Supporting Information

Acid/base responsive assembly / dis-assembly of a family of zirconium(IV) clusters with a cyclic imide-dioxime ligand

Stamatis S. Passadis¹, Sofia Hadjithoma², Michael G. Papanikolaou¹, Anastasios D. Keramidas²*, Haralampos N. Miras³* and Themistoklis A. Kabanos¹*

¹Section of Inorganic and Analytical Chemistry, Department of Chemistry, University of Ioannina, Ioannina 45110, Greece. E-mail: tkampano@uoi.gr

² Department of Chemistry, University of Cyprus, Nicosia 2109, Cyprus. E-mail: <u>akeramid@ucy.ac.cy</u>

³ West CHEM, School of Chemistry, University of Glasgow, Glasgow G12 8QQ, U.K. E-mail: <u>Charalampos.moiras@glasgow.ac.uk</u>

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Fig. S1 The bicapped octahedral coordination environment of Zr(1) atom in 1.



Fig. S1 The bicapped octahedral coordination environment of Zr(1) atom in 1.



Fig. S2 The bicapped octahedral coordination environment of Zr(1) (A) and Zr(2) (B) atoms in **2**.



Fig. S3 2D {¹H} grCOSY NMR of the solid from the reaction of ZrCl₄, H₃pidiox and KOH.



Fig. S4 2D $\{^{1}H, ^{13}C\}$ grHSQC NMR of the solid from the reaction of ZrCl₄, H₃pidiox and KOH.



Fig. S5 2D $\{^{1}H, ^{13}C\}$ grHMBC NMR of the solid from the reaction of ZrCl₄, H₃pidiox and KOH.



Fig. S6 2D $\{^{1}H\}$ grNOESY-EXSY NMR of the solid from the reaction of ZrCl₄, H₃pidiox and KOH. A) EXSY and B) NOESY peaks.



Fig. S7 ¹H NMR spectra of **1** in solution (CD₃OD, 4.00 mM) and DCl (1280 mM) *vs* time.



Fig. S8 2D {¹H,¹³C} grHSQC NMR of 4.



Fig. S9 2D $\{^{1}H\}$ grNOESY-EXSY NMR of 4.