Supporting Information

for

Determination of Absolute Configuration of Acyclic 1,2-Diols with Mo$_2$(OAc)$_4$. 2.

New structural evidence toward a rationale of the method. What remains of Mo$_2$(OAc)$_4$ in DMSO solution?

By

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Plot of CD at 308 nm of 1/Mo$_2$(OAc)$_4$ mixtures in DMSO as a function of addition of water (Figure S1), and $^1$H-NMR TOCSY spectrum of 2/Mo$_2$(OAc)$_4$ mixture in $d_6$-DMSO (Figure S2).

Figure S1. Plot of $-\theta$ (observed ellipticity) at 308 nm vs. equivalents of water added, for ICD spectra at stationary conditions of (R)-phenylethane-1,2-diol (1) 2.7 mM in solution of dimolybdenum tetraacetate 2.7 mM (main graph) and 28.2 mM in solution of dimolybdenum tetraacetate 31.0 mM (insert) in DMSO; cell path length 0.1 and 0.01 cm, respectively.
Figure S2. $^1$H-NMR TOCSY spectrum (300 MHz, $\tau_{\text{mix}}=30$ ms) of (R,R)-butane-2,3-diol (2) 43.7 nM in solution of dimolybdenum tetraacetate 48.6 nM in anhydrified $d_6$-DMSO. Arrows indicate the signals attributed to the major (full line) and the two minor (dotted line) diol/dimolybdenum complexes.