Structural modifications resulting from proton transfer in complexes of phenols with pyridine.

Autorzy

Irena Majerz

Emilia Kwiatkowska

Aleksander Koll

Rok wydania

2005

Czasopismo

Journal of Physical Organic Chemistry

Numer woluminu

18

Strony

833-843

DOI

10.1002/poc.948

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The structural consequences of proton transfer in complexes of phenol (**1**), 2,6-dichlorophenol (**2**), 4-nitrophenol (**3**) and 2,6-dichloro-4-nitrophenol (**4**) with pyridine were analyzed on the basis of results of B3LYP/6–31G** calculations. Three methods of describing the progress of proton transfer are proposed: the O—H [*d*(OH)] and C—O [*d*(CO)] bond lengths and the fraction X_{PT} of the proton transfer form, calculated from the values of the dipole moments. The *d*(OH) parameter reveals behaviour near to X_{PT} and can be used as a universal measure of the degree of proton transfer. The *d*(CO) parameter gives nearly linear dependences for various structural parameters, but independent estimation of the specific effects of the substituents is necessary, as separate correlations for each complex are found. A role of resonance interaction in systems containing a *p*-NO_2 substituent is demonstrated.

Adres publiczny

https://doi.org/10.1002/poc.948

Strona internetowa wydawcy

onlinelibrary.wiley.com