Supporting Information to :

Shestakova et al :

"A First Comparison of Solid State and Solution Structure of a Complex between Lanthanum Nitrate and 1,9-Diaza-18crown6 "

Synthesis of the complex 1 : from commercially available 1,10-diazacrownether and anhydrous lanthanum nitrate in acetonitrile according to a literature procedure [O.A.Gansow, A.R.Kausar, *Inorg.Chim.Acta*, **95**, 1 (1985).]. Crystals suitable for the X-ray studies was obtained by slow evaporation of the acetonitrile solution in an NMR sample tube.

Experimental details for the X-ray analysis: Crystal data for **1** CH_3CN: $C_{14}H_{29}La_1N_6O_{13}$, M=628.34, triclinic, space group $P\bar{1}$, a=8.111(3)Å, b=10.857(4)Å, c=13.849(3)Å, α= 80.55(2)°, β=78.16(2)°, γ=80.90(3)°, V=1167.6(6)Å^3, ρ_{calc}=1.787g/cm^3, μ=19.05 cm^{-1}, for Z=2. Intensities of 7881 reflections (R_{int}= 0.0451) were measured at 153K with a Syntex $P2_1$ automated diffractometer using Mo Kα radiation (λ=0.71073Å, $\theta/2\theta$ scan, $\theta \leq 30°$). The structure was solved by direct method and refined by full-matrix least squares against F^2 in the anisotropic (H-atoms isotropic) approximation. All hydrogen atoms were located from the electron density difference synthesis and were included in the refinement in isotropic approximation. The refinement for **1** converged to wR_2=0.1472 and GOF=1.069 for 7413independent reflections (R_1=0.0561 was calculated against **F** for the 7392 observed reflections with $I>2\sigma(\mathbf{I})$). The number of the refined parameters was 413. All calculations were performed using SHELXTL PLUS 5.1 on a IBM PC/AT.