

Electronic supplementary information

DOI:

Title: Synthesis and crystal structure of nitrosoruthenium complexes *cis*-[Ru(NO)Py₂Cl₂(OH)] and *cis*-[Ru(NO)Py₂Cl₂(H₂O)]Cl. Photoinduced transformations of *cis*-[Ru(NO)Py₂Cl₂(OH)]

Author(s): Alexander N. Makhinya,* Maxim A. Il'in, Ruslan D. Yamaletdinov, Il'ya V. Korolkov, Iraida A. Baidina

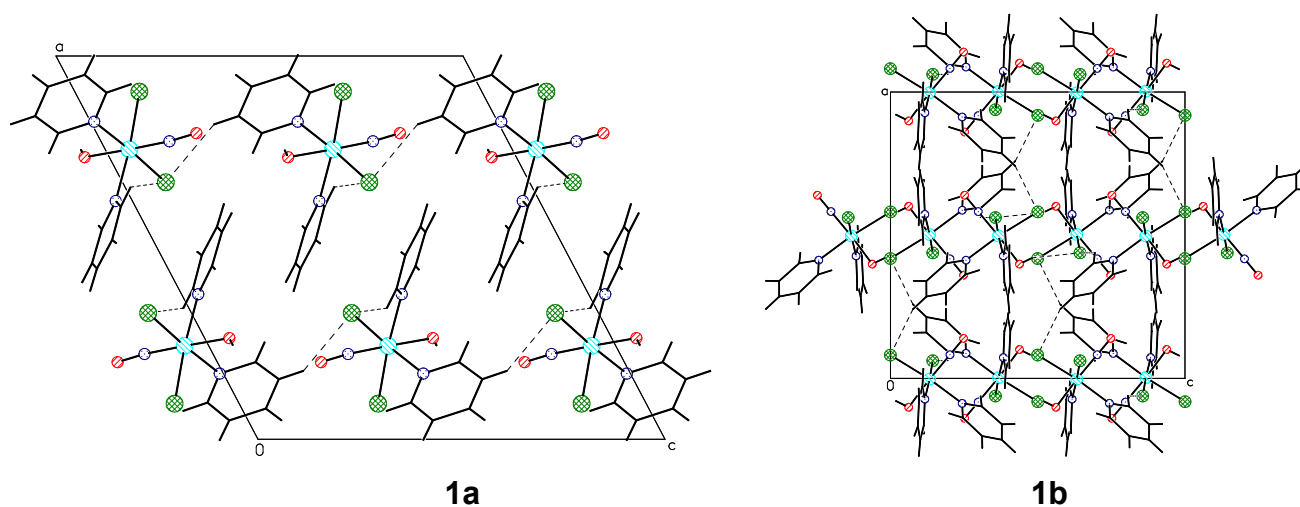


Figure S1. Packing of structural units in the crystals of **1a** and **1b** as viewed along the axis *y*.

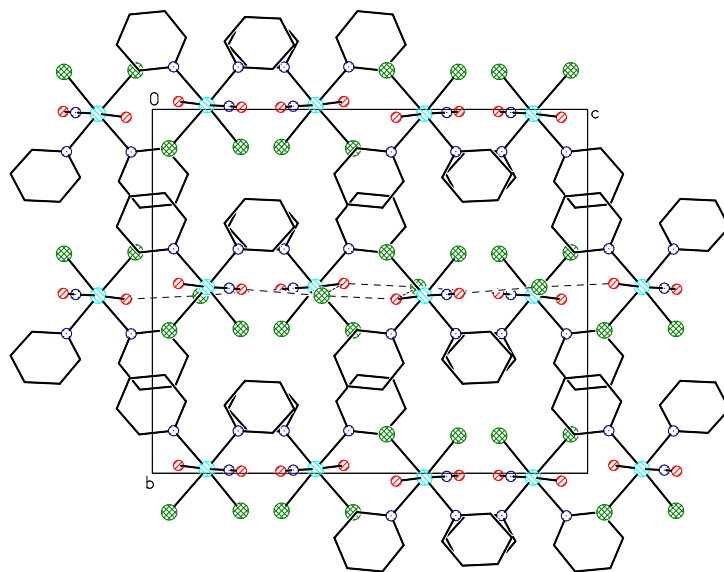


Figure S2. Packing of structural units in the crystal of **2** as viewed along the axis *x*.

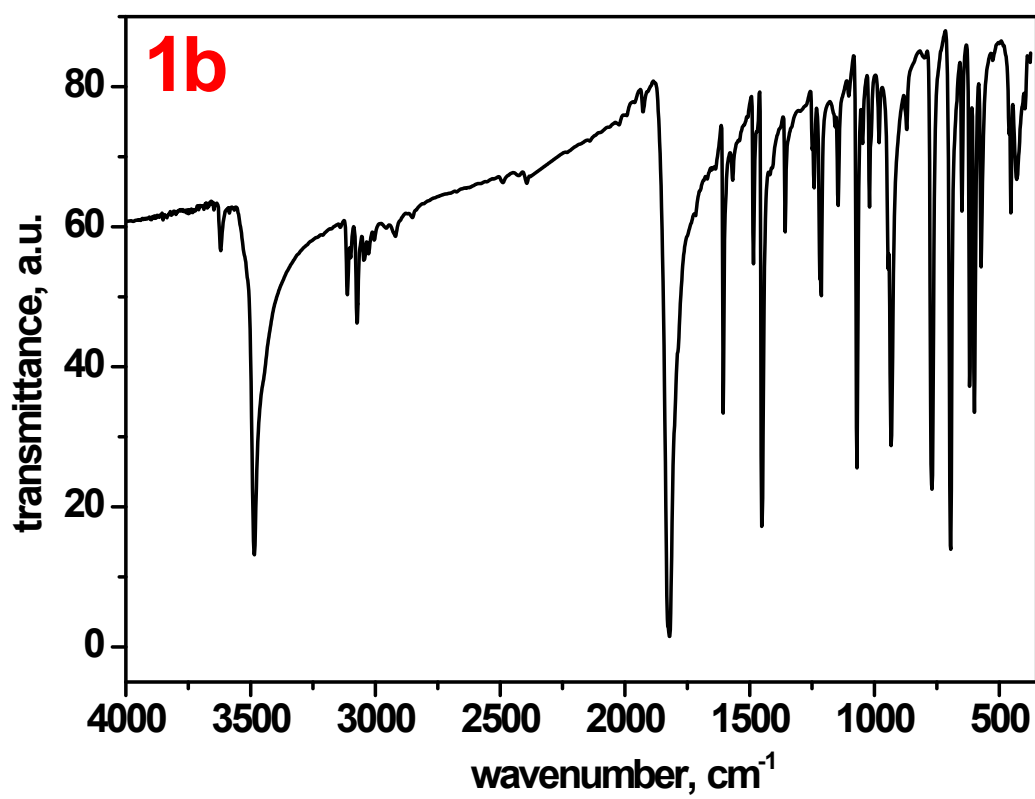
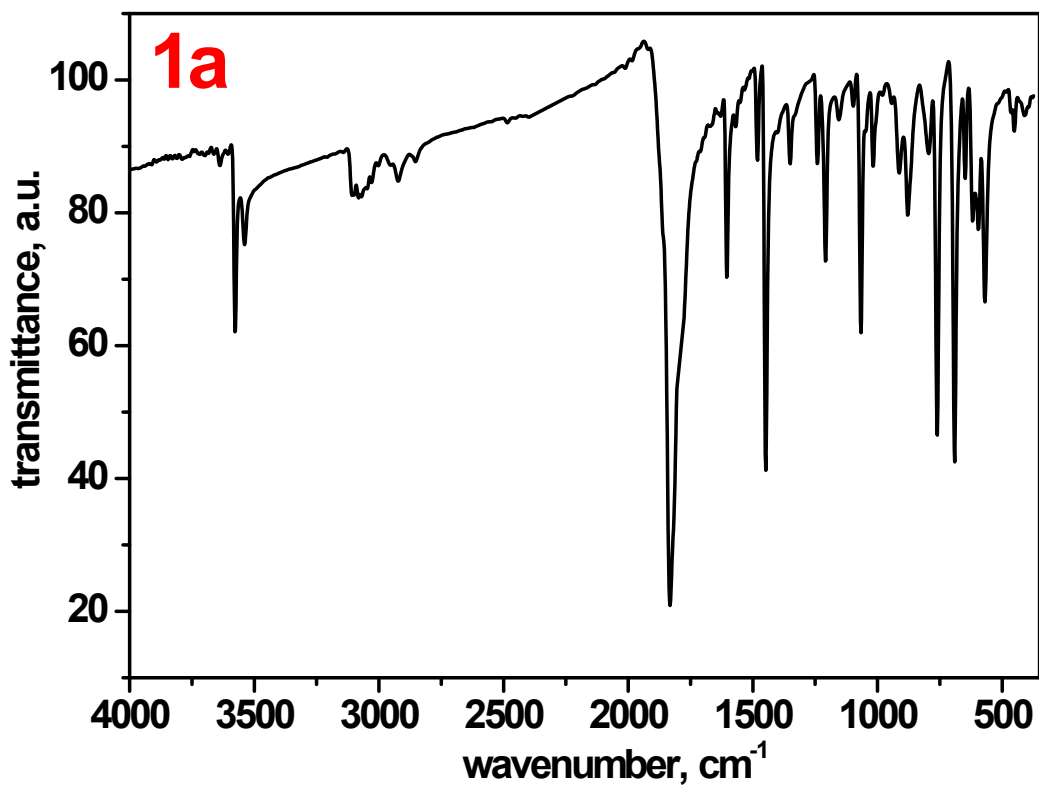


Figure S3. Infrared spectra of 1a and 1b.

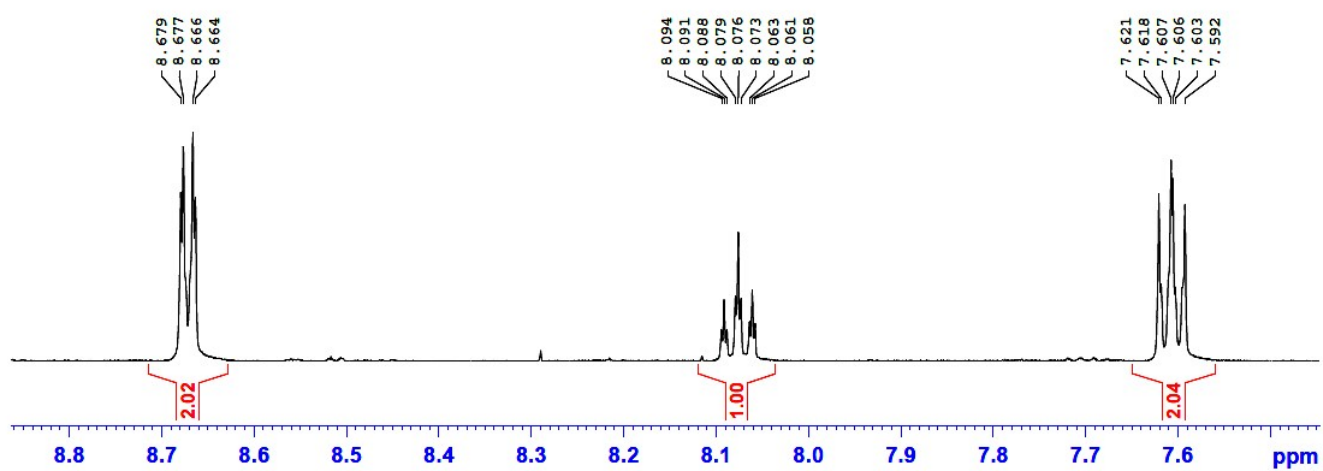


Figure S4. NMR ^1H spectrum of *cis*-[Ru(NO)Py₂Cl₂(OH)] (1a or 1b) in DMSO.

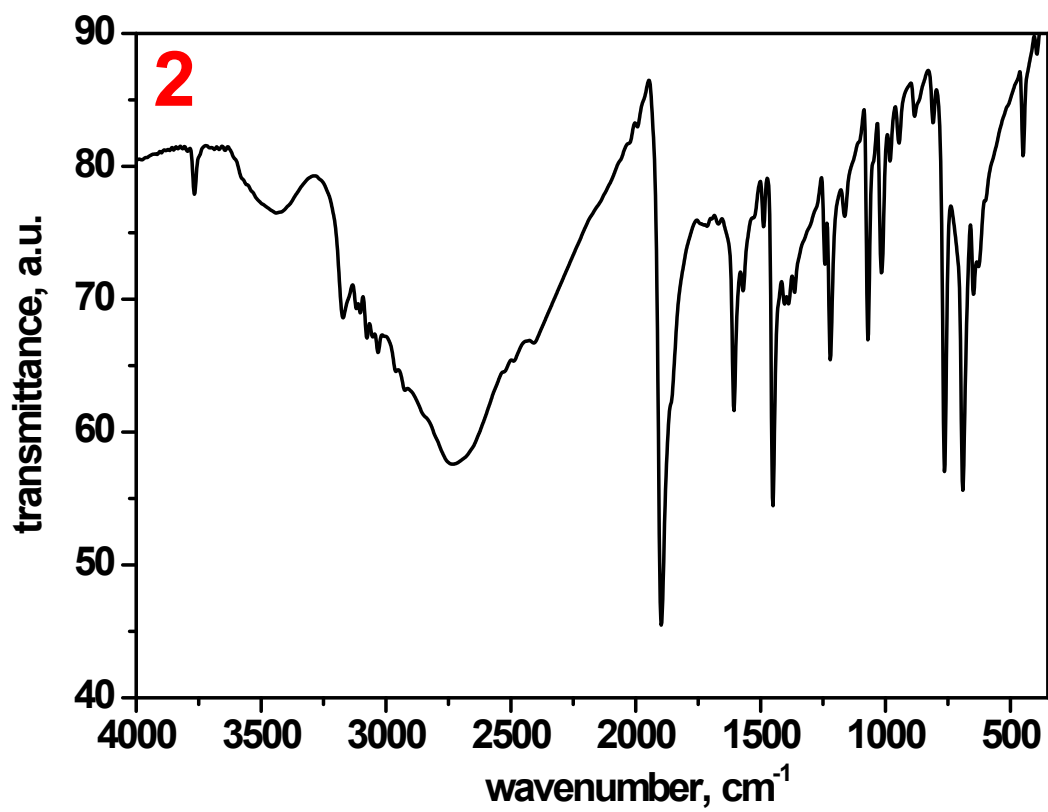


Figure S5. Infrared spectrum of *cis*-[Ru(NO)Py₂Cl₂(H₂O)]Cl (**2**).

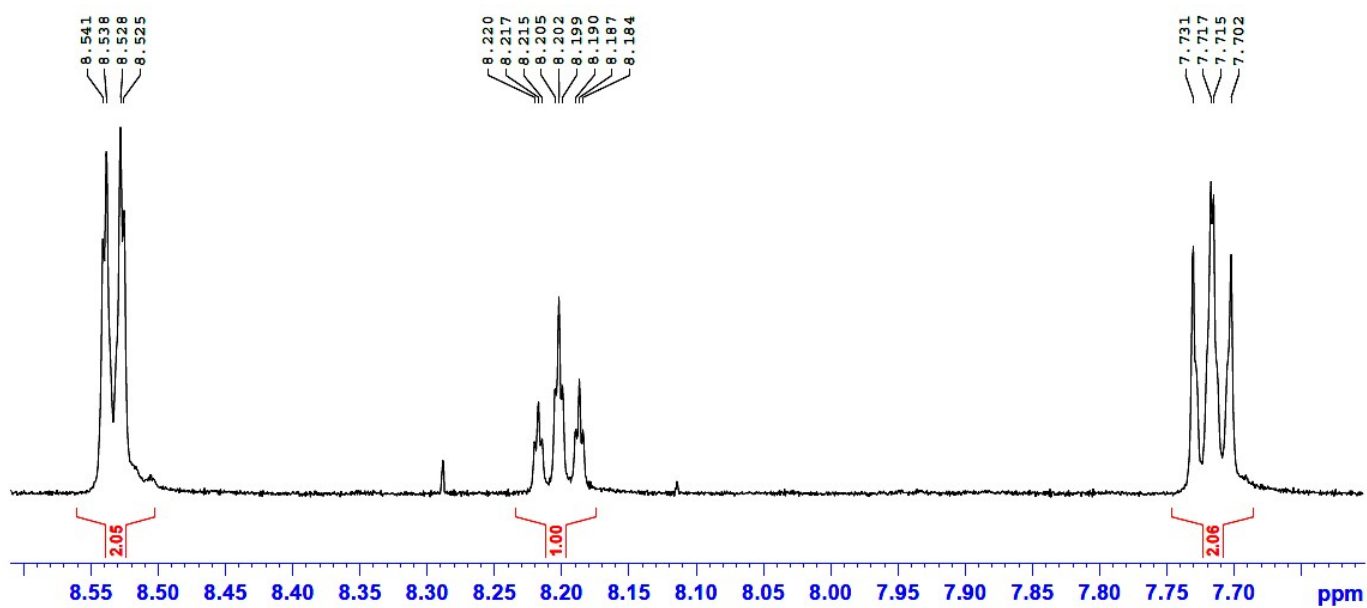
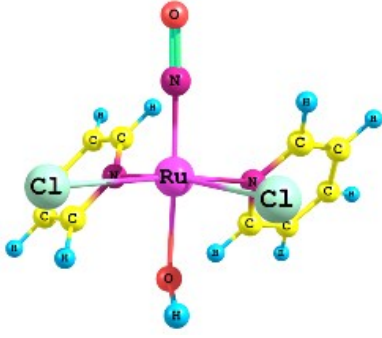
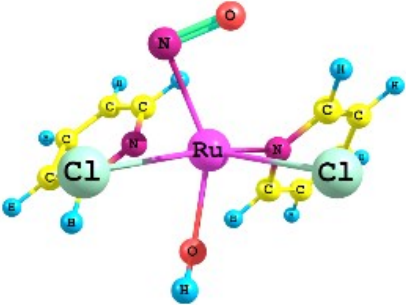
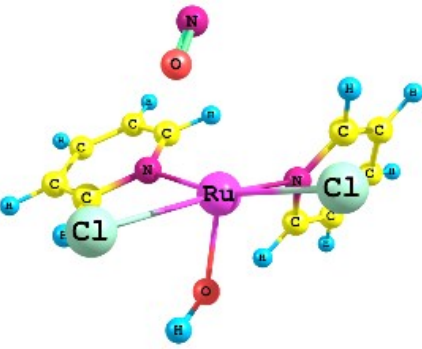



Figure S6. NMR ^1H spectrum of *cis*-[Ru(NO)Py₂Cl₂(H₂O)]Cl (**2**) in DMSO.

Table S1. Optimized geometries of different states for *cis*-[Ru(NO)Py₂Cl₂(OH)].

Geometry	State	N–O [Å]	Ru–NO (Ru–ON for MS1, TS1) [Å]	E _{rel.} GS [eV]
	GS	1.159	1.774	0
	MS2	1.188	1.978	1.24
	TS1	1.160	2.268	2.45
	MS1	1.152	1.883	1.76