

SUPPLEMENTARY MATERIAL

(for the communication “Exclusive Transition State Stabilization in the Supramolecular Catalysis of Diels Alder Reaction by a Uranyl Salophen Complex.” submitted by Antonella Dalla Cort, Luigi Mandolini* and Luca Schiaffino).

Synthesis of compounds **2b** and **3b**.

Materials

Salicylaldehyde (Aldrich) and uranyl acetate dihydrate (Fluka) were commercial samples. 3-Phenylsalicylaldehyde was available from a previous work.¹ 4,5-Bis-dodecyloxy-benzene-1,2-diamine was prepared according to a literature procedure.²

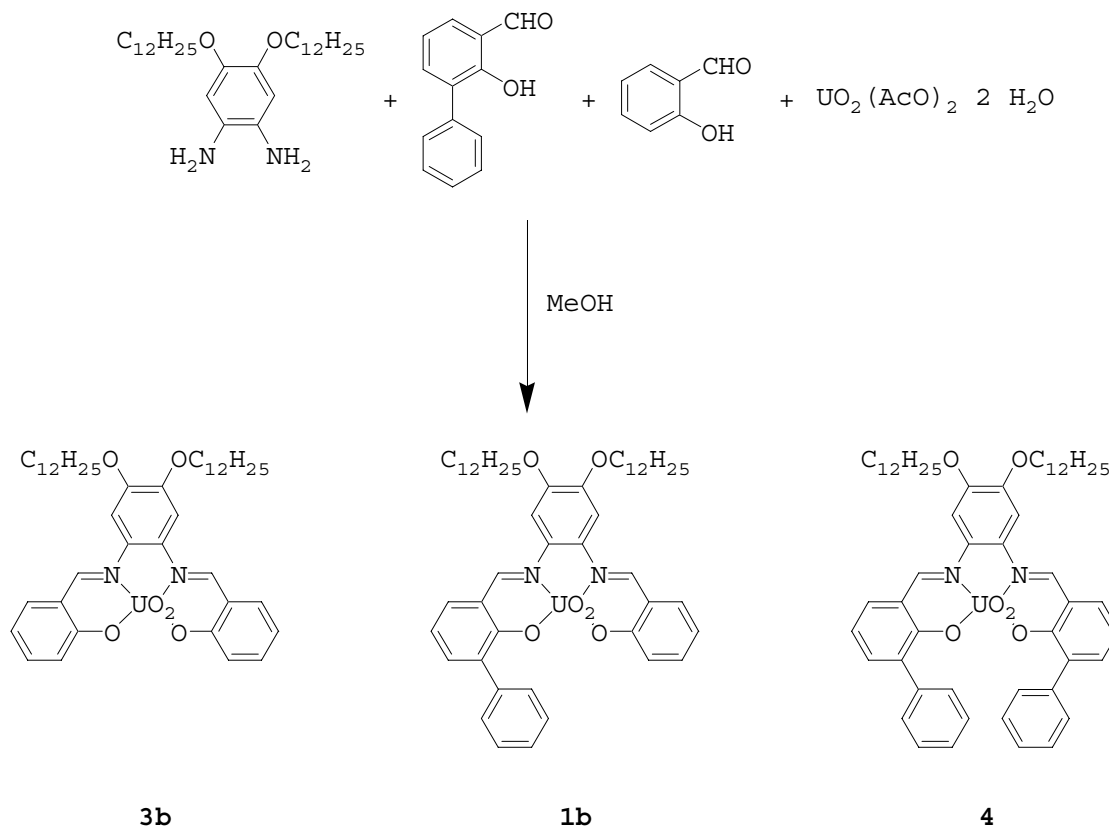
Synthetic procedure

Nonsymmetrical complex **1b** was prepared according to a previously described statistical procedure.³ The three reaction products were separated by flash chromatography on silica gel. Product **4** was eluted with cyclohexane/acetone 80:20, product **1b** with cyclohexane/acetone 50:50, product **3b** with acetone.

¹ A. Dalla Cort, J. I. Miranda Murua, C. Pasquini, M. Pons, L. Schiaffino, *Chem. Eur. J.* **2004**, *10*, 3301-3307.

² M.M.G. Antonisse, M. Martijn, B.H.M. Snellink-Rueel, I. Yigit, J.F.J. Engbersen, D.N. Reinhoudt, *J. Org. Chem.* **1997**, *62*, 9034-9038.

³ A. Dalla Cort, L. Mandolini, G. Calmieri, C. Pasquini, L. Schiaffino, *Chem. Commun.*, **2003**, 2178-2179.



[[4,5-Bis(dodecyloxy)-1,2-bis[nitrilomethylidene(2-hydroxyphenyl)]phenylene](2-)-N,N',O,O']dioxouranium (3b) (yield 21%) showed spectral data consistent with those already reported in the literature.²

[[4,5-Bis(dodecyloxy)-1-[nitrilomethylidene(2-hydroxy-biphenyl-3-yl)]-2-[nitrilomethylidene(2-hydroxyphenyl)]phenylene](2-)-N,N',O,O']dioxouranium (1b).

Yield 45%; ¹H NMR (CDCl₃, 200 MHz): δ 9.58 (1H, s), 9.47 (1H, s), 8.00 (2H, d, J = 3.0 Hz), 7.93-7.62 (3H, m), 7.49-7.13 (7H, m), 6.95 (1H, t, J = 7.4 Hz), 6.81 (1H, t, J = 7.2 Hz), 4.36 (2H, t, J = 6.3 Hz), 4.25 (2H, t, J = 6.3 Hz), 2.05 (4H, m), 1.68 (4H, m), 1.60-1.30 (32H, m), 1.07-0.95 (6H, m); ¹³C NMR (CDCl₃, 75 MHz): δ 167.7, 164.7, 151.1, 151.0, 141.2, 141.1, 139.6, 137.2, 136.8, 135.6, 135.4, 133.1, 130.3, 129.9, 128.5, 127.4, 125.9, 125.8, 124.4, 122.1, 120.1, 118.9, 105.9, 105.5, 70.8, 70.6, 32.6, 30.4, 30.3, 30.2, 30.1, 30.0, 29.9, 26.8, 26.7, 23.4, 14.8. Anal. Calcd C₅₀H₆₆N₂O₆U * 3 H₂O: C, 55.44; H, 6.70; N, 2.59. Found: C, 55.5; H, 7.0; N, 2.4.

Structure of the optimised geometry of the transition state in cartesian coordinates

Calculated with use of the Gaussian 03⁴ package.

⁴ Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B.

C	-0.0061257799	-0.0879723275	-0.0034542754
C	-0.0065154832	-0.0880529854	1.4024445841
C	1.2660173181	-0.0932981542	2.1584775373
C	2.5053780460	0.1495529836	1.3727680588
C	2.5057536594	0.1496379663	0.0276531570
C	1.2668309742	-0.0931149258	-0.7587782051
O	1.3197947791	-0.2941027905	3.3691105666
O	1.3212826426	-0.2937625035	-1.9694068889
C	-0.6452734012	1.9691351029	-0.6611250276
C	-2.0403227906	1.8711010788	-0.0793279083
C	-2.0407183005	1.8710396791	1.4775022471
C	-0.6459654609	1.9690058601	2.0600118182
C	0.3135309632	2.7368200735	1.3997222747
C	0.3138861593	2.7368885753	-0.0002731851
H	3.4176749013	0.2658848317	-0.5530338295
H	3.4169753863	0.2657249280	1.9539785488
H	-0.8479502559	-0.5103852199	-0.5436444348
H	-0.8486480395	-0.5105125064	1.9421172498
H	-0.5552729554	1.8167181960	-1.7338965875
H	-0.5565072275	1.8164766301	3.1328126771
H	-2.5620927031	0.9941989171	1.8746821063
H	-2.5614781267	0.9942808645	-0.4768408890
H	-2.6019139694	2.7421532518	1.8413340082
H	-2.6013477953	2.7422330438	-0.4433777901
H	1.1704621840	3.1262261343	1.9433255363
H	1.1710923384	3.1263481287	-0.5434040371