

## **Unexpected dimerization of 1,3-dimethyl-5-methylenebarbituric acid revealed by a combined experimental and computational study**

### Abstract

A comparison of experimental and calculated  $^{13}\text{C}$ -nuclear magnetic resonance chemical shifts reveals the molecular structure of a dimer that was obtained by an unexpected dimerization of 1,3-dimethyl-5-methylenebarbituric acid. Furthermore, the puckering angle of the cyclobutane unit linking the six-membered rings is discussed in detail. The influence of substituents on 1,3-position of the cyclobutane ring on the puckering angle is demonstrated based on 1,1,3,3-tetramethylcyclobutane. Copyright © 2015 John Wiley & Sons, Ltd.