p-N,N'-tetraacetylodiaminodurene. The structure and vibrational spectra.

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2015

Czasopismo

Chemical Physics

Numer woluminu

459

Strony

148-154

DOI

10.1016/j.chemphys.2015.08.005

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The crystal and molecular structure of p-N,N′-tetraacetylodiaminodurene (TADD) is reported based on the X-ray diffraction studies. The N-acetyl moieties are planar and all N-acetyl groups are perpendicular to the ring plane. Methyl groups both of acetyl moieties and of durene form a number of non-conventional hydrogen bonds with nitrogen and oxygen atoms. The vibrational spectra very well reflect the structure of molecules and their contacts. They are compared with calculated data by using various theoretical approaches. The neutron scattering spectra show two tunnel lines of low energy values (at ±0.9 and ±2.3 μeV at 4 K), which can be ascribed to methyl groups of N-acetyl moieties, which behave more freely than those attached to the phenyl ring.

Słowa kluczowe

Tetraacetylodiaminodurene, Inelastic neutron spectroscopy

Adres publiczny

http://dx.doi.org/10.1016/j.chemphys.2015.08.005

Strona internetowa wydawcy

http://www.elsevier.com