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Study of the mechanism of isopropyl sulfoxide production from isopropyl sulfhide

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Abstract

This paper presents results of a quantum-chemical study of the mechanism for producing diisopropyl sulfoxide. From the literature it is known that many sulfoxides can be obtained by oxidation of dialkyl sulphides in the presence of various acids. The purpose of this study was to computer simulate the mechanism of the interaction of dialkyl sulfides with hydrogen peroxide to determine the role of catalysis in this process. Diisopropyl sulfide was the starting compound. At the first stage, calculations were performed using the Priroda program and the semi-empirical density functional method QM_N3 developed by Dmitry Laikov. A search was made for transition states as well as descents along the reaction coordinate. Were localized minima that correspond to the reagents and products using the shell P-AutoExtremum and the method QM_N3. Then, the found geometrical parameters of transition states were recalculated by the GGA PBE method in the same Priroda program. The enthalpies of activation of the studied reactions are calculated. A comparison of the results was obtained by these two methods. The reaction of diisopropyl sulfide with two molecules of hydrogen peroxide was studied. The QM_N3 method quickly calculates transition states, but significantly overestimates the reaction barriers, as shown by calculations. Thus, according to the QM_N3 method, the enthalpy of activation of the reaction of diisopropyl sulfide with one hydrogen peroxide molecule was 202.9 kJ/mol, while the PBE method gives a value of 81.4 kJ /mol. However, both methods show that adding a second hydrogen peroxide molecule reduces the barrier. The process activation enthalpy is 33.7 kJ/mol according to the PBE method. At the same time, hydrogen peroxide was a reagent and catalyst.

References

[1] G.F. Bolshakov. Organic sulfur compounds of oil. *Novosibirsk: Science.* **1986**. 243p. (russian)
[2] A.Kh. Sharipov. *Chem Technol Fuels Oils.* **1997**. Vol.33. No.3. P.125-137.
[3] Oae Shigeru. Chemistry of organic sulfur compounds. Per. with japan Ed. Prilezhaeva E.N. *Moscow: Chemistry.* **1975**. 512p. (russian)
[4] A.Kh. Sharipov. *Neftekhimiya.* **1991**. Vol.31. No.3. P.275-283. (russian)
[5] A.Kh. Sharipov, Z.A. Suleimanova, I.S. Faizrakhmanov, R.M. Masagutov. *Neftekhimiya.* **1991**. Vol.31. No.1. P.86. (russian)
[6] A.Kh. Sharipov, I.S. Faizrakhmanov, L.F. Zainullina, R.F. Talipov. *Bulletin of Bashkir University*. **2006**. No.2. P.56-58. (russian)
[7] D.N. Laikov. *Journal of Chemical Physics*. **2011**. Vol.135. P.134120.
[8] D.N. Laikov, Yu.A. Ustynyuk. *Russian Chemical Bulletin*. **2005**. Vol.54. P.820-826.
[9] A.G. Shamov, G.G. Garifzianova, I.V. Aristov, G.M. Khrapkovsky. The mechanism of decomposition cyclohexyl phenyl sulfide in the process of aquathermolysis. *Butlerov Communications.* **2016**. Vol.48. No.10. P.156-162. DOI: 10.37952/ROI-jbc-01/16-48-10-156
[10] A.G. Shamov, I.V. Aristov, G.G. Garifzianova, and G.M. Khrapkovsky. Theoretical study of the mechanism of model sulfur aquathermolysis asphaltene using of the Priroda program. *Butlerov Communications.* **2016**. Vol.48. No.11. P.7-11. DOI: 10.37952/ROI-jbc-01/16-48-11-7
[11] J.P. Perdew, K. Burke, M. Ernzerhof. *Phys. Rev. Lett.* **1996**. Vol.77. P.3865-3868.
[12] A.G. Shamov, G.G. Garifzianova, I.V. Atistov, O.D. Fomihyh, G.M. Khrapkovsky. *Herald of Technological University*. **2017**. Vol.20. No.2. P.5-10. (russian)
[13] G.G.Garifzianova, D.V. Chachkov, A.G. Shamov. *Herald of Technological University*. **2011**. No.42. P.7-11. (russian)

[14] D.L. Egorov, A.G. Shamov, G.M. Khrapkovsky. *Herald of Technological University.* **2016**. Vol.19. No.23. P.14-17. (russian)
[15] D.L. Egorov, A.G. Shamov, and G.M. Khrapkovsky. Processing of the results of quantum chemical calculations using P-Analysis Program. *Butlerov Communications.* **2016**. Vol.48. No.11. P.1-6. DOI: 10.37952/ROI-jbc-01/16-48-11-1
[16] http://www.chemcraftprog.com