Structural, Electronic, and Vibrational Properties of Amino-adamantane and Rimantadine Isomers

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(Submitted on 13 Apr 2012)

We performed a first principles total energy investigation on the structural, electronic, and vibrational properties of adamantane molecules, functionalized with amine and ethanamine groups. We computed the vibrational signatures of amantadine and rimantadine isomers with the functional groups bonded to different carbon sites. By comparing our results with recent infrared and Raman spectroscopic data, we discuss the possible presence of different isomers in experimental samples.

Subjects:	**Chemical Physics (physics.chem-ph)**; Other Condensed Matter (cond-mat.other)
Journal reference:	J. Phys. Chem. A, 2010, 114 (44), pp 11977-11983
DOI:	10.1021/jp107496b
Cite as:	**arXiv:1204.2878 [physics.chem-ph]** (or **arXiv:1204.2878v1 [physics.chem-ph]** for this version)

Submission history

From: Joelson Cott Garcia jcgarcia [view email]
[v1] Fri, 13 Apr 2012 04:48:18 GMT (1326kb)

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