Structure and Molecular Motions in Rubidium Tetraphenylborate

A. Pajzderska, H. Małuszyńska, and J. Wąsicki

Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

Reprint requests to A. P.; E-mail: apajzder@main.amu.edu.pl

Z. Naturforsch. **57 a,** 847–853 (2002); received June 12, 2002

By X-ray diffraction it was found that at 293 K the crystals of rubidium tetraphenylborate are tetragonal, space group $I\bar{4}2m$, $a = b = 11.212(2)$ Å, $c = 8.098(2)$ Å, with 2 molecules of $Rb^+[C_{24}H_{20}B]^-$ in the unit cell. The molecular reorientations as functions of temperature were studied by ^{1}H NMR. Two types of motions were detected: an anisotropic reorientation of the tetraphenylborate anions about their mass centres, and small-angle reorientations / oscillations of the phenyl rings. The dependence of the potential energy of the anion in the crystal on the angle of the phenyl ring rotation about the B-Ph bond was obtained on the basis of atom-atom calculations. The dynamics of this compound was compared to that of tetraphenyltin.

Key words: NMR; Ralaxation; Potential Energy; X-ray; Crystal Structure.