

عنوان مقاله:

Effect of External Electric Field and Temperature on Entropy, Heat of Capacity, and Chemical Reactivity with QSAR
Study of Morphonium Chloride and Nitrous Ionic Liquids Crystal Using DFT

محل انتشار:

نشریه متدهای شیمیایی، دوره 4، شماره 5 (سال: 1399)

تعداد صفحات اصل مقاله: 10

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خلاصه مقاله:

Due to the great number of medicinal application of morphine in drugs, the morphonium chloride (IL01) and morphonium nitrous (IL02) were investigated using the computational method to assess their biological activity. The quantitative structure activity relationship (QSAR) parameters for instance, charge density, surface area grid, volume, LogP, polarizability, refractivity, and molecular mass were demonstrated through the density functional theory (DFT) for simulation as well as the chemical reactivity like HOMO, LUMO, and HOMO, LUMO gap were also calculated. In addition, the most important thermodynamic properties such as entropy and heat of capacity were calculated using DFT method. The values of the initial entropy and heat of capacity were zero without applying temperature. At 273 K, the entropy and heat of the capacity are 0.117, 0.113, and 0.062, 0.055 kcal/mol-deg for IL01 and IL02, respectively, which finally increased by 0.177, 0.162 and 0.120, 0.099 kcal/mol-deg at 523 K. When electric field was applied on IL01, and IL02, the entropy was decreased by 32.47% and 2.65% whereas the heat of capacity was decreased by 79.03% and 1.81%, respectively. Finally, in same electric field with increasing temperature, the entropy was enhanced by 16.45% and 45.45% besides the heat of capacity was increased about 100% at 523 K and IL02 was found to be less response compared with that of the IL01 at low temperature for electric filed but almost similar response at high temperature.

کلمات کلیدی:

Morphine, DFT, electric field, QSAR

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