Magnetic Resonance in Chemistry 2015 vol.52 N12, pages 769-778

Dynamic NMR study of cyclic derivatives of pyridoxine

Rakhmatullin I., Galiullina L., Garipov M., Strel'Nik A., Shtyrlin Y., Klochkov V. *Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

Abstract

Copyright © 2014 John Wiley & Sons, Ltd. A series of pyridoxine derivatives was investigated by 1H and 2D nuclear overhauser enhancement spectroscopy (NOESY) NMR. The free energies of activation for the pyridyl-oxygen rotation of the 2,4-dinitrophenyl ether of the seven-membered acetals of pyridoxine were measured by dynamic NMR. A conformational exchange between the chair and twist forms of the seven-membered acetal ring was confirmed by dynamic NMR and STO3G computations.

http://dx.doi.org/10.1002/mrc.4123

Keywords

dynamic 1H NMR, energy barrier, pyridoxine