The crystalline α,ω-dicarboxylate metal complex with the longest aliphatic chain to date: uranyl 1,15-pentadecanedioate

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Supporting Information

Experimental

Synthesis. Caution! *Uranium is a radioactive and chemically toxic element, and uranium-containing samples must be handled with suitable care and protection.*

General. $UO_2(NO_3)_2{\cdot}6H_2O$ (depleted uranium, R. P. Normapur, 99%) was purchased from Prolabo, and 1,15-pentadecanedioic acid was from Alfa Aesar.

Luminescence Measurements. The emission spectrum was recorded on a solid sample using a Horiba-Jobin-Yvon Fluorolog spectrofluorometer. The powdered complex was pressed between two silica plates which were mounted such that the faces were oriented vertically and at 45° to the incident excitation radiation. An excitation wavelength of 420 nm was used and the emission was monitored between 450 and 650 nm.

Infrared spectrum. The spectrum was recorded on a powdered crystalline sample using a Nicolet 6700 FTIR instrument with a Smart Orbit diamond-anvil attachment.

Crystallography

Table S1 Selected bond lengths (Å) and angles (°) in complex **1**.

U(1)-O(1)	1.758(4)
U(1)-O(2)	1.757(4)
U(1)-O(3)	2.439(4)
U(1)-O(6)#1	2.463(4)
U(1)-O(7)	2.465(4)
U(1)-O(5)#1	2.468(4)
U(1)-O(8)	2.474(4)
U(1)-O(4)	2.487(4)
O(1)-U(1)-O(2)	178.93(19)
O(1)-U(1)-O(3)	91.11(19)
O(2)-U(1)-O(3)	89.52(18)
O(1)-U(1)-O(6)#1	94.4(2)
O(2)-U(1)-O(6)#1	84.95(19)
O(3)-U(1)-O(6)#1	173.05(15)
O(1)-U(1)-O(7)	90.2(2)
O(2)-U(1)-O(7)	90.30(19)
O(3)-U(1)-O(7)	118.08(14)
O(6)#1-U(1)-O(7)	66.26(15)
O(1)-U(1)-O(5)#1	86.92(19)
O(2)-U(1)-O(5)#1	92.02(17)
O(3)-U(1)-O(5)#1	123.30(14)
O(6)#1-U(1)-O(5)#1	52.90(14)
O(7)-U(1)-O(5)#1	118.58(15)
O(1)-U(1)-O(8)	88.74(19)
O(2)-U(1)-O(8)	92.31(18)
O(3)-U(1)-O(8)	65.85(14)
O(6)#1-U(1)-O(8)	118.50(14)
O(7)-U(1)-O(8)	52.29(14)
O(5)#1-U(1)-O(8)	169.92(14)
O(1)-U(1)-O(4)	89.28(19)
O(2)-U(1)-O(4)	90.40(17)
O(3)-U(1)-O(4)	52.98(13)
O(6)#1-U(1)-O(4)	122.71(13)
O(7)-U(1)-O(4)	171.02(14)

O(5)#1-U(1)-O(4)	70.33(13)
O(8)-U(1)-O(4)	118.73(13)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,y-1/2,z-1

Torsion angles

O(3)-C(1)-C(2)-C(3)	-177.6(5)
O(4)-C(1)-C(2)-C(3)	4.2(9)
C(1)-C(2)-C(3)-C(4)	-173.0(5)
C(2)-C(3)-C(4)-C(5)	-176.8(5)
C(3)-C(4)-C(5)-C(6)	-178.5(5)
C(4)-C(5)-C(6)-C(7)	-177.0(5)
C(5)-C(6)-C(7)-C(8)	-176.8(5)
C(6)-C(7)-C(8)-C(9)	-179.8(5)
C(7)-C(8)-C(9)-C(10)	-178.0(5)
C(8)-C(9)-C(10)-C(11)	-177.2(5)
C(9)-C(10)-C(11)-C(12)	-172.3(6)
C(10)-C(11)-C(12)-C(13)	-56.8(8)
C(11)-C(12)-C(13)-C(14)	-175.3(6)
C(12)-C(13)-C(14)-C(15)	-169.6(6)
C(13)-C(14)-C(15)-O(5)	-161.0(6)
C(13)-C(14)-C(15)-O(6)	19.4(9)
O(8)-C(16)-C(17)-C(18)	167.0(7)
O(7)-C(16)-C(17)-C(18)	-14.1(11)
C(16)-C(17)-C(18)-C(19)	-178.8(6)
C(17)-C(18)-C(19)-C(20)	179.8(6)
C(18)-C(19)-C(20)-C(21)	-178.4(5)
C(19)-C(20)-C(21)-C(22)	177.2(5)
C(20)-C(21)-C(22)-C(23)	-178.8(4)
C(21)-C(22)-C(23)-C(22)#2	179.0(6)

Symmetry transformations used to generate equivalent atoms:

#2 -x,y,-z+1/2

Fig. S1 Hirshfeld surface calculated on the anionic part of the asymmetric unit and mapped with d_i (top) and curvedness (bottom). Hydrogen bonds with the dimethylammonium cation are shown as dashed lines. Anomalous parts in the vicinity of uranium are due to truncation of the polymer chain.

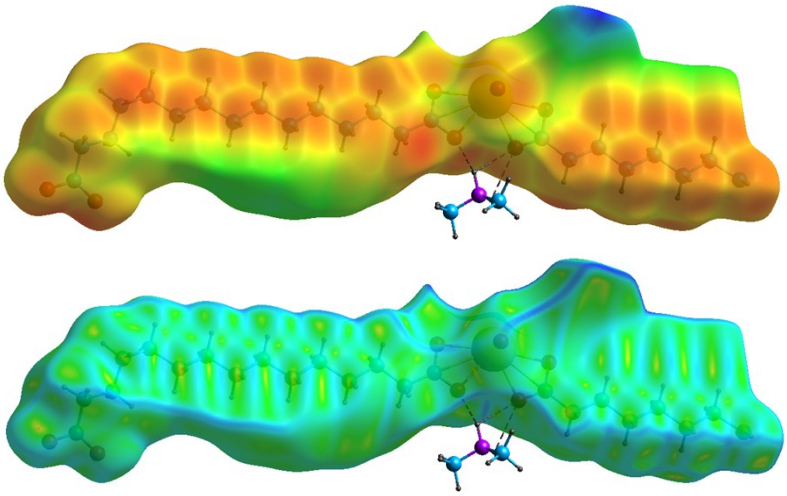

Fig. S2 Emission spectrum of complex **1** in the solid state.

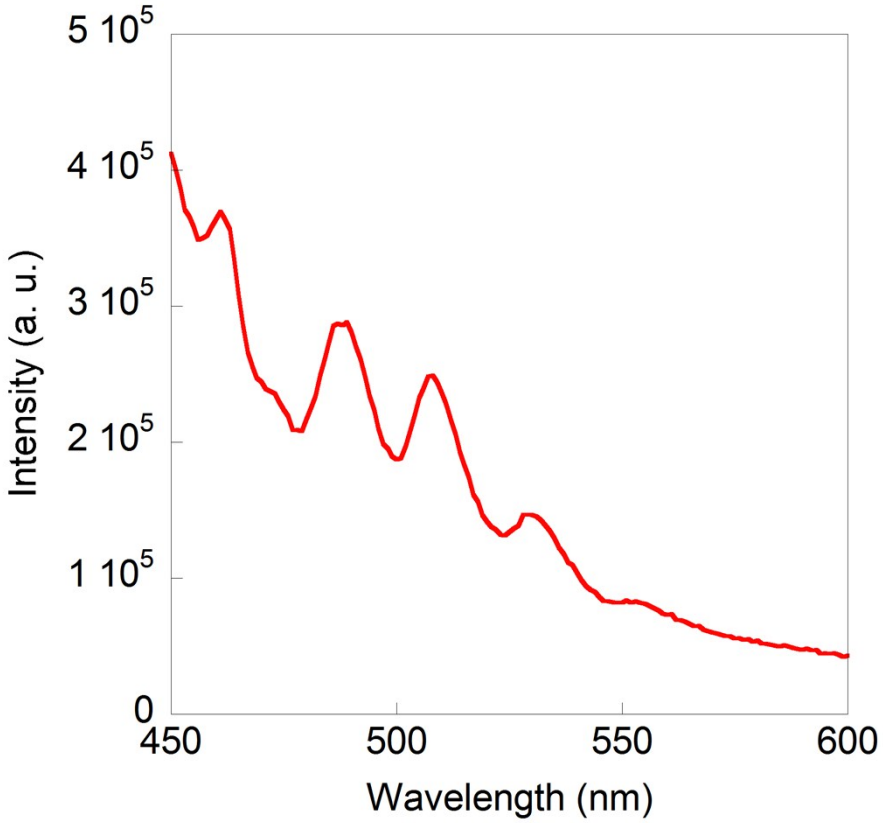

Fig. S3 Infrared spectrum of complex **1**.