The structure of diaminodurene and the dynamics of the methyl groups.

Autorzy

Lucjan Sobczyk

M. Prager

Wanda Sawka-Dobrowolska

Grażyna Bator

Andrzej Pawlukojć

Eugeniusz Grech

L. Van Eijck

A. Ivanov

S. Rols

J. Wuttke

T. Unruh

Rok wydania

2009

Czasopismo

Journal of Chemical Physics

Numer woluminu

130

Strony

164519/1-164519/9

DOI

10.1063/1.3125629

Kolekcja

Naukowa

Streszczenie

Diaminodurene crystallizes in the orthorhombic space group Pbca, with eight molecules in the unit cell. Four inequivalent methyl groups with different environments exist in a molecule. The amino groups are also different, which is well reflected in infrared spectra. Two tunneling modes are resolved at 23.7 and 7.0 μeV at 4.5 K. Their intensities are consistent with the presence of two further unresolved tunneling modes. Quasielastic spectra are composed of three Lorentzians of equal intensities. The two low activation energies and tunnel modes are modeled into consistent rotational potentials. The third activation energy and a librational band are used to guess the strength of the two stronger rotational potentials. The internal modes related to the torsional/librational vibrations mix with ring torsions in the range of 70–220 cm−1. This way the tunnel modes couple to ring torsions whose energy determines the broadening of both tunnel bands. The calculations for free molecules yield mode frequencies a little bit lower than the experimental inelastic neutron scattering (INS) values. Application of theoretical methods elaborated for the crystalline state leads to a satisfactory consistency. It is also valid for bending modes of NH2 groups, which in the solid state show much higher frequencies than in the gas phase, as expected.

Adres publiczny

https://doi.org/10.1063/1.3125629

Strona internetowa wydawcy

https://www.aip.org/

Język

Angielski

Typ publikacji

Artykuł