Computational study on the fragmentation of Benzyl penicillin by AM1 method

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Abstract

Isobutane Chemical-Ionization (CI) mass spectrum of benzyl penicillin[1] has been considered by the comparison of net charges on atoms in the molecule for the mechanism of formation of fragments. The geometry and electronic structure of benzyl penicillin[2,3] (**1,2,3**) and its fragments (**4 to 9**) have been optimized and calculated in the gas phase by using semi-empirical molecular orbital Austin Model-1 (AM1) method, which is included in the MOPAC93 (ver. 5.13). In this connection, the heats of formation (ΔH_f^o), dipole moment (μ), ionization potential (IP), and energies of frontier molecular orbitals (E_{HOMO} and E_{LUMO}) have been performed and discussed. Thus obtained fragmentation of benzylpenicillin is mentioned in the **Figure-1**. It is also observed the stability of investigated fragments are increased in the order of **9 < 5 < 4 < 6 < 3 < 7 < 2 < 8 < 1.** The IP is increased in the order of **1 < 4 < 2 < 3 < 5 < 8 < 6 < 9 < 7**. The dipole moment is increased in the order of **6 < 3 < 1 < 8 < 7 < 2 < 9 < 5 < 4**.

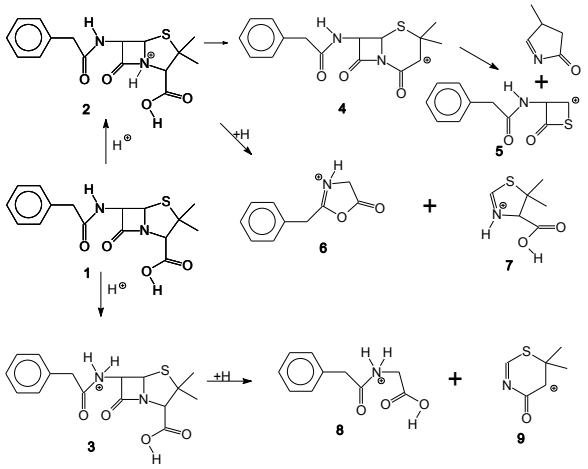

Figure-1:- Isobutane CI-mass spectrum of Benzyl penicillin - Fragmentation

1. L.A. Mitscher, H.D.H Showalter, K. Shirahata and R.L. Foltz, ***J Antibiotics***, 28(9), 668-675, **1975**.

2. M. Venugopal, P. Raveendra Reddy and B. Rajeshwar Rao, ***Int J Org and Bio-org Chem,*** 2(1), 1-6, **2012**. www.urpjournals.com

3. M Venugopal, P Raveendra Reddy and B Rajeshwar Rao, ***Int J Pharm and Chem Sci,*** 2(3), 1150-1156, **2013**. www.ijpcsonline.com