Dynamics of some *n*-Alkanes Adsorbed in the Micropore of (±)-[Co(en)$_3$]Cl$_3$ as Studied by ^{2}H NMR

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The dynamic behavior of *n*-hexane-d$_{14}$ and *n*-decane-d$_{22}$, adsorbed in the micropore of [Co(en)$_3$]Cl$_3$ crystal was studied by ^{2}H NMR at 144 - 345 K. The quadrupole coupling constants (QCC) are 160 kHz for the methylene group and 60 kHz for methyl group below 144 K for hexane and below 178 K for decane, suggesting that the molecular reorientation about the molecular long axis is frozen below these temperatures. The QCC of CD$_2$ group in hexane decreases from 160 kHz to 80 kHz on heating up to 170 K. Similar reduction of QCC of CD$_2$ observed above 280 K for decane. Assuming the three-site jump model of the guest molecule about its molecular long axis, we reproduced the experimental spectrum, and obtained the rate of the molecular motion in each guest. The temperature dependence of jump rates leads to the activation energies for the molecular reorientation of 20 kJ mol^{-1} and 30 kJ mol^{-1} for *n*-hexane and *n*-decane, respectively, suggesting that the length of the guest molecule influences greatly its dynamics in the micropore.

Key words: (±)-[Co(en)$_3$]Cl$_3$; ^{2}H NMR; Micropore; Host-guest Interaction; Molecular Motion.