

- [8] Teixeira, A.L., Santos, R.C., Leal, J.P., Simoes, J.A.M., Falcao A.O., ThermInfo: *Collecting, Retrieving, and Estimating Reliable Thermochemical Data*, From: <http://arxiv.org/ftp/arxiv/papers/1302/1302.0710.pdf>.
- [9] *NIST Chemistry WebBook. NIST Standard Reference Database Number 69*. From: <http://webbook.nist.gov/chemistry/>
- [10] Yager, R., Filev D.P., *Essentials of Fuzzy Modeling and Control*, USA: John Wiley & Sons, 1994.
- [11] Thierauf, R.J., *Effective Business Intelligence Systems*, Westport. Quorum Books, 2001.
- [12] Allison, T., *The NIST Chemical Kinetics Database/* From: <http://www.auburn.edu/~stanbdm/Alison27s20report/files/NISTKineticsDB-TomAllison.pdf>.
- [13] Frenklach M., *PRIME Update: Workflow 2.0 and Automated UQ Predictive Modeling of Hydrogen Combustion*. From: http://kinetics.nist.gov/RealFuels/maccr/maccr2011/MACCCR_2011_Frenklach.pdf
- [14] Tumanov, V.E., Data Warehousing and Data Mining in Thermochemistry of Free Radical Reactions, *Fourth Winter Symposium on Chemometrics "Modern Methods of Data Analysis"*, Chernogolovka, 2005, pp. 28-29.
- [15] Denisov, E.T., New Empirical Models of Radical Abstraction Reactions, *Russian Chemical Reviews*, Vol. 66, No. 10, 1997, pp. 859-876.
- [16] Denisov, E.T., Tumanov, V.E., Transition-State Model as the Result of 2 Morse Terms Crossing Applied to Atomic-Hydrogen Reactions, *Zurnal fiziceskoj himii*, Vol. 68, No. 4, 1994, pp. 719-725.
- [17] Hemmer, M.C., *Expert System in Chemistry Research*, CRC Press, Taylor & Francis Group, 2008.
- [18] Gasteinger, J., Jochum, C., EROS - A Compute Programm for Generating Sequences of Reactions, *Topics Curr. Chem.*, Vol. 74, 1978, pp. 93-126.
- [19] Long, J. M., *SPARC: An Expert System for Estimating Physical and Chemical Reactivity: User Manual for Calculating Ionization pKa*, Ecosystems Research Division, National Exposure Laboratory, U.S. Environmental Protection Agency: Athens, GA, 1996.
- [20] Himmelblau ,D.M., Applications of Artificial Neural Networks in Chemical Engineering, *Korean Z Chem. Eng.*, Vol. 17, No. 4. 2000, pp. 373-392.
- [21] Gasteiger, J., Zupan, J., Neural Networks in Chemistry, *Angev. Chem. Int. Ed. Engl.*, Vol. 32, 1993, pp. 503-527.
- [22] Tumanov, V.E., Application of the Artificial Neural Networks and Fuzzy Logic for the Prediction of Reactivity of Molecules in Radical Reactions, *Computational Problems in Engineering. Series: Lecture Notes in Electrical Engineering*, Switzerland: Springer International Publishing, Vol. 307, 2014, pp. 261-269.
- [23] Tumanov, V.E., Hybrid Algorithm of Application of Artificial Neuronets for an Evaluation of Rate Constants of Radical Bimolecular Reactions, *Advances in Neural Networks, Fuzzy Systems and Artificial Intelligence. Recent Advances in Computer Engineering Series*, WSEAS Press. Gdansk, Poland, Vol. 21, 2014, pp. 58-61.
- [24] Tumanov ,V.E., Gaifullin, B. N., Evaluation of the Rate Constants of Reactions of Phenyl Radicals with Hydrocarbons with the Use of Artificial Neural Network, *Current Approaches in Applied Artificial Intelligence*, Springer International Publishing Switzerland, Vol. 9101, 2015, pp. 394-403.
- [25] Tumanov, V., Gaifullin, G., Application of the Artificial Neural Networks for the Prediction of Reactivity of Molecules in Radical Reactions, *Mathematical Modelling and Simulation in Applied Sciences. Proc. of the 3rd International Conference on Energy, Environment, Devices, Systems, Communications, Computers* (INEEE '12). Rovaniemi, Finland, 2012, pp. 62-65.
- [26] Lazarev, D. Yu., Tumanov, V.E., Prediction of Bond Dissociation Energies of Organic Molecules by Kinetic Data of the Radical Reactions Using the Fuzzy Knowledge Base, *BIT,s 3rd Annual Conference and EXPO of AnalytiX-2014*, Dalian, China, 2014, p. 379.
- [27] Dutot, A.-L., Rude, J., Aumont, B., Neural Network Method to Estimate the Aqueous Rate Constants for the OH Reactions with Organic Compounds, *Atmospheric Environment*, Vol. 37, 2003, pp. 269-276.
- [28] Luo, Y.-R., *Comprehensive Handbook of Chemical Bond Energies*, London - New York: CRC Press, Boca. 2007.
- [29] Denisov, E.T., Tumanov, V.E., Estimation of the Bond Dissociation Energies from the Kinetic Characteristics of Liquid-Phase Radical Reactions, *Russian Chemical Reviews*, Vol. 74, No. 9, 2005, pp. 825-858.

- [30] Larose, D.T., *Data Mining Methods and Models*, John Wiley & Sons, 2006.
- [31] Rouvray, D.H., *Fuzzy Logic in Chemistry*, Academic Press, 1997.