3-Oxy-5-phenyl-1*H*-1,2,3-triazole-4-carboxylic Acid. Synthesis, Structure, and Properties

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Abstract—The structure of 3-oxy-5-phenyl-1*H*-1,2,3-triazole-4-carboxylic acid was determined both experimentally (by the X-ray diffraction method) and by quantum-chemical calculations. Alkylation of 3-oxy-5-phenyl-1*H*-1,2,3-triazole-4-carboxylic acid (as crystal hydrate) with methyl iodide, depending on the reactant ratio, gives 1-methoxy-4-phenyl-1*H*-1,2,3-triazole-5-carboxylic acid and methyl 1-methoxy-4-phenyl-1*H*-1,2,3-triazole-5-carboxylate. Nitration of the title compound under mild conditions occurs at the 5-phenyl group with formation of *meta*-nitro derivative, while under more severe conditions 3,5-dinitrobenzoic acid is obtained. 3-Oxy-5-phenyl-1*H*-1,2,3-triazole-4-carboxylic acid was also converted into the corresponding acid chloride and substituted amide.