Theoretical Study on Amines Structures

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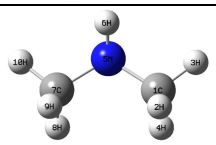
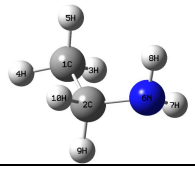
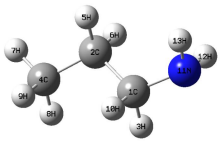
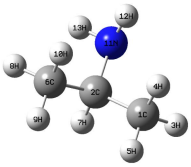
Abstract

The acetylation of amines is one of the most frequently used transformations in organic synthesis as it provides an efficient means for protecting amino groups in a multistep synthetic process. Geometric parameters of reactants: methylamine, dimethylamine, ethylamine, propylamine and isopropylamine were performed in the gas phase using the DFT (Density Functional Theory)/B3LYP (Becke, 3-parameter, Lee-Yang-Parr) method and was adopted the 3-21+G* basis set. Enthalpies of formation were determined using the AM1 (Austin Model 1) method. Theoretical study on amines structures was carried out [1]. The table lists the energies, lengths and angles values obtained.

Amines	Structures	Bond Lengths (Å)	Bond Angles (°)	Energies kcal mol^{-1}
Methylamine		C-H = 1.12 C-N = 1.43 N-H = 1.00	H-C-H = 107.95 H-C-N = 109.03 C-N-H = 111.33	- 7.42
Dimethylamine		C-H = 1.12 C-N = 1.44 N-H = 1.00	C-N-C = 114.38 H_3-C-N = 108.78 H-N-C = 110.58	- 5.69
Ethylamine		C_1-C_2 = 1.52 C_2-N = 1.44 N-H_7 = 1.00 C_2-H_9=1.13	C_1-C_2-N = 116.79 H_5-C_1-C_2 = 111.04 H_9-C_2-N = 107.54 C_2-N-H_8 = 110.89	-15.20
Propylamine		C_1-C_2 = 1.53 C_1-N = 1.44 N-H_{12} = 1.00 C_2-H_5 =1.12 C_1-H_3 =1.13	C_2-C_1-N = 116.58 H_3-C_1-N = 107.75 H_{12}-N-C_1 = 110.95 H_5-C_2-C_1 = 109.76 C_4-C_2-C_1 = 110.81	-22.16
Isopropylamine		C_1-C_2 = 1.53 C_2-N = 1.48 N-H_{12} = 0.99 C_2-H_7 =1.12 C_1-H_3 =1.10	C_1-C_2-N = 110.17 H_7-C_2-N = 107.15 H_{13}-N-C_2 = 109.61 H_5-C_1-C_2 = 110.67 N-C_2-C_6 = 112.45	-22.46

References:

[1] J. Nascimento, M. Pelegrini, L.F.A. Ferrão, O. Roberto-Neto, F.B.C. Machado, J. Braz. Chem. Soc. 22 (2011) 968.