structures were ranked by energy and the geometry of the ten lowest energy structures has been optimized using PBEh-3c method, which is more accurate than the widely used B3LYP/6-31G(d). Obtained global minimum dimer structure (Fig.) is more than 150 kJ/mol lower in energy than the kanamycin A monomer in the gas phase. For this lowest energy structure electronic properties, NMR and IR spectra have been calculated.

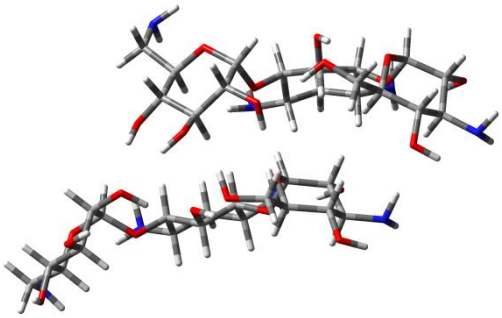

Fig. The calculated lowest energy structure of kanamycin A dimer

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Formation enthalpies of five-membered nitrogen-containing aromatic heterocycles. Quantum chemical calculations

Vadim E. Matulis, Mikhail G. Dzianisik, Oleg A. Ivashkevich
Research Institute for Physical Chemical Problems, Belarusian State University, Minsk, Belarus, *e-mail*:*matulisvad@gmail.com*

Five-membered nitrogen-containing aromatic heterocycles are important due to their wide application in various fields of technology, medicine, agriculture. In addition, tetrazoles and nitrotriazoles have a sufficiently high thermal stability along with considerable energetics and high nitrogen content, therefore they are effective components of composite propellants, explosive and gas-generating compositions. So, it is especially important to have information on the enthalpy of formation of these substances. Thermodynamic properties are also useful for developing methods of selective azole ring functionalization or introduction of azole fragment into more complex molecules. However, in literature there are a few data on the formation enthalpies of these compounds.

In this work, the standard gas-phase formation enthalpies of five-membered nitrogen-containing aromatic heterocycles have been calculated using isodesmic or atomization reactions. The first method requires knowledge of the experimental gas-phase formation enthalpies of all substances participating in the corresponding reaction, while determination of the formation enthalpies via atomization reactions does not have these shortcomings. The values of the gas-phase formation enthalpies of azoles, calculated using both methods, are in good agreement with the experimental ones. The only exception is 2-methyltetrazole. The experimental value of the gas-phase formation enthalpy of 2-methyltetrazole [1] is higher than that of 1-methyltetrazole, which also contradicts the results of our calculations. This indicates that further experimental studies of the formation enthalpy of 2-methyltetrazole are necessary.

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Design and synthesis of pyrazole amide derivatives assuccinate dehydrogenase inhibitors

N. B. Sun, Y. Lu, J. Yu, S. L. Wang, W. Ke, L. Wang
Research Department of Chemistry and Chemical Engineering, College of Biology and Environmental Engineering, Zhejiang Shuren University, Hangzhou, China, *e-mail:yj313513@sina.com*

Succinate dehydrogenase inhibitors affect the respiratory chain electron transport system of pathogens by acting on the protein complex II (succinate dehydrogenase), hinder its energy metabolism, thereby inhibiting the growth of pathogenic bacteria, leading to its death. It is a method for prevention and treatment of diseases. Due to this unique mechanism of succinate dehydrogenase inhibitors and the characteristics such as low toxicity, high activity, variable structures of these inhibitors, it has gradually attracted the attention of pesticide companies and scientists in recent years [1]. As pathogens have gradually produced different degrees of resistance to existing inhibitor products [2, 3] including pyridine-ethyl-benzamides, furan amides, pyrazole-amides and others [4, 5, 6], the development of novel succinate dehydrogenase inhibitors is increasingly showing its necessity and urgency. Hereby we report the design, synthesis, fungicidal activity and SAR study of novel fluorinated pyrazole amide derivatives as succinate dehydrogenase inhibitors, which can be divided into the following parts.

1. Virtual screening model establishment (Fig. 1) of those organic molecules that can be used as candidate inhibitors via computer softwares for the likes of