Supplementary Information

Bismuth and antimony halometalates containing photoswitchable ruthenium nitrosyl complex

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Table S1. Experimental and refinement details.

Complex	$[RuNOPy_4Br]_4[Sb_2Br_8][Sb_3Br_{12}]_2$ (**1**)	$(H_3O)[RuNOPy_4Br]_4[Bi_2Br_9]_3{\cdot}3H_2O$ (**2**)
Empirical formula	$C_{20}H_{20}Br_9N_5ORuSb_2$	$C_{80}H_{89}Bi_6Br_{31}N_{20}O_8Ru_4$
Formula weight	1410.17	5593.07
Temperature/K	100	150
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
a/Å	12.0218(11)	15.1913(13)
b/Å	22.4544(19)	17.2926(12)
c/Å	26.372(2)	27.970(3)
α/°	90	96.349(3)
β/°	92.506(3)	103.183(3)
γ/°	90	105.167(3)
Volume/Å^3	7112.2(11)	6790.4(10)
Z	8	2
ρ_{calc}g/cm^3	2.634	2.735
μ/mm^{-1}	12.064	17.348
F(000)	5152	5062
Crystal size/mm^3	0.217 × 0.205 × 0.106	0.055 × 0.055 × 0.055
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.846 to 66.504	2.876 to 51.362
Index ranges	-18 ≤ h ≤ 18, -34 ≤ k ≤ 34, -32 ≤ l ≤ 40	-18 ≤ h ≤ 18, -21 ≤ k ≤ 21, -34 ≤ l ≤ 31
Reflections collected	256633	73912
Independent reflections	27174 [R_{int} = 0.0953, R_{sigma} = 0.0588]	25709 [R_{int} = 0.0590, R_{sigma} = 0.0793]
Data/restraints/parameters	27174/2/685	25709/12/1374
Goodness-of-fit on F^2	1.053	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0393, wR_2 = 0.0780	R_1 = 0.0525, wR_2 = 0.1066
Final R indexes [all data]	R_1 = 0.0747, wR_2 = 0.0885	R_1 = 0.0754, wR_2 = 0.1150
Largest diff. peak/hole / e Å^{-3}	1.36/-1.82	3.25/-1.93

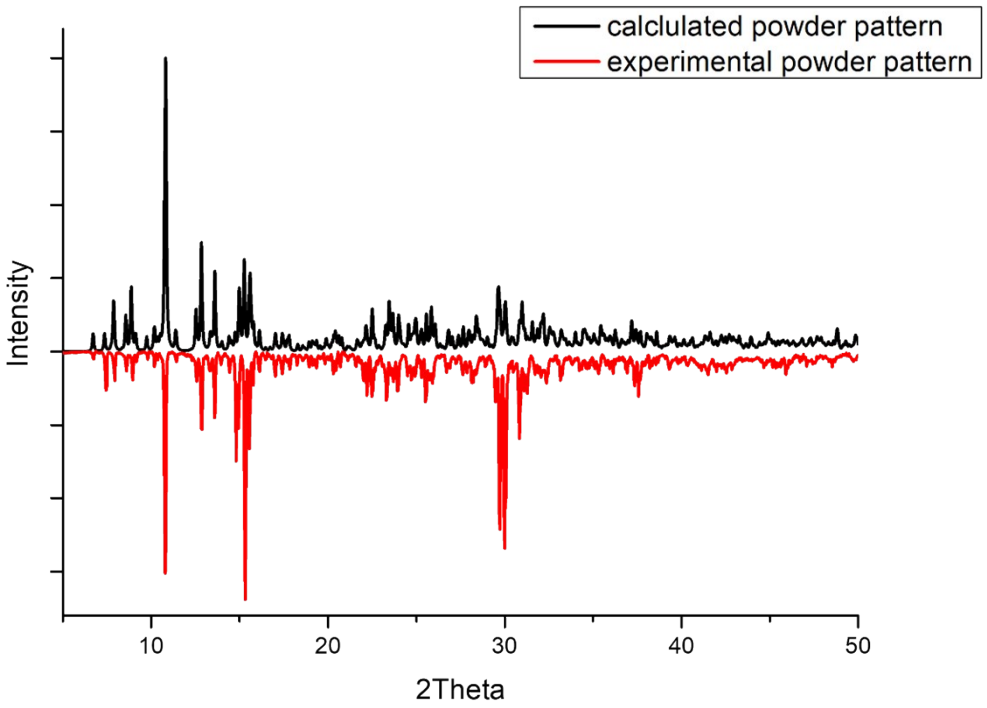

Fig. S1. PXRD data of **1**.

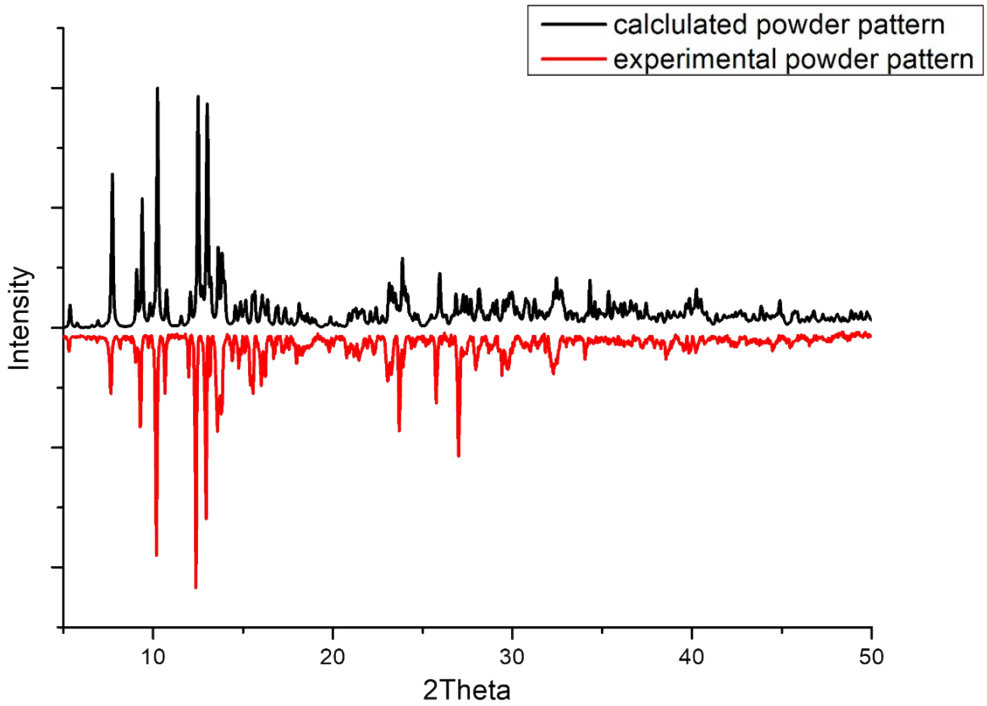

Fig. S2. PXRD data of **2**.

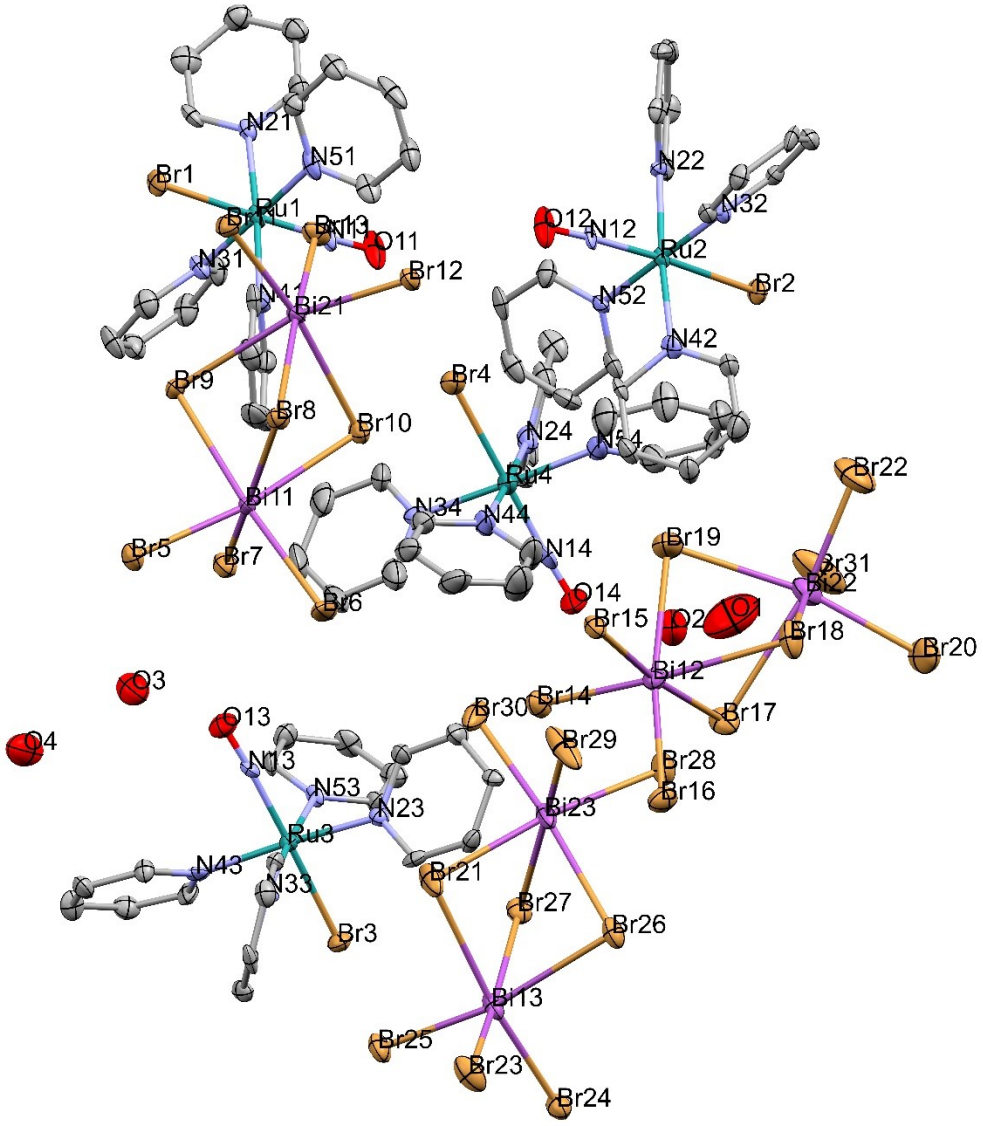

Fig. S3. The asymmetric unit of the structure of $(H_3O)[RuNOPy_4Br]_4[Bi_2Br_9]_3 \cdot 3H_2O$ (**2**). Hydrogen atoms are omitted for clarity.

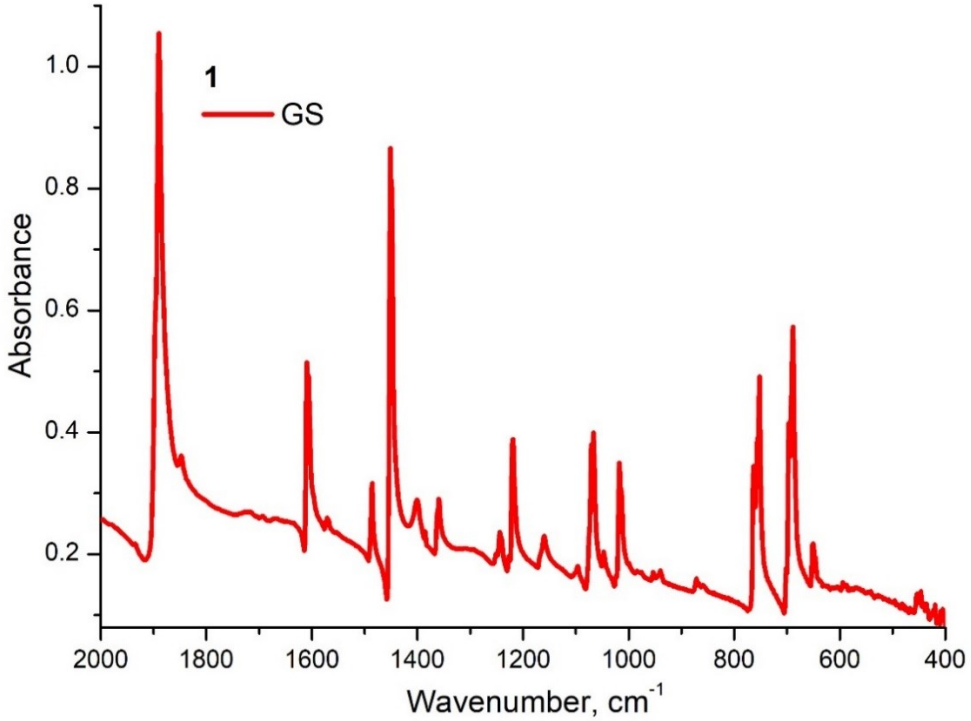

Fig. S4. IR-spectrum of **1** at 100 K.

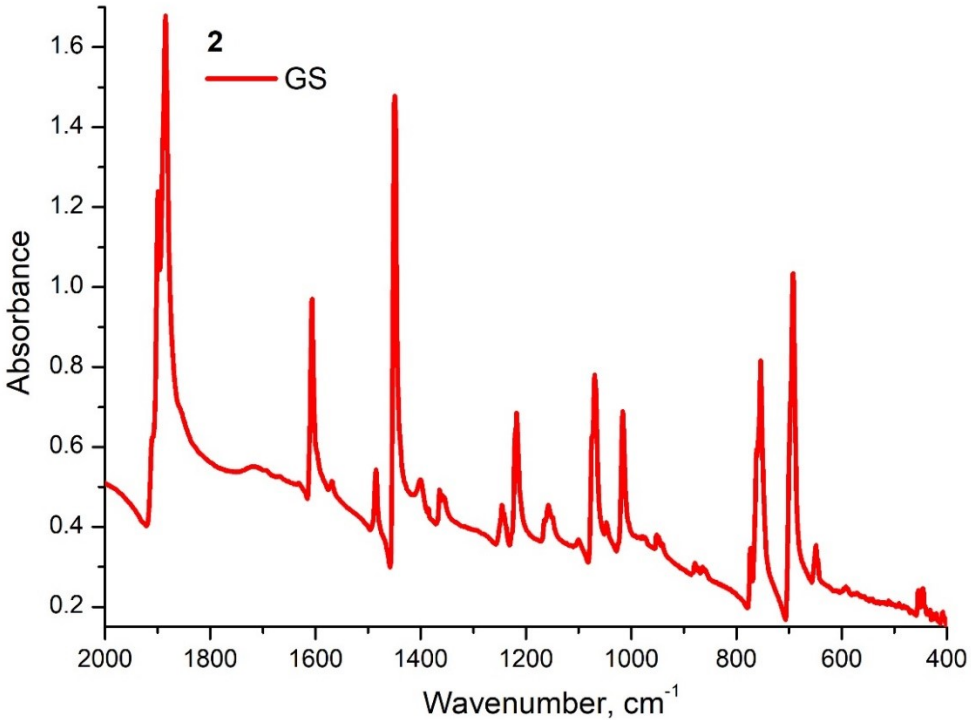

Fig. S5. IR-spectrum of **2** at 100 K.

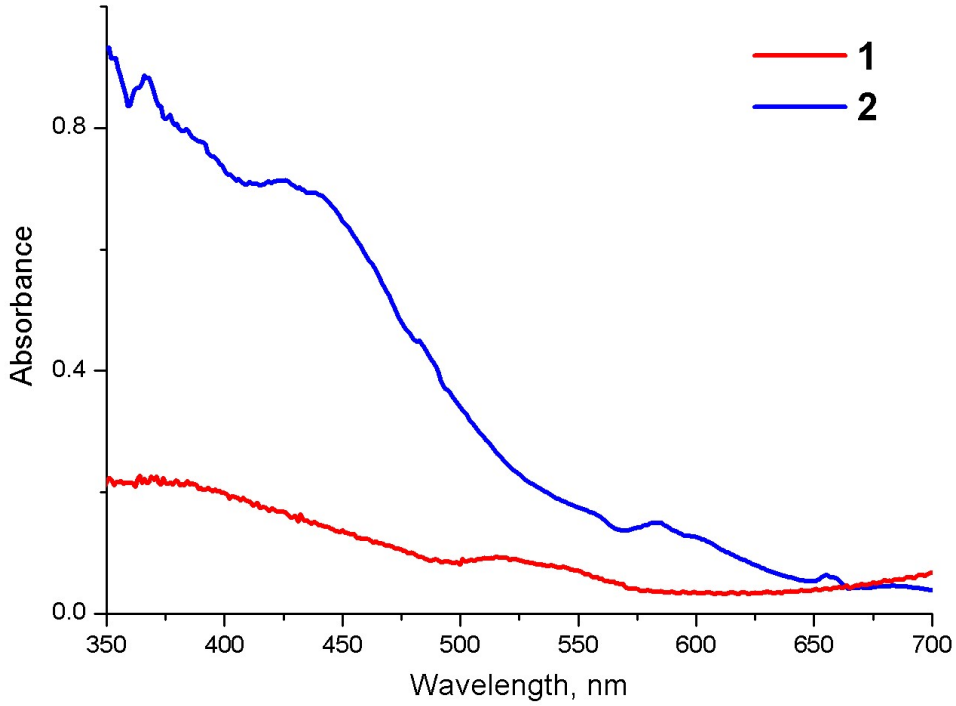

Fig. S6. UV-vis spectra of **1** and **2** in GS embedded into KBr matrix.