Dynamic NMR study of dinitrophenyl derivatives of seven-membered cyclic ketals of pyridoxine

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

Abstract

© 2015 John Wiley & Sons, Ltd. Two pyridoxine derivatives containing a dinitrophenyl moiety were investigated by ¹H NMR spectroscopy. Conformational dynamics in solution were studied for each compound using dynamic NMR experiments. It was shown that both compounds studied are involved into two conformational exchange processes. The first process is a transformation of the seven-membered cycle conformation between the enantiomeric P-twist and M-twist forms, and the second is a rotation of the dinitrophenyl fragment of the molecules around the C-O bond. Energy barriers of both conformational transitions were determined.

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Keywords

conformational exchange, dynamic ¹H NMR, energy barrier, ketal, pyridoxine