A structural and theoretical investigation of equatorial *cis* and *trans* uranyl-phosphinimine and -phosphine oxide complexes, $UO_2Cl_2(Cy_3PNH)_2$ and $UO_2Cl_2(Cy_3PO)_2$

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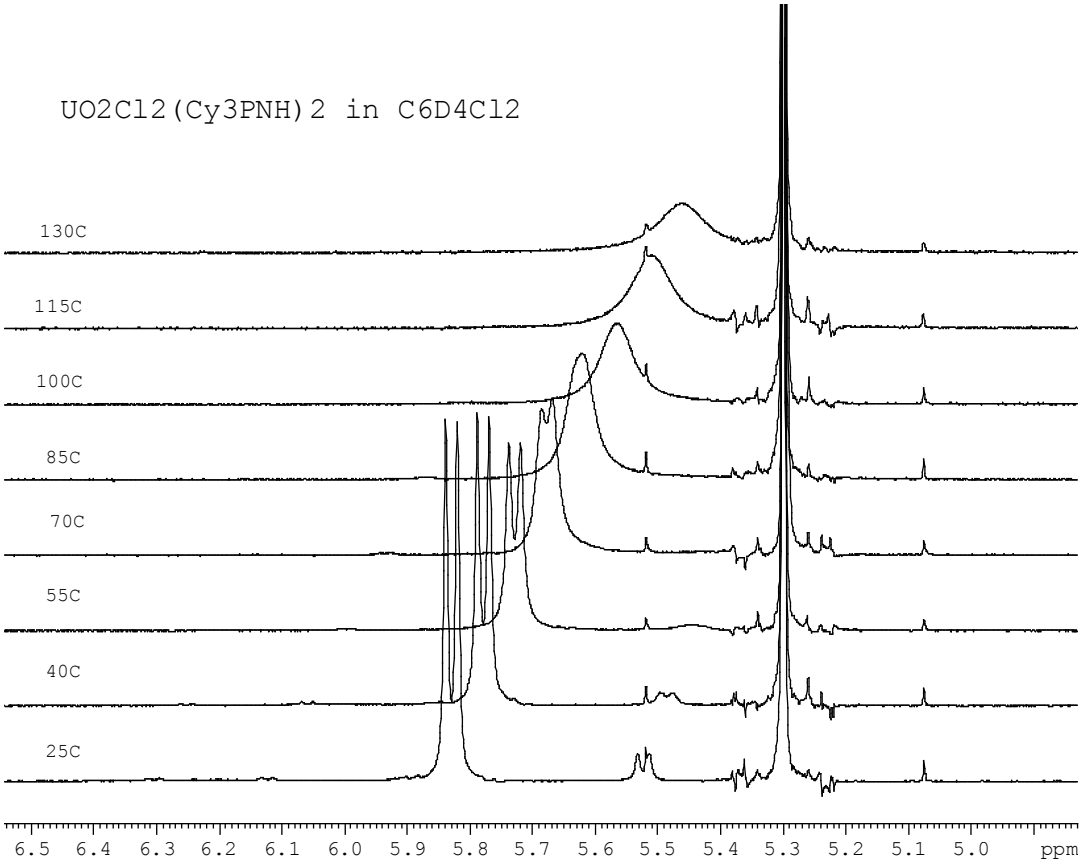
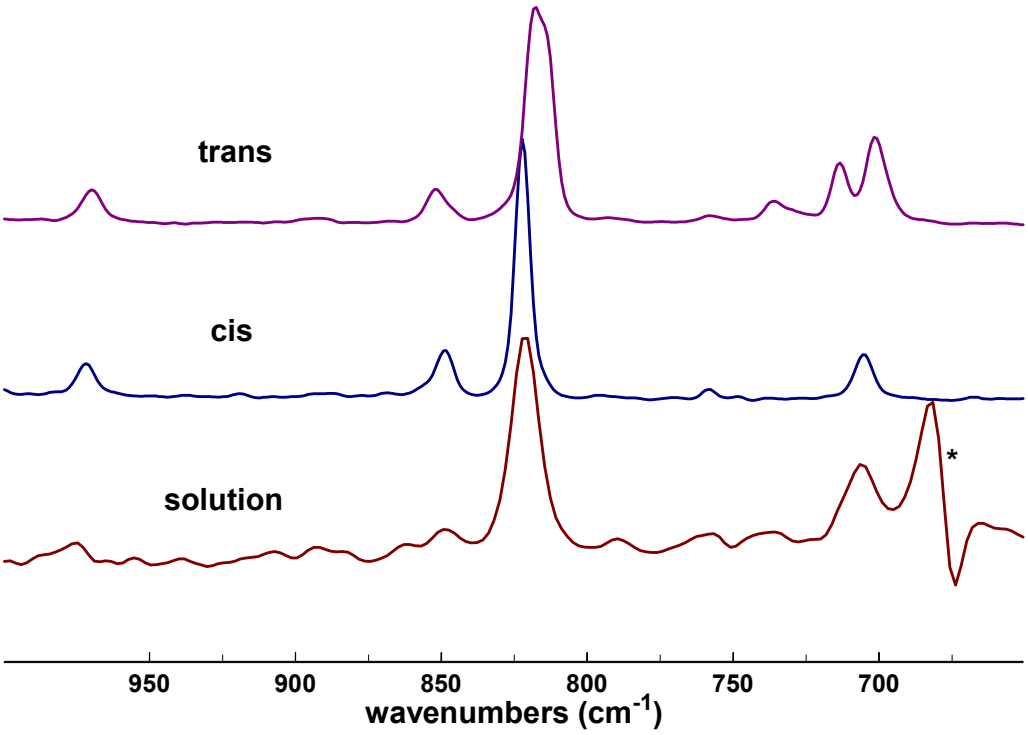
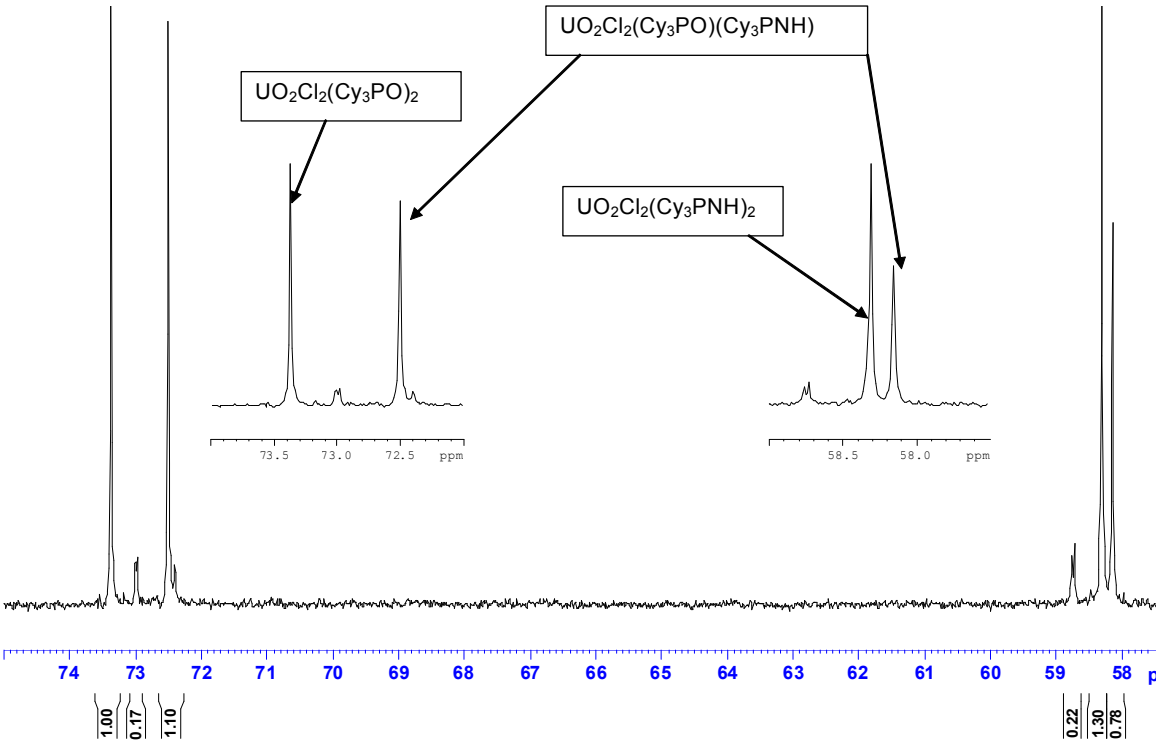
Supporting Information including ^{1}H, ^{31}P and Raman spectra.



^{1}H Variable Temperature NMR spectra(P=N*H* region) of $UO_2Cl_2(Cy_3PNH)_2$ (**1**) in $C_6D_4Cl_2$.



Solid state Raman spectra of crystals of *trans* and *cis* $UO_2Cl_2(Cy_3PNH)_2$ (**1**) (top and middle) and the solution spectrum of $UO_2Cl_2(Cy_3PNH)_2$ in CD_2Cl_2 (solvent subtracted and * indicates artifact of subtracted CD_2Cl_2 peaks).



$^{31}P\{^{1}H\}$ NMR spectrum of $UO_2Cl_2(Cy_3PNH)_2$ + $UO_2Cl_2(Cy_3PO)_2$ (1:1) in CD_2Cl_2. The spectrum shows there is a distribution of ligands and formation of the mixed ligand species $UO_2Cl_2(Cy_3PO)(Cy_3PNH)$.