2. Показано, что триацилгидразон выступает в роли тринуклеирующего лиганда; каждая молекула диацилгидразона является бинуклеирующей и содержит свободную карбоксильную группу.

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GADOLINIUM(III) MIXED-LIGAND COMPLEX WITH HYDRAZONES OF 1,3,5-BENZENETRICARBOXYLIC ACID AND 4-FORMYL-3-METHYL-1-PHENYLPYRAZOL-5-ONE

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Gadolinium(III) mixed-ligand complex with hydrazones of 1,3,5-benzenetricarboxylic acid and 4-formyl-3-methyl-1-phenylpyrazol-5-one was obtained by the next procedure. 4-Formyl-3-methyl-1-phenylpyrazol-5-one (0,77 g, 3,81 mmol) had

been added into suspension of 0.32 g of the mixture (ratio 1:2) of 1,3,5-benzenetricarboxylic acid trihydrazide and 5-methoxycarbonyl-1,3-benzenedicarboxylic acid dihydrazide in 15 mL DMFA heated to 65-70 °C. This mixture was stirred on 30 min, and then 1.27 mmol of gadolinium chloride in ethanol (15 mL) and 0.8 mL of pyridine were added. The reaction mixture was stirred on 30 min, cooled to room temperature and filtered. In few days from resulting solution formed trigonal X-ray suitable crystals with composition $Gd_3C_{141}H_{105}N_{36}O_{24}\cdot 6DMF\cdot 5.5H_2O$.

The crystal structure was solved by the direct methods and refined by means of Bruker Smart APEX II diffractometer (150 K, using MoK_α radiation; wavelength 0.71073 Å) for 15099 unique reflections. Space group $R\bar{3}$, a = 30.8057(9); b = 30.8057(9); c = 39.117(2) Å; V = 32148(3) Å^3, M = 3624.95 g/mol, Z = 6, d_{calc} = 1.123 g·cm^{-3}, μ = 0.984 mm^{-1}, F(000) = 11076; R_1 = 0.0671 и R_w = 0.1330, *GOOF* = 0.923.

The molecule of complex $Gd_3(L^1)(HL^2)_3$ (H_3L^1 - 1,3,5-benzenetricarboxylic acid trihydrazone; H_3L^2 - 5-carboxy-1,3-benzenedicarboxylic acid dihydrazone) is based on Gd triangle with distances Gd…Gd 9.838 Å. The acyltrihydrazone is coordinated as a tritopic ligand and placed ander basal plane; three acyldihydrazones occupe the faces and are bitopic. The pyrazole moieties of the ligands of both types are coordinated in deprotonated enol form; the hydrazone moieties are coordinated in molecular form. Each of the acyldihydrazone molecules has one protonated non-coordinated carboxyl group. Molecules of solvents – N,N-dimethylformamide and water, are non-coordinated and fill the cavities of the crystal lattice. The geometry of gadolinium coordination polyhedron can be considered as tricapped trigonal prism, which consists of combination of DyN_3 triangle and DyO_6 trigonal prism.

Keywords: hydrazone, 1,3,5-benzentricarboxylic acid, 4-formyl-3-methyl-1-phenylpyrazol-5-one, X-Ray study.

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