

Supporting Information for
Uranyl Stabilized Schiff base Complex

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Experimental Section

General Procedure: $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, 1,3-diamino, 2-propanol, Salicylaldehyde, triethylamine and ethylenediamine were purchased from Acros and used as received. The ligand, SalproH₃ was synthesized according to the literature method.¹ The ¹H/¹³C NMR were recorded on a Bruker AV 400 spectrometer operated at 400 MHz with d₆-DMSO as solvents with tetramethylsilane as the reference. The IR data were recorded as KBr pellets on SHIMSDZU Inc. IR, Prestige-21 Fourier Transform Infrared Spectrophotometer in the range 400 – 4000 cm⁻¹. Electrospray ionization mass spectrometry was performed on a Micromass QTOF mass spectrometer.

X-ray Crystallography: Crystals of compounds **1(S)₂** and **2(S)** were obtained in good yield from DMF and pyridine by slow evaporation at room temperature. Crystals of Salen (N, N-ethylenebis(salicylideneimine)) were obtained by slow evaporation of d₄-MeOH solution. X-ray diffraction data were collected at -80 °C on a Bruker SMART APEX CCD X-ray diffractometer unit using Mo K α radiation from crystals mounted in Paratone-N oil on glass fibers. SMART (v 5.624) was used for preliminary determination of cell constants and data collection control. Determination of integrated intensities and global cell refinement were performed with the Bruker SAINT Software package using a narrow-frame integration algorithm. The program suite SHELXTL (v 5.1) was used for space group determination, structure solution, and refinement.² Refinement was performed against F^2 by weighted full-matrix least square, and empirical absorption correction (SADABS³) was applied. H atoms were placed at calculated positions using suitable riding models with isotropic displacement parameters derived from their carrier atoms. Crystal data, selected bond distances and angles, are provided in Tables S1 – S3.

Synthesis of [(UO₂)₂(Salpro)(OH)(MeOH)₂] (1'(MeOH)₂): Uranyl nitrate (2 mmol, 1.0 g) was added to a stirring solution of MeOH/CHCl₃ (50 mL) (1:1) containing SalproH₃ (2 mmol, 0.6 g) and triethylamine (2 mmol, 0.2 g) and heated to reflux temperature for 6 - 7 hours. The resulting orange precipitate was filtered, washed with cold MeOH/CHCl₃ (1:1) mixture and dried under vacuum (0.9 g, 98 %). X-ray quality orange crystals were obtained from supersaturated DMF or DMSO solutions. δ_{H} (400 MHz, d₆-DMSO, ppm): 2.7 and 2.9 (s, 2DMSO, 12H), 4.7, 4.9 and 5.8 (m, CH₂-CH-CH₂, 5H), 6.7 – 7.9 (m, 2C₆H₄, 8H), 9.4 (s, CHN, 2H), 11.7 (s, OH, 1H). δ_{C} (400 MHz, d₆-DMSO, ppm): 31 and 36 (CH₂N), 71 (CHO), 115-163 (phenyl), 167 and 170 (CHN). IR (KBr, ν_{max} /cm⁻¹): 2919,

1629, 1541, 1469, 1447, 1383, 1309, 1202, 1151, 1030, 895, 801. m/z (EI): 980 ($M^+ + 2\text{MeOH}$) (10 %).

Synthesis of $[\text{UO}_2(\text{Salen})(\text{S})] \cdot (2 \cdot (\text{S}))$ ($\text{S} = \text{MeOH}, \text{Py}$)⁴: Uranyl nitrate (1 mmol, 0.5 g) was added to a stirring solution of MeOH/ CHCl_3 (50 mL) (1:1) containing SalproH₃ (1 mmol, 0.3 g) and ethylenediamine (2 mmol, 0.12g) and heated to reflux temperature for 2 - 3 hours. The resulting orange precipitate was filtered, washed with cold MeOH/ CHCl_3 (1:1) mixture and dried under vacuum (0.37 g, 66 %). X-ray quality crystals were obtained from slow evaporation of pyridine at room temperature. δ_{H} (400 MHz, d_6 -DMSO, ppm): 2.7 (s, DMSO, 3H), 4.5 (t, CH_2 , 2H), 6.7, 6.9 and 7.6 (m, C_6H_4 , 4H), 9.5 (s, CHN, 1H). δ_{C} (400 MHz, d_6 -DMSO, ppm): 42.8 (DMSO), 64 (CH_2), 116 – 135 (phenyl) and 169 (CHN). IR (KBr, $\nu_{\text{max}}/\text{cm}^{-1}$): 2956, 1626, 1436, 1385, 1256, 1014, 896, 799. m/z (EI): 1072 ($2M^+ - 2\text{MeOH}$) (2%); 536 ($M^+ - \text{MeOH}$) (65 %).

Reaction of $1 \cdot (\text{S})_2$ with excess of EDA: Ethylenediamine (3 mmol, 0.18 g) was added to the methanolic suspension of $1 \cdot (\text{MeOH})_2$ (1 mmol, 0.1 g) and the resulting reaction mixture was refluxed for 6 – 7 hours. The solvent was completely removed and the precipitate was washed with cold MeOH/ CHCl_3 (1:1) mixture and dried under vacuum. The precipitate was dissolved in either DMF or DMSO, which yielded orange crystals of $1 \cdot (\text{DMF/DMSO})_2$.

Reaction of SalproH₃ with EDA: EDA (0.1 mmol) was added to a suspension of SalproH₃ (0.1 mmol) in MeOH (5 mL) and shaken until the latter dissolved completely. The solution was slowly evaporated which yielded orange crystals of Salen.

Table S1. Crystal Data for Compounds **1** and **2**.

Compounds	1	2
Empirical formula	$\text{C}_{11.5}\text{H}_{15}\text{N}_2\text{O}_5\text{U}$	$\text{C}_{21}\text{H}_{19}\text{N}_3\text{O}_4\text{U}$
Fw	499.29	615.42
Wavelength (Å)	0.71073	0.71073
Crys syst	Monoclinic	Orthorhombic
Space group	P1 21/n 1	P c a 21
a (Å)	11.797(3)	18.427(2)
b (Å)	9.784(2)	9.0712(1)
c (Å)	24.594(5)	11.8143(1)
α (deg)	90.00	90.00
β (deg)	94.811(4)	90.00
γ (deg)	90.00	90.00
V (Å ³)	2828.7(2)	1974.8(4)
Z	8	4
density calcd (mg/m ³)	2.345	2.070
abs coeff (mm ⁻¹)	11.495	8.252
F(000)	1840	1160
Cryst size (mm ³)	0.1x0.1x0.05	0.1x0.1x0.1

Reflns collected	18601	10662
Indep reflns	4058 ($R_{\text{int}} = 0.0687$)	2838 ($R_{\text{int}} = 0.0569$)
Refinements method	Full-matrix least squares on F^2	Full-matrix least squares on F^2
GOF of F^2	0.858	0.968
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0272$	$R_1 = 0.0254$
R indices (all data)	$wR_2 = 0.0539$ $R_1 = 0.0364$ $wR_2 = 0.0557$	$wR_2 = 0.0574$ $R_1 = 0.0286$ $wR_2 = 0.0588$
Largest diff peak and hole ($e/\text{\AA}^3$)	1.177 and -0.691	1.146 and -0.606

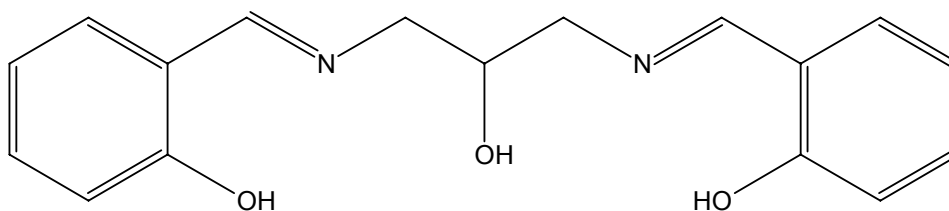
Table S2. Selected bond distances (\AA) and angles ($^\circ$) for compound **1**(DMF)₂.

U1-O2	1.783(4)	U1-O1	1.792(4)
U1-O6	2.241(5)	U1-O8	2.327(4)
U1-O7	2.380(5)	U1-N1	2.544(5)
U2-O3	1.778(4)	U2-O4	1.794(4)
U2-O5	2.235(5)	U2-O8	2.343(4)
U2-O7	2.364(4)	U2-N2	2.579(5)
U2-O1D1	2.400(5)	U1-O1D2	2.461(4)
U1-U2	3.869(8)		
O2-U1-O1	178.7(2)	O2-U1-O6	88.0(2)
O1-U1-O6	90.76(2)	O2-U1-O8	91.90(2)
O1-U1-O8	89.29(2)	O6-U1-O8	154.81(2)
O2-U1-O7	88.5(2)	O1-U1-O7	92.34(2)
O6-U1-O7	136.31(2)	O8-U1-O7	68.84(2)
O3-U2-O4	179.5(2)	O3-U2-O5	92.0(2)
O4-U2-O5	87.80(2)	O3-U2-O8	89.20(2)
O4-U2-O8	90.83(2)	O5-U2-O8	155.83(2)
O3-U2-O7	91.60(2)	O4-U2-O7	88.85(2)
O5-U2-O7	135.22(2)	O8-U2-O7	68.83(2)

Table S3. Selected bond distances (\AA) and angles ($^\circ$) for compound **2**(Py).

U1-O1	1.783(4)	U1-O2	1.777(4)
U1-O3	2.242(4)	U1-O4	2.230(3)
C1-O3	1.314(6)	C12-O4	1.323(6)
O2-U1-O1	177.3(2)	O2-U1-O4	89.86(2)
O1-U1-O4	91.40(2)	O2-U1-O3	88.97(2)
O1-U1-O3	91.02(2)	O4-U1-O3	152.42(2)

O2-U1-N2	88.49(2)	O1-U1-N2	89.66(2)
O4-U1-N2	71.01(2)	O3-U1-N2	136.48(2)
O2-U1-N1	92.46(2)	O1-U1-N1	84.98(2)
O4-U1-N1	136.72(2)	O3-U1-N1	70.86(2)
N2-U1-N1	65.87(2)	O2-U1-N3	95.62(2)
O1-U1-N3	87.01(2)	O4-U1-N3	75.93(2)
O3-U1-N3	76.77(2)	N2-U1-N3	146.67(2)
N1-U1-N3	146.44(2)		



SalproH₃

Fig S1. Chemical structure of SalproH₃.

Reference:

1. Nishida, Y.; Kida, S., *Dalton Trans.* **1986**, 2633.
2. Sheldrick, G. M., *SHELXTL PC, version 6.12, An Integrated System for Solving, Refining, and Displaying Crystal Structures from Diffraction Data; Siemens Analytical X-ray Instruments, Inc. Madison, WI, 2001.*
3. Sheldrick, G. M., *SADABS-An empirical absorption correction program; Bruker Analytical X-ray Systems Madison, WI, 1996.*
4. This compound has been reported and characterized earlier with EtOH/DMF/DMSO as coordinating solvents.