Electronic Supplementary Information (ESI)

Systematic Investigation on the Coordination Chemistry of a Sulfonated Monoazo Dye:

Ligand Dominated d- and f-Block Derivatives

Jian Lü,^a Shui-Ying Gao,^a Jing-Xiang Lin,^a Lin-Xi Shi,^a Rong Cao,^{*a} and Stuart R. Batten^b

^aState Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of

Matter, Chinese Academy of Sciences, Fujian, Fuzhou, 350002, P. R. China; ^bSchool of

Chemistry, Monash University 3800, Australia

Table S1 Hyd	lrogen bond le	engths (Å) for	compounds 1-5.
--------------	----------------	----------------	----------------

		Compound 1	
N(1)-H(4A)····O(1)W	2.792	N(4)-H(4E)O(4)W	2.753
$O(2)_W - H(1D) - O(2)$	2.844	$O(2)_{W}-H(1C)\cdots O(6)$	2.876
$O(3)_{W}-H(1E)\cdots O(3)$	2.914	$O(2)_W-H(1H)\cdots O(5)$	2.846
		Compound 2	
N(4)-H(1X)····O(1)	3.024	N(4)-H(1F)O(1)W	2.804
N(4)-H(1C)····O(5)	2.930	$O(1)_W - H(1E) - O(6)$	2.722
$O(2)_W-H(1I)\cdots O(4)$	2.838	$O(1)_W$ -H(1D)····O(4)	2.893
		Compound 3a	
$O(1)_W$ -H···O(2)	2.740	$O(1)_W$ -H···O(3)	2.744
N(1)-H…O(2)	3.087		
		Compound 3b	
$O(1)_W$ -H···O(1)	2.740	$O(1)_W$ -H···O(2)	2.759
N(1)-H…O(3)	3.046		
		Compound 3c	
$O(1)_W$ -H···O(2)	2.776	$O(1)_W$ -H···O(3)	2.672
N(1)-H…O(3)	3.031		
		Compound 3d	
$O(1)_{W}$ -HO(2)	2.734	$O(1)_W$ -H···O(3)	2.767
$O(1)_{W} \Pi O(2)$			
$N(1)-H\cdots O(2)$	3.098		
$N(1)-H\cdots O(2)$	3.098	Compound 3e	
$O(1)_{W} H^{-}O(2)$ $N(1)-H\cdots O(2)$ $O(1)_{W}-H\cdots O(1)$	3.098 2.742	Compound 3e O(1) _W -H…O(2)	2.733
$O(1)_{W} H^{-}O(2)$ $N(1)-H\cdots O(2)$ $O(1)_{W}-H\cdots O(1)$ $N(1)-H\cdots O(2)$	 3.098 2.742 3.066 	Compound 3e $O(1)_W$ -H···O(2)	2.733
$O(1)_{W}$ H $O(2)$ N(1)-HO(2) $O(1)_{W}$ -HO(1) N(1)-HO(2)	3.098 2.742 3.066	Compound 3e O(1) _W -H…O(2) Compound 3f	2.733
$O(1)_{W} H^{-}O(2)$ $N(1)-H^{}O(2)$ $O(1)_{W}-H^{}O(2)$ $O(1)_{W}-H^{}O(2)$	3.0982.7423.0662.771	Compound 3e $O(1)_W$ -H···O(2) Compound 3f $O(1)_W$ -H···O(3)	2.733 2.719
$O(1)_{W} H^{-}O(2)$ $N(1)-H^{}O(2)$ $O(1)_{W}-H^{}O(2)$ $O(1)_{W}-H^{}O(2)$ $N(1)-H^{}O(2)$	 3.098 2.742 3.066 2.771 3.024 	Compound 3e $O(1)_W$ -H···O(2) Compound 3f $O(1)_W$ -H···O(3)	2.733 2.719
$O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(1) N(1)-H···O(2) $O(1)_{W}$ -H···O(2) N(1)-H···O(2)	 3.098 2.742 3.066 2.771 3.024 	Compound 3e $O(1)_W$ -H···O(2) Compound 3f $O(1)_W$ -H···O(3) Compound 5a	2.733 2.719
$O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(1) N(1)-H···O(2) $O(1)_{W}$ -H···O(2) N(1)-H···O(2) $O(3)_{W}$ -H···O(9)	 3.098 2.742 3.066 2.771 3.024 2.840 	Compound 3e $O(1)_W$ -H···O(2) Compound 3f $O(1)_W$ -H···O(3) Compound 5a $O(3)_W$ -H···O(2)	2.7332.7192.950
$O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) N(1)-H···O(2) $O(3)_{W}$ -H···O(9) $O(2)_{W}$ -H···O(3)	 3.098 2.742 3.066 2.771 3.024 2.840 2.837 	Compound 3e $O(1)_W$ -H···O(2) Compound 3f $O(1)_W$ -H···O(3) Compound 5a $O(3)_W$ -H···O(2) $O(1)_W$ -H···O(2) _W	 2.733 2.719 2.950 2.688
$O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) N(1)-H···O(2) $O(3)_{W}$ -H···O(2) $O(3)_{W}$ -H···O(3) $O(1)_{W}$ -H···O(5)	 3.098 2.742 3.066 2.771 3.024 2.840 2.837 2.731 	Compound 3e $O(1)_{W}$ -H···O(2) Compound 3f $O(1)_{W}$ -H···O(3) Compound 5a $O(3)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2)_{W} $O(2)_{W}$ -H···O(6)	 2.733 2.719 2.950 2.688 2.788
$O(1)_{W} H^{-}O(2)$ $N(1)-H\cdots O(2)$ $O(1)_{W}-H\cdots O(2)$ $O(1)_{W}-H\cdots O(2)$ $N(1)-H\cdots O(2)$ $O(3)_{W}-H\cdots O(2)$ $O(3)_{W}-H\cdots O(3)$ $O(1)_{W}-H\cdots O(5)$	 3.098 2.742 3.066 2.771 3.024 2.840 2.837 2.731 	Compound 3e $O(1)_W-H\cdots O(2)$ Compound 3f $O(1)_W-H\cdots O(3)$ Compound 5a $O(3)_W-H\cdots O(2)_W$ $O(1)_W-H\cdots O(2)_W$ $O(2)_W-H\cdots O(6)$ Compound 5c	 2.733 2.719 2.950 2.688 2.788
$O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2) $O(3)_{W}$ -H···O(3) $O(1)_{W}$ -H···O(5) $O(3)_{W}$ -H···O(5)	 3.098 2.742 3.066 2.771 3.024 2.840 2.837 2.731 2.901 	Compound 3e $O(1)_{W}$ -H···O(2) Compound 3f $O(1)_{W}$ -H···O(3) Compound 5a $O(3)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2)_{W} $O(2)_{W}$ -H···O(6) Compound 5c $O(3)_{W}$ -H···O(8)	 2.733 2.719 2.950 2.688 2.788 2.852
$O(1)_{W} H^{-}O(2)$ $N(1)-H^{}O(2)$ $O(1)_{W}-H^{}O(2)$ $O(1)_{W}-H^{}O(2)$ $O(3)_{W}-H^{}O(2)$ $O(3)_{W}-H^{}O(3)$ $O(1)_{W}-H^{}O(5)$ $O(3)_{W}-H^{}O(5)$ $O(3)_{W}-H^{}O(2)$	 3.098 2.742 3.066 2.771 3.024 2.840 2.837 2.731 2.901 2.753 	Compound 3e $O(1)_{W}$ -H···O(2) Compound 3f $O(1)_{W}$ -H···O(3) Compound 5a $O(3)_{W}$ -H···O(2) $O(1)_{W}$ -H···O(2)_{W} $O(2)_{W}$ -H···O(2)_{W} $O(2)_{W}$ -H···O(4)_{W}	 2.733 2.719 2.950 2.688 2.788 2.852 2.659

Fig. S1 XRPD patterns of complexes La/Pr/Nd/Sm-L, showing the identical characteristics of the samples.

Fig. S2 Simulated and experimental XRPD patterns of 5c, and a comparison of experimental

XRPD patterns of **5b** and **5c**.

Fig. S3 IR spectra on CaF_2 slides of PEI-BW₁₂ (a), PEI-BW₁₂/5c-Ho (b), and PEI-(PW₁₂/5c-Ho)₆ (c).

Fig. S4 AFM images of 5c on mica slide.

Fig. S5 UV-vis spectra of the PEI-(PEG/**5c-Ho**)_{*n*} multilayer films on a quartz slide.



Fig. S1

Electronic Supplementary Information for Dalton Transactions This journal is The Royal Society of Chemistry 2009



Fig. S2



Fig. S3

Electronic Supplementary Information for Dalton Transactions This journal is The Royal Society of Chemistry 2009



0 Data type Z range 1.73 μm Height 10.000 nm



0 Data type Z range 10.0 µm Height 30.00 nm

Fig. S4

Electronic Supplementary Information for Dalton Transactions This journal is The Royal Society of Chemistry 2009



Fig. S5