

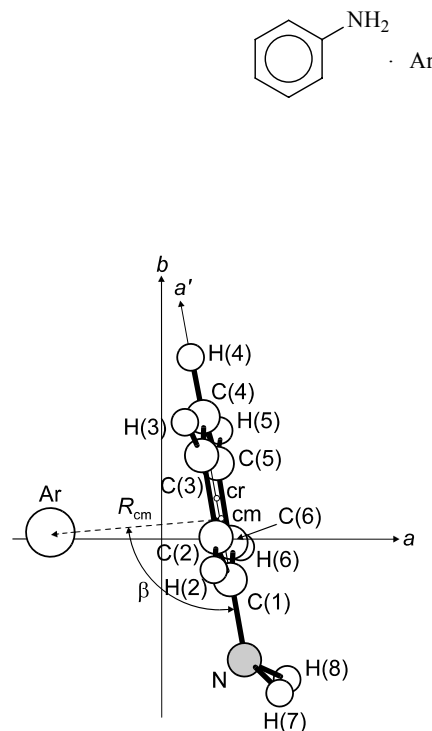
723
MW C_6H_7ArN

Aniline – argon (1/1)

Benzenamine – argon (1/1)
(weakly bound complex) C_s (effective symmetry class)
(large-amplitude motion)

r_0	\AA	θ_0	deg
R_{cm}	3.546(1)	β^a	93.31(11)
a'^b	0.287(5)	$ \varphi ^c$	4.64(11)
c'^b	3.534(2)		
R_{\perp}^d	3.519(2)		

Atom	a_0 [\AA]	b_0 [\AA]	c_0 [\AA]
C(1)	1.1997	-0.8190	0.0
C(2)	1.0844	-0.1238	-1.2062
C(3)	0.8564	1.2514	-1.2023
C(4)	0.7404	1.9512	0.0
C(5)	0.8564	1.2514	1.2023
C(6)	1.0844	-0.1238	1.2062
H(2)	1.1738	-0.6630	-2.1400
H(3)	0.7691	1.7781	-2.1446
H(4)	0.5638	3.0166	0.0
H(5)	0.7691	1.7781	2.1446
H(6)	1.1738	-0.6630	2.1400
N	1.4290	-2.2021	0.0
H(7)	2.0206	-2.6633	-0.6628
H(8)	2.0206	-2.6633	0.6628
Ar	-2.4631	-0.2435	0.0
cm ^e	1.0654	0.1054	0.0
cr ^f	0.9700	0.5661	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.

^a) See figure for the definition.

^b) Coordinates of Ar in the principal axis system of aniline.

^c) Angle between the c' axis of aniline and R_{cm} .

^d) Normal distance between Ar and the aromatic ring.

^e) Center of mass of aniline.

^f) 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.