



جمهورية العراق  
وزارة التعليم العالي والبحث العلمي  
جامعة القادسية  
كلية العلوم

**search about**

**Computational chemistry investigation  
for the stability of substituted  
anthracene compounds by semi  
empirical approximation methods**

(بحث مقدم الى مجلس كلية العلوم / قسم علوم الكيمياء / جامعة القادسية وهو  
جزء من متطلبات نيل درجة البكالوريوس في علوم الكيمياء)

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**بإشراف الدكتورة**

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

وَقُلْ رَبِّيَ رَبُّنَا عَلَيْنَا

حُذِرُوا اللَّهَ الْعَظِيمَ

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# Abstract

Semi-empirical computational methods have been widely applied for theoretical investigations of various organic molecules.

In this study, we report the computational investigation of substituted anthracene compounds using GAUSSIAN 03 software in semi empirical PM3-level

All optimized geometry of compounds has been determined then Bonds length, bonds angle, HOMO, LUMO and HOMO-LUMO energy gap were calculated

The result shown that the withdrawing group increasing the activity of compound by decreasing the HOMO-LUMO energy gap, on the other hand the donating group decrease the activity of compound by increasing the HOMO-LUMO energy gap

The results shown that for the compounds substitute by donating group the activity were increase when it was substituted on the terminal ring as a result to decrease the HOMO-LUMO energy gap.

On the contrary for the compounds substitute by withdrawing groups the activity of compounds were decrease when it was substituted on the terminal ring as a result to increase of the HOMO-LUMO energy g

# أهداء

إلى من كلله الآله بالهيبة والوقار .. إلى من علمني العطاء بدون انتظار ..  
إلى من أحمل أسمه بكل افتخار .. أرجو من الآله أن يمد في عمرك لتري  
ثماراً قد حان قطافها بعد طول انتظار وستبقى كلماتك نجوم أهدتي بها  
اليوم وفي الغد وإلى الأبد

والدي الحبيب...