

2'-Oxoethyl Flavin Revisited

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The present work investigates the possibility of using 2'-oxoethyl flavin (**2**) as a starting material for the construction of more complicated flavin-based molecules. 2'-Oxoethyl flavin (**2**), prepared by oxidative degradation of commercially available riboflavin **1**, is however a rather untypical aldehyde. It prefers the hydrated *gem*-diol form **4** in aqueous solution. *Ab initio* electronic structure calculations, carried out at the level of Møller-Plesset perturbation theory of second order (MP2), predict the existence of an intramolecular hydrogen bond between one of the hydroxy groups of the diol and the N1 atom of the flavin skeleton. This result is supported by ¹H NMR measurements which indicate an interaction between the hydroxy groups and the conjugated ring system. We postulate that this rather strong intramolecular hydrogen bond is the origin of the enhanced stability of the *gem*-diol over the aldehyde form **2**.

Synthetic applicability of 2'-oxoethyl flavin **2** is limited by low solubility in most organic solvents and sensitivity to basic conditions. The aldehyde functional group is surprisingly reluctant to nucleophilic attack, and several reactions quite typical for aldehydes failed. Nevertheless, reductive amination led to the expected secondary amine **7**. Solubility of the molecule thus increased, and a new amino group was introduced.

Key words: Flavin, Aldehyde, Hydration, Nucleophilic Attack, Reductive Amination, Local MP2