Supporting Information:

Structural Control in Nano-assembly of Tungsten and Molybdenum Dithiolene Complex Analog

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Table S1. X-ray crystallographic data for **1** and **2**.

Compound	**1**	**2**
Empirical formula	$C_{26}H_{58}N_{12}O_{10}S_8W_2$	$C_{20}H_{36}Mo_2N_{10}O_8S_8$
Formula weight	1323.02	992.95
Temperature (K)	100(2)	100(2)
Radiation	MoK_α	MoK_α
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	monoclinic
Space group	*P-1*	*P2/c*

a (Å)	9.311(2)	15.613(5)
b (Å)	9.420(2)	8.603(5)
c (Å)	15.955(4)	16.257(5)
α (deg)	72.834(4)	90
β (deg)	74.371(5)	112.417(5)
γ (deg)	62.447(3)	90
Volume ($Å^3$)	1170.9(5)	2018.6(15)
Z	1	2
$d_{calc.}$ (mg/cm^3)	1.876	1.634
F (000)	654	1004
θ range (deg)	2.49 to 26	2.37 to 26
Reflections collected	6552	11043
Independent refl.	4489	3951
$R_{int.}$	0.0320	0.0438
GOF	1.105	1.286
Final R indices [I >2sigma(I)]	R1 = 0.0692, wR2 = 0.1723	R1 = 0.1009, wR2 = 0.2892
R indices (all data)	R1 = 0.0786, wR2 = 0.1835	R1 =0.1233, wR2 =0.3254

Table S2. Selected Bond lengths [Å] for **1**

W(2)-S(2)	2.416(4)	W(2)-S(1)	2.433(5)
W(2)-S(4)#1	2.457(5)	W(2)-S(4)	2.541(5)
S(3)-W(1)	2.131(5)	S(4)-W(1)#1	2.335(3)
S(4)-W(1)	2.335(3)	S(4)-W(2)#1	2.457(5)
W(1)-S(4)#1	2.335(3)	W(1)-S(2)	2.380(3)
W(1)-S(1)	2.418(3)	W(1)-W(1)#1	2.9444(12)
S(1)-C(1)	1.734(12)	S(2)-C(2)	1.754(11)

Selected Bond angles [º] for **1**.

S(2)-W(2)-S(1)	79.63(15)	S(2)-W(2)-S(4)#1	77.63(14)
S(1)-W(2)-S(4)#1	135.6(2)	S(2)-W(2)-S(4)	131.8(2)

S(1)-W(2)-S(4)	74.96(15)	S(4)#1-W(2)-S(4)	92.94(17)
W(1)#1-S(4)-W(1)	78.19(9)	W(1)#1-S(4)-W(2)#1	39.18(12)
W(1)-S(4)-W(2)#1	70.55(12)	W(1)#1-S(4)-W(2)	69.07(12)
W(1)-S(4)-W(2)	38.28(11)	W(2)#1-S(4)-W(2)	87.06(17)
S(3)-W(1)-S(4)#1	106.34(15)	S(3)-W(1)-S(4)	106.08(16)
S(4)#1-W(1)-S(4)	101.81(9)	S(3)-W(1)-S(2)	104.18(15)
S(4)#1-W(1)-S(2)	80.77(10)	S(4)-W(1)-S(2)	147.43(11)
S(3)-W(1)-S(1)	107.27(15)	S(4)#1-W(1)-S(1)	144.62(12)
S(4)-W(1)-S(1)	79.13(10)	S(2)-W(1)-S(1)	80.66(9)
S(3)-W(1)-W(1)#1	116.28(14)	S(4)#1-W(1)-W(1)#1	50.91(7)
S(4)-W(1)-W(1)#1	50.90(8)	S(2)-W(1)-W(1)#1	122.75(8)
S(1)-W(1)-W(1)#1	119.80(7)	C(1)-S(1)-W(1)	07.7(4)
C(1)-S(1)-W(2)	102.3(4)	W(1)-S(1)-W(2)	38.77(11)
C(2)-S(2)-W(1)	108.2(4)	C(2)-S(2)-W(2)	102.6(4)

Selected Bond lengths [Å] for **2**

Mo(1)-S(4)	1.900(6)	Mo(1)-S(3)	2.323(2)
Mo(1)-S(3)#1	2.348(3)	Mo(1)-S(2)	2.393(2)
Mo(1)-S(1)	2.420(2)	Mo(1)-Mo(1)#1	2.8310(16)
S(3)-Mo(1)#1	2.348(3)	S(1)-C(1)	1.733(9)

Selected Bond angles [º] for **2.**

S(4)-Mo(1)-S(3)	111.16(18)	S(4)-Mo(1)-S(3)#1	108.21(17)
S(3)-Mo(1)-S(3)#1	99.30(9)	S(4)-Mo(1)-S(2)	107.49(18)
S(3)-Mo(1)-S(2)	139.46(11)	S(3)#1-Mo(1)-S(2)	79.53(8)
S(4)-Mo(1)-S(1)	101.40(16)	S(3)-Mo(1)-S(1)	79.30(9)
S(3)#1-Mo(1)-S(1)	148.51(10)	S(2)-Mo(1)-S(1)	81.62(8)
S(4)-Mo(1)-Mo(1)#1	100.76(14)	S(3)-Mo(1)-Mo(1)#1	53.11(6)
S(3)#1-Mo(1)-Mo(1)#1	52.28(6)	S(2)-Mo(1)-Mo(1)#1	129.86(7)
S(1)-Mo(1)-Mo(1)#1	132.09(6)	Mo(1)-S(3)-Mo(1)#1	74.61(8)

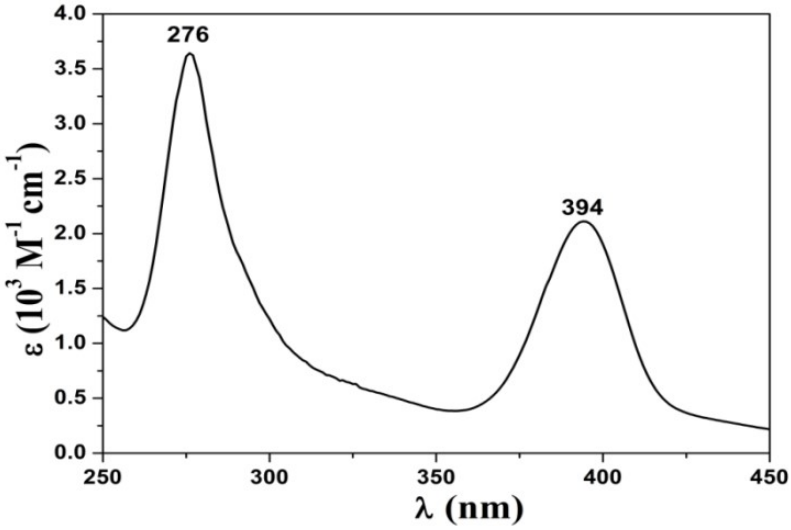

Fig. S1 Electronic absorption spectrum of **1** in water.

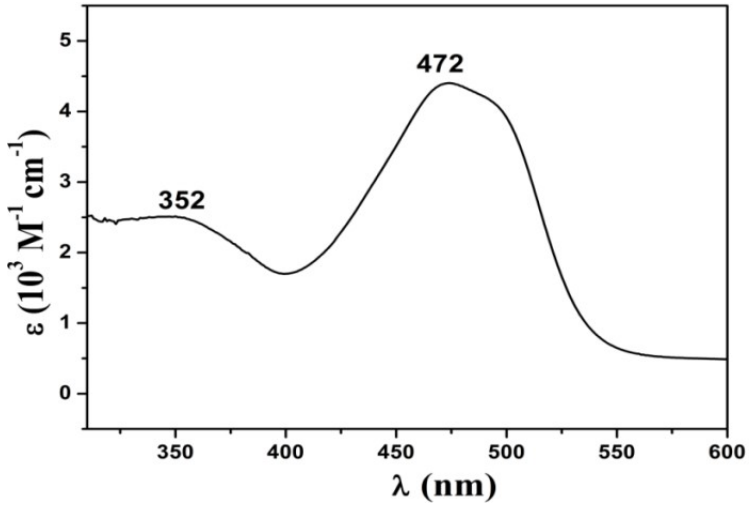

Fig. S2 Electronic absorption spectrum of **2** in water.

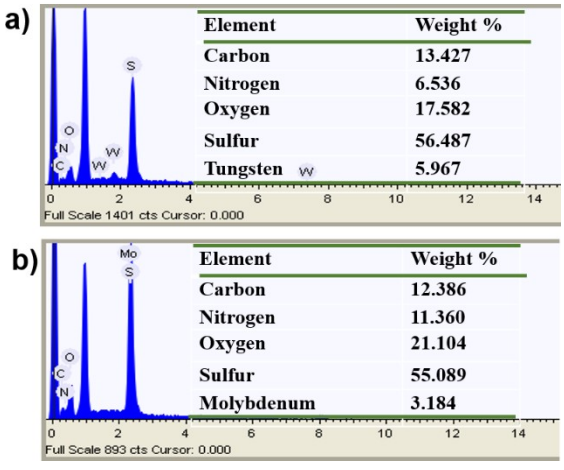

Fig. S3 EDAX analysis with percentage elemental compositions of the nanoflowers of the **1 (a)** and **2 (b)**.

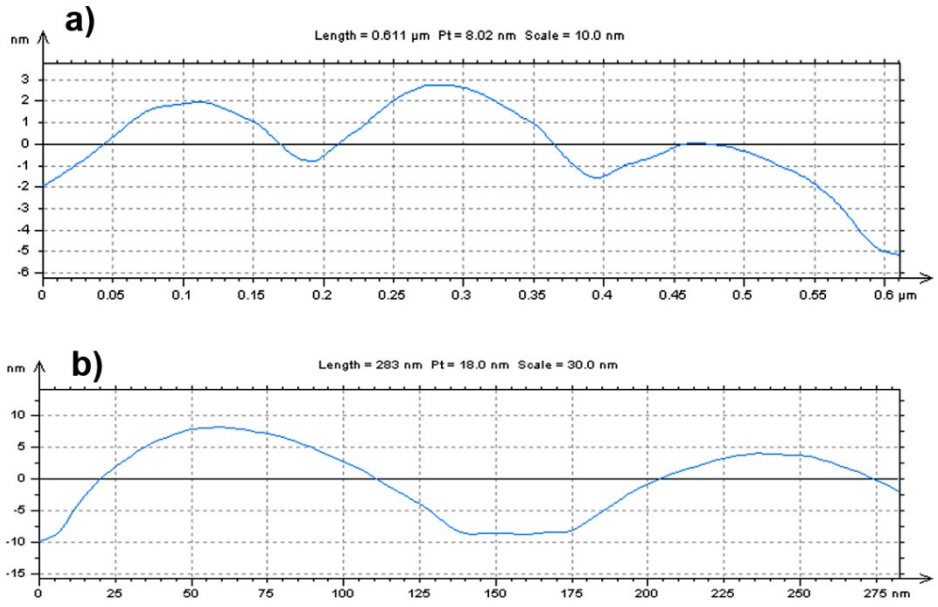

Fig. S4 (a) AFM line profile of **1**, and **(b) 2** on HOPG matrix.