

Structural and Vibrational Study of Maprotiline

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Maprotiline (Ludimil, N-Methyl-9, 10-ethanoanthracene-9(10H)-propanamine) is a tetra cyclic antidepressant (Fig. 1). It is a highly selective inhibitor of norepinephrine reuptake. The solid and solution (CCl₄ and ethanol) infrared spectra of maprotiline have been recorded.

The fully optimized equilibrium structure of maprotiline has been obtained from DFT calculations by using the B3LYP functional in combination with 6-31G and 6-311G (d,p) basis sets. The results of harmonic and anharmonic frequency calculations on maprotiline are presented. The vibrational spectra were interpreted, with the aid of normal coordinate analysis based on a scaled quantum mechanical (SQM) force field [1]. The infrared spectrum was also predicted from the calculated intensities. Vibrational assignment of all the fundamentals was made using the total energy distribution (TED).

The possible interaction between maprotiline and local anesthetic citanest (prilocaine) and neurotransmitter serotonin (5-HT) were investigated.

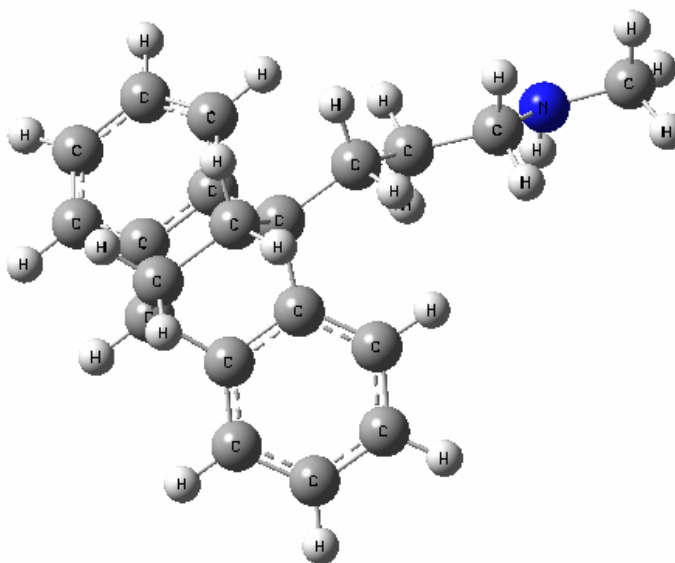


Fig. 1: DFT/6-311G(d,p) structure of maprotiline

[1] J. Baker, A.A. Jarzecki, P. Pulay, J Phys Chem A 102 (1998) 1412–1424.