^{2}H and ^{195}Pt NMR Studies of Molecular and Electron Spin Dynamics in Paramagnetic $[Cu(H_2O)_6][PtCl_6]$*

Takahiro Iijima, Kengo Orii, Motohiro Mizuno, and Masahiko Suhara

Department of Chemistry, Faculty of Science, Kanazawa University, Kanazawa 920-1192, Japan.

Z. Naturforsch. **53 a,** 447–452 (1998); received December 31, 1997

The temperature dependences of ^{2}H and ^{195}Pt NMR spectra and the spin-lattice relaxation time T_1 were measured for $[Cu(H_2O)_6][PtCl_6]$. From the simulation of ^{2}H NMR spectra, the jump rate of 180° flips of the water molecules (k), the nuclear quadrupole interaction parameters ($e^2Qq/h, \eta$) and the electron-nucleon dipolar interaction parameter (ν_D) were obtained. By measuring ^{2}H T_1, k was estimated in the temperature range where the spectrum is insensitive to the motion of the water molecules. Above the phase transition temperature, the pre-exponential factor $k_0 = 8\times10^{11}\,s^{-1}$ and the activation energy E_a=15 kJmol^{-1} for 180° flips of the water molecules were obtained from the spectral simulation and T_1. ^{195}Pt NMR spectra showed an axially symmetric and unsymmetric powder pattern of the chemical shift anisotropy at the high and low temperature phase, respectively. For the deuterated compound, the correlation times of the electron spin in Cu^{2+} were estimated from ^{195}Pt T_1 and the activation energy for jumping between the different configurations of Jahn-Teller distortion Δ = 200 K was obtained.

Reprint requests to Dr. M. Mizuno; E-mail: mizuno@wriron1.s.kanazawa-u.ac.jp