Structural, spectroscopic and theoretical studies on 3,4,7,8-tetramethyl-1,10-phenantroline complex with picric acid.

Autorzy

Grażyna Bator

Lucjan Sobczyk

Wanda Sawka-Dobrowolska

J. Wuttke

Andrzej Pawlukojć

Eugeniusz Grech

J. Nowicka-Scheibe

Rok wydania

2013

Czasopismo

Chemical Physics

Numer woluminu

410

Strony

55-65

DOI

10.1016/j.chemphys.2012.10.012

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The almost planar molecular complex, formed by 3,4,7,8-tetramethyl-phenantroline (Me_4phen) and picric acid (2,4,6-trinitrophenol, PA), has been investigated by using X-ray diffraction, vibrational spectroscopy, tunnel splitting and theoretical analysis. In the crystal of Me_4phen·PA two short bifurcated hydrogen bonds N^+–H···O^- [2.6238(14) Å] and N^+–H···N [2.6898(15) Å] are created. Infra-red spectra show the hydrogen bonds are short. The neutron backscattering spectrum of Me_4phen·PA at 3 K shows two tunneling peaks at *ca*. 1 and 3 μeV. The number of the peaks is consistent with X-ray diffraction studies, which disclosed the inequivalence of methyl groups in the crystal structure. The comparison of the tunnel splitting for neat Me_4phen and for its complex with picric acid indicates that in the latter case the methyl groups are more strongly engaged in the intermolecular interactions, particularly with nitro group oxygen atoms of picric acid, leading to an increase of the CH_3 rotational barrier height.

Słowa kluczowe

Molecular complexes, Ion, lanthanides, symmetry, 8-tetramethyl-1, 10-phenantroline, molecule, 6-trinitrophenol, X-ray diffraction, crystal structure, Infrared spectroscopy, Neutron backscattering, DFT

Adres publiczny

http://dx.doi.org/10.1016/j.chemphys.2012.10.012

Strona internetowa wydawcy

http://www.elsevier.com