# ELECTROOPTICAL PROPERTIES AND STRUCTURE
OF SOME HETARYL PHENYL KETONES

A. S. Kuzharov, V. N. Sheinker,
N. F. Pedchenko, Z. N. Nazarova,
V. F. Lavrushin, and O. A. Osipov

UDC 541.67.634:543.52:547.724'733

We have measured the dipole moments (μ_D) and Kerr molar constants (∞mK_2) of 2-furyl and 2-thienyl phenyl ketones in CCl_4 solution at 25°C: I (X = O, R^5 = CH_3, R^4 = H, μ_D = 3.81, and 10^{12}', ∞ mK_2 = 293), II (O, H, H, 3.25, 182),* III (O, Br, H, 3.33, 64),† IV (S, CH_3, H, 3.73, 250), V (S, Cl, H, 3.57, 191), VI (S, Br, H, 3.12, 133), VII (S, NO_2, N, 5.26, 1508), VIII (S, H, H, 3.66, 213), IX (S, H, CH_3, 3.81, 188), X (S, H, Cl, 3.08, 155), XI (S, H, Br, 3.10, - 6.0), and XII (S, H, NO_2, 4.28, 1187).

$\theta = 130°$, $\mu_{C=O}^{-1\rightarrow} = 2.95$ D
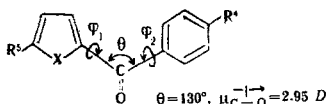
On comparison of the data obtained with the μ and $_\infty mK_2$ values calculated via an additive scheme [1] for the possible mutual orientations of the hetaryl and phenyl fragments, we found that the furan ring in 2-furyl phenyl ketones (I—III) lies in the trigonal plane of the carbonyl groups with the following varying ratios of the O,O-cis $(\varphi_1 = 0°)$, and O,O-trans $(\varphi_1 = 180°)$ conformers, depending on the nature of substituent R^5: I (100%, O,O-cis), II (75%), and III (65%). The existence of two three-dimensional isomers with angles of rotation of the phenyl fragment of $\sim \pm$ (50-70°), the choice between the signs of which is impossible from the available data, is possible for each conformation.

The hetaryl and phenyl fragments in 2-thienyl phenyl ketones IV—XII deviate from the trigonal plane of the carbonyl group in opposite directions with $\varphi_1 \sim 30°$ and $\varphi_2 = \sim - (40-70°)$, and this leads to the minimum steric interactions of the rings between them and the carbonyl group.

These differences in the orientation of the hetaryl fragments are in agreement with the Del Re rule [2], in accordance with which the aromatic system is more strongly conjugated with the π-electron systems attached to it, the lower its internal conjugation.

LITERATURE CITED

1. A. S. Kuzharov, Master's Dissertation [in Russian], Rostov-on-Don (1974).
2. Del Re, J. Chem. Soc., 3324 (1962).

---

*Here and subsequently, X, R^5, R^4, μ_D, and ∞mK_2 are presented in parentheses for all of the compounds.
† Measured in benzene.