XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Accurate pK_a Determination of Alcohols with BMK And G3(MP2)//B3-CEP

Cleuton de Souza Silva[a] and Rogério Custodio[b]

[a] Instituto de Ciências Exatas e Tecnologia, Universidade Federal do Amazonas, Campus de Itacoatiara, 69100-021 Itacoatiara, Amazonas, Brazil ; [b]Instituto de Química, Universidade Estadual de Campinas, Barão Geraldo, P.O. Box 6154, 13083-970 Campinas, São Paulo, Brazil

Abstract: There is much interest in the development of reliable quantum chemical methods for the prediction of thermochemical data. In the last few years, extensive research has been conducted to determine the pK_a value of molecules in a solution. Different theoretical alternatives have been adopted to incorporate the solvation effect for that property. This work presents some theoretical calculations of pK_a for Alcohols by applying SMD (Solvation Model - Density) [1] at the G3(MP2)//B3-CEP [2], and BMK [3] levels of theory. The calculations were carried out with BMK functional with cc-pvtz basis set for the compounds in gas phase and in the presence of the solvent with three waters. The G3(MP2)//B3-CEP theory was also used to estimate the same property in identical conditions. Table 1 shows the results with BMK/cc-pvtz, and G3(MP2)//B3-CEP for calculated and experimental pK_a values. Comparing both theories shows that BMK/cc-pvtz achieved the worst results when compared with the experimental data. The G3(MP2)//B3-CEP theory presented the best pK_a values for the compounds studied. The four results present an absolute error lower than 0.55 units of pKa. Only the $(CH3)_2$─CH─O provided a large deviation of 0.88.

Table 1. Calculated and measured pK_a values for some Alcohols with three waters.

Substance	BMK	G3(MP2)//B3-CEP	Exp.
CH_3CH_2OH	14.42	15.72	15.90
$CH_3CH_2CH_2OH$	13.38	16.52	16.10
$(CH3)_2$─CH─O	15.89	17.98	17.10
$(CH3)_3$─C─OH	18.65	15.45	16.00

Key-words: G3(MP2)//B3-CEP, Alcohols and BMK.
Support: This work has been supported by FAPESP, CNPq, FAEPEX-UNICAMP, CENAPAD-UFC and FAPEAM.

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