ENERGETICS OF 3-(1,5-DIPHENYL-1*H*-PYRROL-2-YL)PROPANOIC ACID DERIVATIVES

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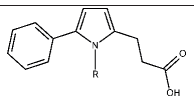
Polysubstituted pyrrole derivatives, in particular arylpyrroles, are capable of exhibiting biological activity. Such compounds are part of a number of drugs characterized by antitumor, antibacterial, analgesic, antioxidant and anti-inflammatory properties. In the chemical industry, such compounds can be used in the production of electrically conductive and optoelectronic materials, plant protection products. A key aspect of their potential use as drug components is the diversification of biological activity due to electrophilic substitution reactions, which is caused by the aromatic nature of the pyrrole ring. Among these compounds, the ability to exhibit biological activity was predicted for 3-(1,5-diphenyl-1*H*-pyrrol-2-yl)propanoic acid derivatives [1]. The lack of values of the enthalpy of formation in the condensed state in the reference literature prompted us to determine them experimentally. The availability of this fundamental thermodynamic parameter will allow to carry out optimization calculations for synthesis and processing processes for technological purposes.

The determination of $\Delta_f H^0_{298.15}$ was performed experimentally using a precision combustion calorimeter B-08-MA and a static calorimetric bomb. To establish the energy equivalent of the calorimetric system (W = 10347±7 J/V), a series of combustions of standard reference benzoic acid was performed. Before the experiments on the combustion of the acids under study, each sample was powdered in a chalcedony mortar, tableted, placed in a platinum cup and tied with a cotton thread. The bomb was filled with 1 ml of distilled water. The cup with the tablet was placed in a calorimetric bomb, which was filled with oxygen to 30 atmospheres. The sample was set on fire with a cotton thread by discharging capacitors through a nichrome wire. After each experiment, a quantitative analysis of combustion by-products was performed to detect the presence of mono- and dioxide, soot, and nitric acid. First, using the standard Rossini method (accuracy $\pm 2 \cdot 10^{-4}$ g), the mass of carbon dioxide formed during combustion was determined. Since the studied acids are nitrogen-containing, after opening the calorimetric bomb, the resulting aqueous solution of nitric acid was titrated using 0.1N KOH. The soot formed on the side surfaces of the platinum cup was determined by weighing with an accuracy of $\pm 5 \cdot 10^{-6}$ g before and after calcining the cup over an open burner.

Thus, the determined enthalpies of combustion ($\Delta_c H^0_{298.15}$) and calculated on their basis the enthalpies of formation in the condensed state ($\Delta_f H^0_{298.15}(cr)$) (Table 1) can be used for optimization calculations of synthesis and processing processes.

Table 1. Determined standard heats of combustion and formation of the studied acids, kJ/mol

Structure	Substitute (-R)	$\Delta_c H^0_{298.15}$	$\Delta_f H^0_{298.15}(cr)$
	C_6H_5	–9618.0±3.5	–287.9±3.5
	4-$CH_3C_6H_4$	–10226.5±3.1	–359.1±3.1
	4-$CH_3OC_6H_4$	–10120.8±4.2	–464.8±4.2

[1] Sitar A., Shevchenko D., Matiichuk V., Skrypska O., Lesyuk O., Khomyak S., Lytvyn R., Sobechko I., Horak Yu. (**2024**). Synthesis of 3-(1R-5-phenyl-1*H*-pyrrol-2-yl)propanoic acids and prediction of their biological activity. *Visnyk of the Lviv University. Series Chemistry*, 65(1), 223–230. https://doi.org/10.30970/vch.6501.223 (in Ukrainian)