# Silne wiazania wodorowe w kompleksach wybranych kwasów organicznych z tetrametylopirazyną=Strong hydrogen bonds in selected complexes of organic acids with teramethylpyrazine.

Autorzy

Grażyna Bator

Lucjan Sobczyk

Rok wydania

2011

Czasopismo

Wiadomości Chemiczne

Numer woluminu

65

Strony

869-885

Kolekcja

Naukowa

Język

Polski

Typ publikacji

Artykuł

Streszczenie

in the present review our interest is focused on the hydrogen bonded complexes of tetramethylpyrazine (TMP) with strong proton donors, in particular with chlorani-lic (CLa) or squaric (H2sQ) acid. The x-ray diffraction studies show that, depending on the proton donor, various assemblies with the acid are formed, e.g. the infinite o-H...N hydrogen bonded chains without proton transfer in the case of the complex with CLa. on the other hand with H2sQ the assemblies of [HsQ]22–-2TMP·H+ com-position are created, in which the ionized HsQ–1 molecules are present in the form of dimers. These dimers are bound with the TMP·H+cations on its both sides viathe +N-H...o– hydrogen bonds. Picric acid forms with TMP the complex of the 2:1 composition with a double protonated TMP molecule. in the case of Hi3 acid the inte-resting units of the (TMP·H+)2·TMP composition are formed, in which two TMP·H+cations are coordinated with one TMP molecule through the +N-H...N bridges. in the infrared spectra of the TMP complexes, both with CLa and H2sQ, the similar absorption continua are observed. They can be interpreted in terms of an asymmetric potential for the proton motion, with either the double minimum or the single broad minimum potential for the CLa and H2sQ complexes, respectively.an analysis of the neutron scattering spectra concerns the phenomena of the tun-neling splitting, quasielastic neutron scattering (QNs) and inelastic (iNs) scattering. in the case of tunneling splitting neat TMP does not show any tunneling transitions in the μeV energy region, because they are overlapped by the elastic scattering band. in the case of the TMP·CLa complex four tunneling transitions are seen correspon-ding to the four crystallographically nonequivalent CH3 groups in the TMP molecule. in the spectrum of the complex with squaric acid the observed two transitions are ascribed to the two different CH3 groups. The two remaining CH3 group tunneling transitions are overlapped by the elastic scattering. The measurements in various low temperature ranges yield information about the shape of the CH3 group rotational potential. The shape of the potential is also reflected in the spectra of quasielastic scattering. in particular the

temperature dependence of the quasielastic band allows us to find the activation energy for the CH3 rotations. Finally the inelastic neutron scattering spectra are analyzed in the energy range of the CH3 torsional modes (below 200 cm–1 = 25 meV). The analysis shows that for the complexes the torsional vibration frequencies are markedly lower than those for neat TMP. in the case of the TMP·CLa complex frequencies found are particularly low. They are close to the frequencies cal-culated for the TMP+ cation. a general conclusion can be drawn that in the complexes the CH3 groups behave more loosely than in neat TMP

Słowa kluczowe

tetramethylpyrazine, chloranilic acid, squaric acid, x-ray diffraction, infra- red spectra, neutron scattering spectra

Adres publiczny

https://www.dbc.wroc.pl/dlibra/publication/14817/edition/13040/conte
ref=desc