عنوان مقاله:

pKa prediction of some anilines using ab initio methods

محل انتشار:

دوازدهمین سمینار شیمی فیزیک ایران (سال: 1388)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Acidity constant prediction in aqueous solution is an active subject that contains growing researches and an exciting topic in computational quantum chemistry. These predictions involve either QSPR modeling [1] or microscopic quantum calculations based on a thermodynamic cycle of the process [2]. The first method is simple but has some .limitations such as the description selection. On the other hand, the second approach requires more CPU time

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا: