

terms of absorbance units using the relation $A_1 - A_r$ (CD in absorbance units) = θ (ellipticity in $^\circ$)/33.0.

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On the Structure of Gaseous Anisole

H. M. SEIP and R. SEIP

Department of Chemistry, University of Oslo, Oslo 3, Norway

Anisole is usually assumed to have a planar heavy atom skeleton,¹ but some authors have suggested that the carbon in the methyl group does not lie in the ring plane.²⁻⁵ Aroney *et al.*² measured the dipole moments and molar Kerr constants for anisole and some *para* substituted derivatives. They give an apparent torsional angle (ϕ) around the C₁-O₇ bond (see Fig. 1) of 18 $^\circ$ for anisole. An extended Hückel calculation⁴ gave minimum in energy for $\phi = 75^\circ$, while $\phi = 0^\circ$ was obtained by the CNDO/2 method if the methyl group was oriented to give minimum steric interac-

tion between the methyl hydrogens and the *ortho* hydrogens in the ring.⁵

Electron diffraction data of anisole were recorded for two nozzle temperatures, the low temperature data (about 55 $^\circ$ C) with Balzers Eldigraph KD-G2,^{6,7} and the high temperature data (about 250 $^\circ$ C) with the Oslo apparatus.⁸ In both cases two nozzle-to-plate distances were used, and composite intensity curves covering the *s*-ranges 2.0 - 28.5 \AA^{-1} and 2.0 - 40.0 \AA^{-1} were calculated in the usual way.⁹ The experimental radial distribution functions⁹ calculated by Fourier inversion of the intensity curves, are shown in Fig. 1.

The mean amplitudes of vibration (*u*) for both temperatures computed as described by Stølevik *et al.*,¹⁰ are included in Table 1. A simple force field, found to give *u* values for benzene in good agreement with more refined calculations,¹¹ was used for the phenyl group. The other force constants were also estimated from force constants found in related molecules.

Least-squares refinements of the structural parameters were then carried out with a diagonal weight matrix. Except for the CO bond the phenyl group was assumed to have hexagonal symmetry, and the methyl group to have a threefold symmetry axis coinciding with the CO bond. For the low temperature data good agreement between experimental and theoretical intensity values was obtained for a model with planar skeleton and mean amplitudes computed as described above. The angle α (Fig. 1) was first assumed to be zero, but better agreement was obtained for $\alpha = 4^\circ$. The most important *u* values were then refined as shown in Table 1. A slightly better fit was obtained. The radial distribution curve calculated with these parameters is given in Fig. 1A. A very slight improvement was obtained if ϕ was increased to about 10 $^\circ$.

For the high temperature data the fit was not satisfactory if ϕ was assumed to be zero and the mean amplitudes kept at the computed values (Fig. 1). Much better agreement was obtained if the *u* values were refined. However, the mean amplitudes for the distances from C₆ to the carbon atoms in the ring, became then considerably larger than the computed values.

Refinements were then carried out for various fixed values of ϕ ; the best agreement was obtained for $\phi = 40^\circ$. It seemed likely that the torsional oscillations about C₁-O₇ resulted in an apparent large devia-

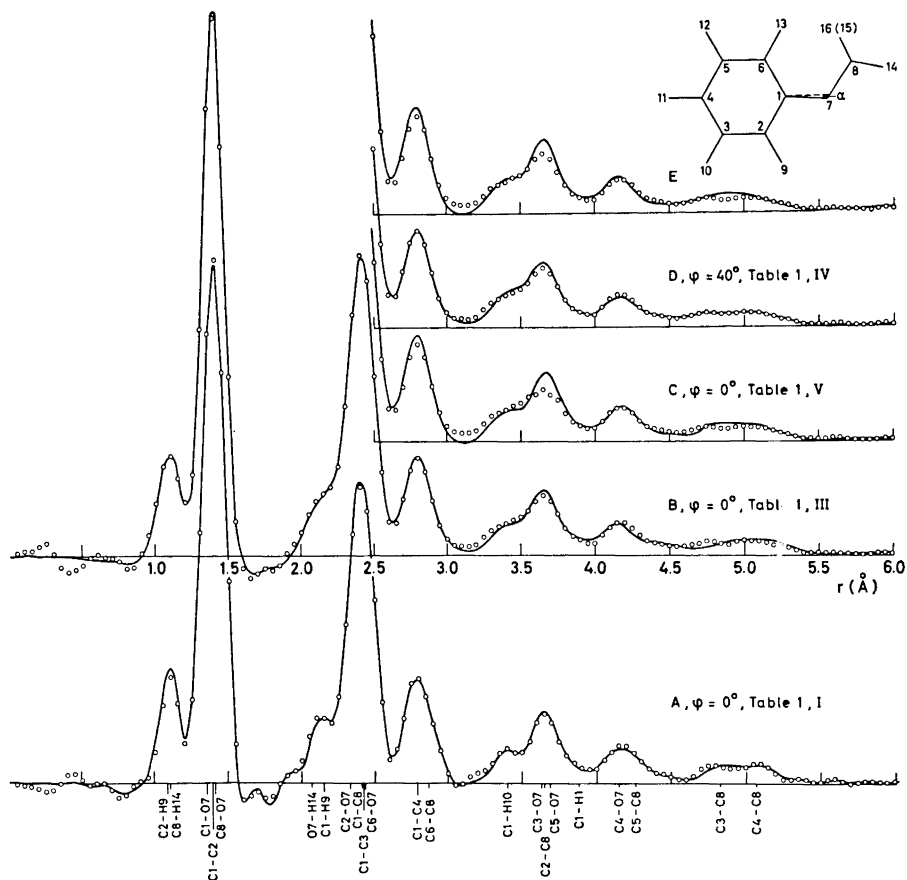


Fig. 1. Experimental (dotted) and theoretical radial distribution curves calculated with an artificial damping constant $k=0.0015 \text{ \AA}^2$. Curve A corresponds to the low temperature data, curves B–E to the high temperature. The parameters used to calculate the theoretical curves are given in Table I. The theoretical curve in E was calculated by using eqn. (1) with $V_0=3 \text{ kcal/mol}$.

tion from planarity. We therefore assumed a potential for internal rotation of the form

$$V(\phi) = (V_0/2)[1 - \cos(2\phi)] \quad (1)$$

The corresponding probability distribution was calculated classically. Owen and Hester have reported a barrier of about 6 kcal/mol.¹ We found that if the computed mean amplitudes were used, satisfactory agreement was not obtained with this barrier. $V_0=3 \text{ kcal/mol}$ and $V_0=2 \text{ kcal/mol}$ gave only a slight improvement (Fig. 1E).

It is not possible from the electron-diffraction data to determine the potential for rotation about the C_1-O_7 bond accurately. However, it seems very likely that $\phi=0^\circ$ corresponds to minimum in energy. This is in agreement with the result of a microwave investigation of *p*-fluoroanisole.¹² The simple function (1) is probably not a good description of the potential. The large difference between the u values obtained for the two temperatures and the good agreement for the high temperature data for $\phi=40^\circ$ may be caused by

Table 1. Bond distances (r_a), angles and mean amplitudes of vibration in anisole.^a The standard deviations given in parentheses apply to the last decimal place.

	Temperature 55°C		Temperature 250°C		
	I	II	III	IV	V
	exp. u values	comp. u values	exp. u values	exp. u values	comp. u values
Distances (Å)					
C ₁ -C ₂	1.397	1.398	1.398(8)	1.398(11)	1.398
C ₈ -O ₇	1.423(7)	1.418(4)	1.434(7)	1.422(6)	1.406
C ₁ -O ₇	1.357(6)	1.359(3)	1.351(5)	1.365(6)	1.379(3)
C ₂ -H ₉	1.09	1.09	1.09	1.09	1.09
C ₈ -H ₁₄	1.11	1.11	1.11	1.11	1.11
Angles (degrees)					
α	4.0	4.0	4.0	4.0	4.0
\angle COC	120.9(6)	120.9(6)	123.6(12)	119.2(11)	119.0
\angle CCH	110.0	110.0	110.0	110.0	110.0
ϕ	0.0	0.0	0.0	40.0	40.0
Mean amplitudes ^b (Å)					
C ₁ -C ₂	0.045	0.046	0.040	0.043	0.047
C ₈ -O ₇	0.048	0.047	0.043	0.046	0.050
C ₁ -O ₇	0.046	0.046	0.041	0.044	0.048
C ₁ ...C ₄	0.064	0.059	0.062	0.065	0.064
C ₁ ...C ₃	0.058	0.054	0.056	0.059	0.058
C ₂ ...O ₇	0.066	0.060	0.061	0.066	0.068
C ₃ ...O ₇	0.068	0.062	0.063	0.068	0.070
C ₄ ...O ₇	0.069	0.063	0.064	0.069	0.071
C ₆ ...O ₇	0.064	0.060	0.059	0.064	0.066
C ₆ ...O ₇	0.062	0.057	0.057	0.062	0.064
C ₁ ...C ₈	0.056	0.064	0.113	0.098	0.073
C ₂ ...C ₈	0.059	0.067	0.116	0.101	0.076
C ₃ ...C ₈	0.066	0.072	0.123	0.108	0.083
C ₄ ...C ₈	0.083	0.085	0.140	0.125	0.100
C ₅ ...C ₈	0.098	0.097	0.155	0.140	0.115
C ₆ ...C ₈	0.098	0.094	0.155	0.140	0.115

^a Parameters given without standard deviations were not refined with the other parameters.

^b The mean amplitudes were refined in groups, the differences between the values in one group were assumed.

a secondary minimum in the potential function. The low resolution microwave spectra have given indications of the existence of conformers with non-planar skeletons for *p*-anisaldehyde¹³ and *m*-bromoanisole.¹⁴

The bond distances and angles found by least-squares refinements are given in Table 1. The best values and error limits for the most important parameters seem to be: $r_a(\text{C}-\text{C}) = 1.398 \pm 0.003$ Å, $r_a(\text{C}_1-\text{O}_7) = 1.361 \pm 0.015$ Å, $r_a(\text{C}_8-\text{O}_7) = 1.423 \pm 0.015$ Å, $\angle \text{COC} = 120.0 \pm 2.0^\circ$. The average

C-C bond distance is the same as in benzene¹⁵ and the CO distances close to the values found in methyl-vinyl-ether, 1.358 Å and 1.424 Å.¹⁶

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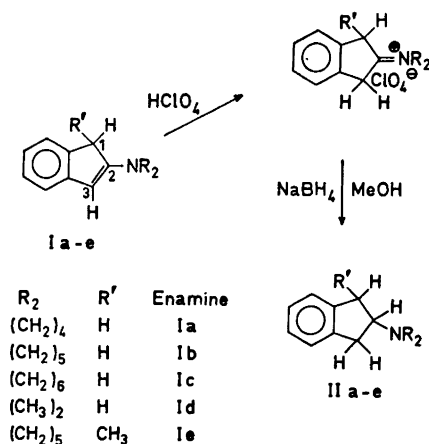
Preparation of Some N-Substituted 2-Aminoindanes

ULF EDLUND

*Department of Organic Chemistry,
University of Umeå, S-901 87 Umeå, Sweden*

In connection with the studies of enamines of 2-indanones^{1,2} we want to report a versatile method for the preparation of some N-substituted 2-aminoindanes. Some of these compounds have been synthesized previously by catalytic reduction of the corresponding enamines at high pressure.³ Structurally these indanamines form an interesting group of compounds since the presence of a phenethylamine skeleton relates them to the pharmacologically and physiologically well-known phenylisopropylamines. Thus these compounds are indane analogs corresponding to amphetamine. The pharmacological effect upon N-alkylation of 2-aminoindanes has earlier been reported.^{4,5}

2-Indanone and 1-methyl-2-indanone are most conveniently prepared by oxidation of the corresponding indenenes with performic acid.^{1,6} The syntheses of the enamines are then easily achieved by mixing the ketone and the desired secondary amine in methanol at room temperature.^{1,7} Since the reduction of enamines by hydride depends on the prior generation of an immonium salt,⁸ we have prepared the stable perchlorate salts of our enamines.



Scheme 1.