

## Charakterystyka mocy poszczególnych wiązań wodorowych w parach zasad DNA = Characterizing strength of individual hydrogen bonds in DNA base-pairs.

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### Rok wydania

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### Czasopismo

Wiadomości Chemiczne

### Numer woluminu

73

### Strony

53-74

### Kolekcja

Naukowa

### Język

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### Typ publikacji

Artykuł

### Streszczenie

The main idea of the current review is to present methods useful to characterize the strength of individual hydrogen bonds in nucleic acids base-pairs. In the paper, the Authors discuss the energy definition of intermolecular interactions taking into account the presence of one intermolecular hydrogen bond (HB) as well as the situation when several intermolecular interactions (namely intermolecular hydrogen bonds) are present. In the Section 2 of the review a general overview of methods developed to estimate the strength of the individual intermolecular hydrogen bond in DNA/RNA base-pairs is presented. Thus, the reader can find detailed information on the methods used so far: the rotational method (2003), compliance constants method (2004), the EML equation application (2006), the atom replacement method (2007), the estimation of hydrogen bond energy on the basis of electron density (calculated by using the AIM theory) at BCP values (2009), the application of NBO method (2010), the comparison of HB strength based on the last two approaches (2015) and the application of coordinates interaction approach (2017). It should be emphasized, that these methods allow to estimate the strength of intermolecular interactions both in the model base-pairs and in other systems with several intermolecular hydrogen bonds. The discussion of the presented methods is supported by Tables 1-10, containing numerical values characteristics of the strength of the particular HB, and Figures 1–2. The section 3 contains a critical comparison of results based on the presented methods. Concluding remarks are given in the last Section.

## Słowa kluczowe

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hydrogen bond, Watson-Crick base pairs, NBO, natural bond orbital method, AIM, atoms in molecules

wiązanie wodorowe, pary zasad Watsona-Cricka, NBO, koncepcja naturalnych orbitali wiązań, AIM, metoda atomy w cząsteczce

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### OTHER

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