Ab Initio Calculation On "2-Amino-Ethyl-Acetate" ($CH_3COOCH_2CH_2NH_3^+$) Ion

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The important role that acetylcholine (Ach) plays in biology (muscarinic activity) stimulated much theoretical research [1] on it. It is known [2] that the biological importance drops when the methyl groups are replaced by H atoms. This study is devoted to $[CH_3C(O)OCH_2CH_2NH_3]^+$ (Fig. 1), a molecule

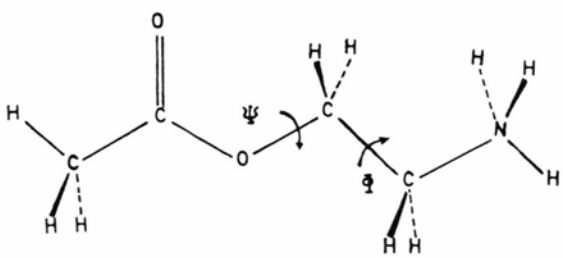

Fig. 1. Scheme of $[CH_3C(O)OCH_2CH_2NH_3]^+$ ion.

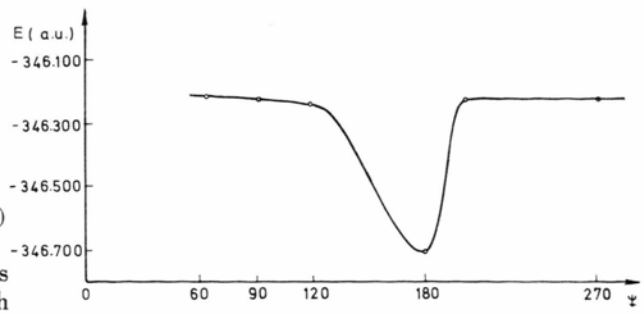

Fig. 2. Total energy vs. Ψ at $\Phi=50°$.

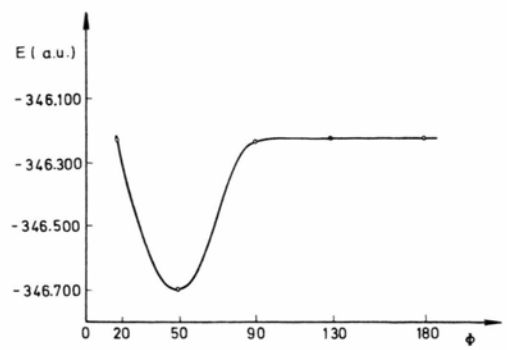

Fig. 3. Total energy vs. Φ at $\Psi=180°$.

where all methyl groups of Ach are replaced by H atoms. An ab initio procedure was used with the minimum basis set STO-2G of Pople et alias [3]. All bond lengths reported in the Ach bromide crystal structure [4] were adapted for our calculation except the standard bond length for N-H bonds [5]. Only two angles [1] Φ and Ψ were varied. The results are shown in Figs. 2 and 3. The calculations use a small basis set, but we believe that the relative values of energies remain the same with larger basis sets. This was partially confirmed by the calculations at a few selected points with the basis set [3] STO-3G. Though the angle optimization (Φ, Ψ) was not done with the STO-3G basis set one can expect that the general picture of the conformation would be the same. It is interesting to compare our results with the calculations on Ach. The most interesting result of these calculations [1] is that there are many configurations within an acceptable range of energies (~ 10 kcal/mol). The molecule we have studied is completely different in this respect. It is quite rigid with an enormous difference of energy between a very shallow minimum at (180°, 180°) and an absolute minimum at (50°, 180°). The effect of conformation on the electronic structure is roughly similar to that observed [1] in Ach. The four highest occupied orbitals and the lowest unoccupied one are all located in the ($H_3CCOOCH_2CH_2$) moiety. The energies of these orbitals depend to some extent (0.02 a.u.) on the conformation. The variations of population matrices are very small (atomic charge density variation to 0.01).

Acknowledgements

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