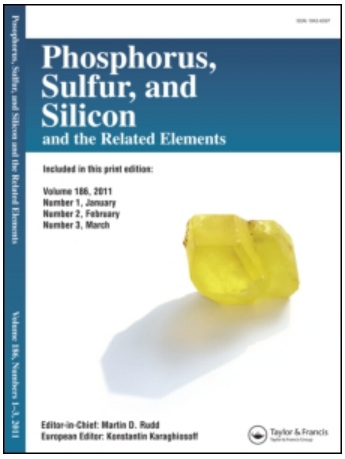

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Structure and Dynamical Behaviour of Bis(N-Diisopropoxy-Phosphorylthiobenzamido) Copper(II)

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Structure and Dynamical Behaviour of Bis(N-Diisopropoxy-Phosphorylthiobenzamido) Copper(II)

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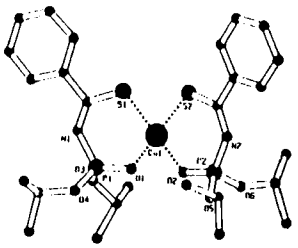
Among the new compounds of N-(thio)phosphorylthioamides, the copper(II) complex with N-diisopropoxyphosphorylthiobenzamide (CuL_2) exhibits series of unusual properties which have been extensively investigated in the present work. The X-ray structure of CuL_2 has been determined. Crystals of CuL_2 are monoclinic, $P2_1/c$, a = 15.610, b = 11.880, and c = 18.320 Å, β = 106.74°, Z = 4. The CuL_2 complex has the *cis*-structure with Cu-S distances ranging from 2.238 to 2.253 Å and Cu-O distances being from 1.919 to 1.937 Å (Figure).



The distinctions of the g and A components for the CuL_2 monocrystal ($g_{x,y}$ = 2.046, $A_{x,y}$ = 11 G, the Q-band EPR data) and frozen benzene solution ($g_{x,y}$ = 2.053, $A_{x,y}$ = 22 G) suggest the *trans*-isomer presence in solutions. For CuL_2 solutions in non-coordinating solvents (hexane, toluene, benzene, and 1,4-dioxane) the correlation times ($4 \div 14 \cdot 10^{-11}$ s, 300 K) and activation energy of rotation (6÷12 kJ/mol) have been derived from the X-band EPR linewidths as functions of temperature. In solutions of CuL_2 with electron-donor solvents the adducts were discovered as well as the thermodynamic and kinetic parameters of adduct formation determined by EPR over a wide range of temperature.

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