Development of a Transition State Database from Chemical Reactions

Introduction

Studies of computational chemistry in recent decades have been growing exponentially, a simple Google search with the phrase 'Computational chemestry' in generates approximately 11,500,000 results and tends to increase more and more.

Currently, there are several theoretical methods based on computational chemistry, such as density functional theory and the semi-empirical method[1,2], which became a great choice for the prediction of some properties such as vibrational frequencies, potential energy surface, electronic parameters and energies, molecular properties and perhaps the most difficult of them, transition states structures.

Currently there are some recognized data banks and that are cataloged critical information in the molecular field, one can cite the crystallography data bank of Cambridge (CCDC), one facing in the area solid state, Virtual Atomic and Molecular Data Center (VAMDC). There are two national examples, the first database pharmacokinetics (PK / DB) and a second that is being developed with the approach of cataloging a database of natural products from Brazil[3,4].

Considering examples of molecular properties data bank and the great difficulty of calculating state transitions, this paper propose the built of a online system that supplemente this lack.

Methods

DFT and semiempirical methods combined with STQN method (Synchronous Transit-Guided Quasi-Newton)[5] were used to find the transition states. All theoretical calculations were carried out using the G09[6] program suite.

The reactions used to implementation in the data base were: hydrogens transfers, adding halide hydrogens in alkenes following Markovnikov mechanism, reaction aromatic nitration reaction of Morita-Baylis-Hilman, atmospheric reactions and obtaining inorganic cycles involving sulfur-phosphorus-nitrogen bond.

The database will be built in tables with descriptions of the reactions, their mechanism and downloads will be available at website.

Results and Discussion

The intention of the Transition Stats Data Bank (TSDB) is the user has the facility to find the transition state of the reaction of interest and describe analogues transition states with different functional groups. In the data bank, first, it is showed a generic description of the reaction and a second page shows the detailed mechanism, which it is available a Gaussian input file with transition state optimized in the PM6 or B3LYP/6-31G, see Figure 1. In addition, it will be possible to the user, also, deposit own transition states. The website will be hosted in the www.qtea.ueg.br/tsdb.
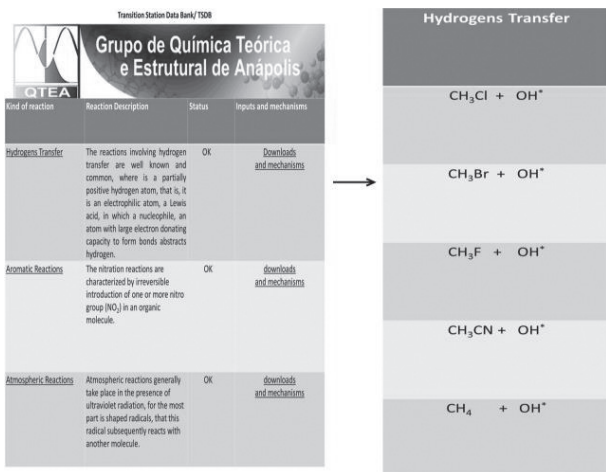
Figure 1: Website framework to find the optimized transition state.

To composition of the data bank, preliminary, we propose several transition states which are shown in a Table 1. The geometric parameters such as length bond formed and broken, angles and torsion angles are presented.

Conclusion

In summary, we propose the online framework of the data bank and we describe some transition states for specific chemical reactions. These transition states obtained assisted in the build on framework of the data bank.

The theory of the transition state is a great alternative to having theoretical results, such as electronic and thermodynamic properties with such perfect accuracy as those using experimental results. It can be observed that for the transition state calculation requires a long time because its difficulty requires the researcher a robust chemical sense. . In this sense, the data bank can assist researchers to elucidate others reactions mechanism.

Acknowledgments

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Table 1: Geometric parameters obtained from chemical reactions studied

Reaction	d1	d2	A1	A2	T1	A2	T1
CH3Cl + OH-	1.25	1.24	108.4	103.3	0.00	103.34	0.00
CH3Br + OH*	1.31	1.18	107.8	99.4	0.00	99.44	-0.00
CH3F + OH*	1.19	1.30	107.8	95.6	-0.03	95.62	-0.03
CH3CN + OH*	1.22	1.24	106.7	99.7	0.10	99.71	0.10
CH4 + OH*	1.19	1.29	107.3	96.9	59.2	96.98	59.21
C2H7 + HX	1.87	1.30	150.6	100.7	33.3	100.70	33.30
C6H6 + NO2	-	2.01	-	107.0	60.4	107.03	60.46
C8H9N2O + C6H10O3	-	1.96	-	108.9	84.3	108.93	84.31
O3 + NO2	1.23	1.83	116.8	107.1	7.0	107.13	7.03
P2N2S2	1.50	2.19	129.3	90.2	179.9	90.24	179.9

d1 = distance broken bond; d2 = distance connection formed; A1 = lead angle being broken; A2 = lead angle being formed; T1= Twist angle between the planes.

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F. O. S Neto & V. H Carvalho*

Grupo de Química Teórica e Estrutural de Anápolis, Campus de Ciências Exatas e Tecnológicas, Universidade Estadual de Goiás, 75001-970, Anápolis, Brasil

*E-mail: fatioleg@ueg.com