Pemilihan Metode Perhitungan Kimia Komputasi Semi-empiris untuk Pengembangan 1,3,4-Thiadiazole

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Abstract	Computational chemistry methods are those used to help researchers design chemical compounds optimally, so that experiments and mistakes do not need to be done in the laboratory. This is a very important step because it can save costs, chemicals, and also the time spent. The method used in this study is semi-empirical, while the parameters used in this study are the infrared (IR) spectrum and the core magnetic resonance (NMR) spectrum which will be matched with the results of the study. The compound to be investigated is 1,3,4-Thiadiazole is a heterocyclic compound which is very useful in the field of medicines which contain anti-inflammatory, anticancer, glaucoma drugs etc. The results showed the most appropriate calculation method is PM3 based on infrared variation values of 1697.44 and the PRESS value of nuclear magnetic resonance variation of 21.170.
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