

Neutral vs. zwitterionic form of dipicolinic acid: A DFT study

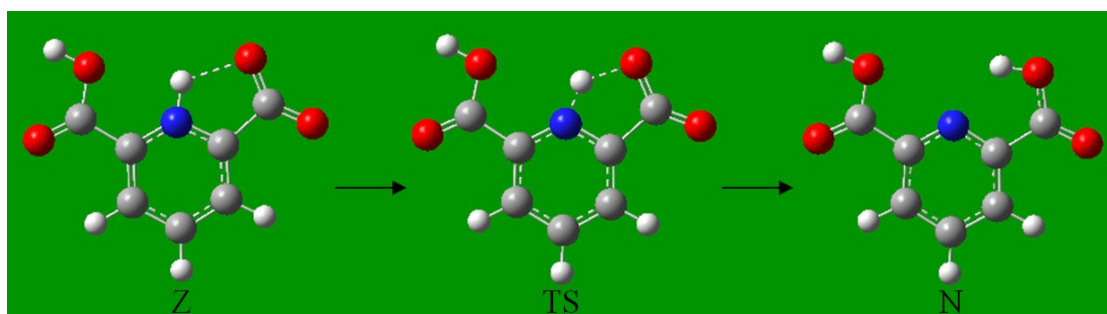
Seyed Hasan Kazemi^a, Hossein Eshtiagh-Hosseini^a and Masoud Mirzaei^a

^a Department of Chemistry, Ferdowsi University of Mashhad, Mashhad 917791436, Iran

E-mail: kazemi7@gmail.com; kazemi-r@staff.um.ac.ir

Dipicolinic acid (DPA) is well known as a chelate, eliminating radioactivity and antibacterial substance [1]. It has drawn attention recently for its inhibitory effects on the anti-platelet aggregation activity of blood, with those effects per weight being stronger than those of aspirin [2]. It was also found that when DPA is added to the culture solution of *Bacillus subtilis natto*, the concentration of vitamin K₂ increased [3].

Since proton transfer (PT) is one of the most important reactions in chemical and biological processes [4-6] in this paper, we report on our investigation of the PT reaction between the zwitterionic (Z) and neutral (N) form of DPA with density functional theory (DFT) at the B3LYP/6-31G(d) basis set level. Nonspecific solvent effects have also been taken into account by using the continuum model (IPCM) of four different solvent. The barrier height for the PT reaction of DPA decreases upon shifting from the water to the gas phase. As a result, the PT reaction between Z and N is thermodynamically and kinetically very easier in the gas phase than in solution. We hope that our study provides an enhanced interpretation of DPA and its derivatives.



References

- [1] H. Sumi, T.Ohsugi, *Nippon Nogeikagaku Kaishi*. **1999**, 73, 1289.
- [2] T. Ohsugi, S. Ikeda, H. Sumi, *Food Sci Technol Res*. **2005**, 11, 308.
- [3] H. Sumi, S. Ikeda, T.Ohsugi, *The Open Food Science Journal*. **2009**, 3, 10.
- [4] DÖ. Isin, N. Karakus, *J Mol Model*. **2010**, 16, 1877.
- [5] M. Mirzaei, H. Aghabozorg, H. Eshtiagh-Hosseini, *J Iran Chem Soc*. **2011**, 8, 580.
- [6] RD. Massaro, E. Blaisten-Barojas, *Computational and Theoretical Chemistry*. **2011**, 977, 148.