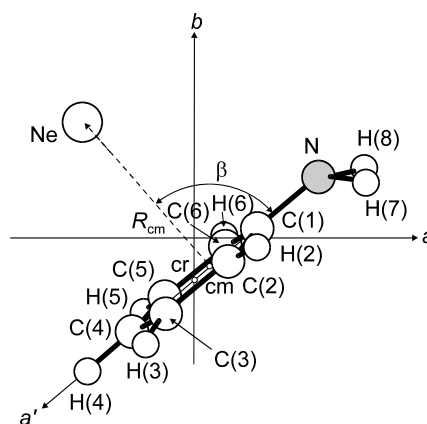
 $\text{C}_6\text{H}_7\text{NNe}$ 
**Aniline – neon (1/1)**  
Benzenamine – neon (1/1)  
(weakly bound complex)

 $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}$	$\theta_0$	deg
$R_{\text{cm}}$	3.434(3)	$\beta^{\text{a}}$	91.62(8)
$a'^{\text{b}}$	0.177(5)	$ \varphi ^{\text{c}}$	2.95(8)
$c'^{\text{b}}$	3.429(3)		
$R_{\perp}^{\text{d}}$	3.413(3)		



Atom	$a_0 [\text{\AA}]$	$b_0 [\text{\AA}]$	$c_0 [\text{\AA}]$
C(1)	1.1093	0.1936	0.0
C(2)	0.5837	-0.2758	1.2062
C(3)	-0.4560	-1.2044	1.2023
C(4)	-0.9850	-1.6769	0.0
C(5)	-0.4560	-1.2044	-1.2023
C(6)	0.5837	-0.2758	-1.2062
H(2)	0.9914	0.0883	2.1400
H(3)	-0.8542	-1.5601	2.1446
H(4)	1.7905	-2.3964	0.0
H(5)	-0.8542	-1.5601	-2.1446
H(6)	0.9914	0.0883	-2.1400
N	2.1549	1.1275	0.0
H(7)	2.9050	1.1160	0.6628
H(8)	2.9050	1.1160	-0.6628
Ne	-1.9537	2.0343	0.0
$\text{cm}^{\text{e}}$	0.4252	-0.4425	0.0
$\text{cr}^{\text{f}}$	0.0621	-0.7417	0.0



The structural analysis leads to a most probable structure with the rare gas atom in *anti* position. It is on the side of the lone pair and shifted away from the nitrogen with respect to the center of mass of aniline.

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

<sup>b)</sup> Coordinates of the Ne in the principal axis system of aniline.

<sup>c)</sup> Angle between the  $c'$  axis of aniline and  $R_{\text{cm}}$ .

<sup>d)</sup> Normal distance between the Ne and the aromatic ring.

<sup>e)</sup> Center of mass of aniline.

<sup>f)</sup> Center of the phenyl ring of aniline.

Consalvo, D., Storm, V., Dreizler, H.: Chem. Phys. **228** (1998) 301.

Storm, V., Dreizler, H., Consalvo, D.: Chem. Phys. **237** (1998) 395.