

## عنوان مقاله:

Theoretical studying of green synthesis of ۱,۲ disubstituted benzimidazole and quinoxaline derivatives by Bronsted acid ionic liquid in water at ambient temperature

## محل انتشار:

همایش منطقه ای شیمی (سال: ۱۳۸۹)

تعداد صفحات اصل مقاله: ۱

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## خلاصه مقاله:

This work has done by experimentally methods [۱, ۲] and because of importance of Benzimidazole and quinoxaline derivatives in biological systems we have made an effort to consider this case by theoretical studying with Gaussian ۹۸ Code. In this work we have calculated the prediction of productive by HF, BLYP and B<sup>3</sup>LYP methods and ۶-۳۱G, ۶-۳۱G\* and ۶-۳۱G\*\* are used as basis sets. We have then compared our results to experimental results and there is good agreement between them. We calculated enthalpy reaction and Gibbs free energy and other thermodynamics properties to predict. We also used Hyper Chem Code to prepare our calculations in Gaussian Code.

## کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/۸۲۸۹۳۸>