Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# A chiral lactate reporter based on total and circularly polarized Tb(III) luminescence

Marco Leonzio,[1] Andrea Melchior,*[2] Georgina Faura,[2] Marilena Tolazzi,[2] Marco Bettinelli,[1] Francesco Zinna,[3]† Lorenzo Arrico,[3] Lorenzo Di Bari,*[3] and Fabio Piccinelli*[1]

# Supporting information

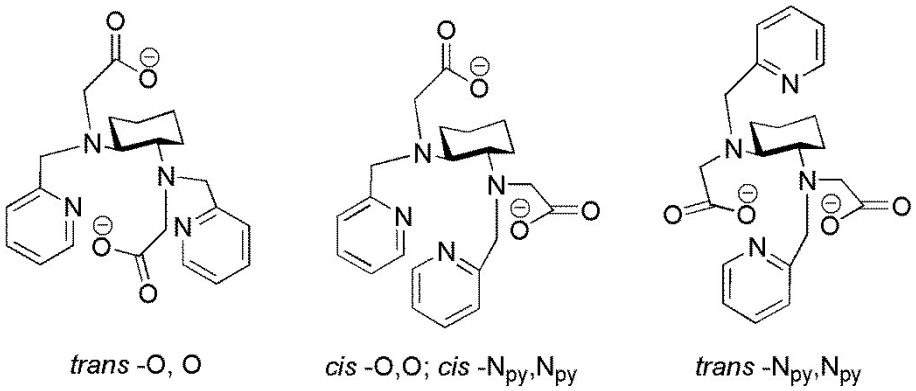


**Chart S1**. The possible coordination geometries of $bpcd^{2-}$ ligand.

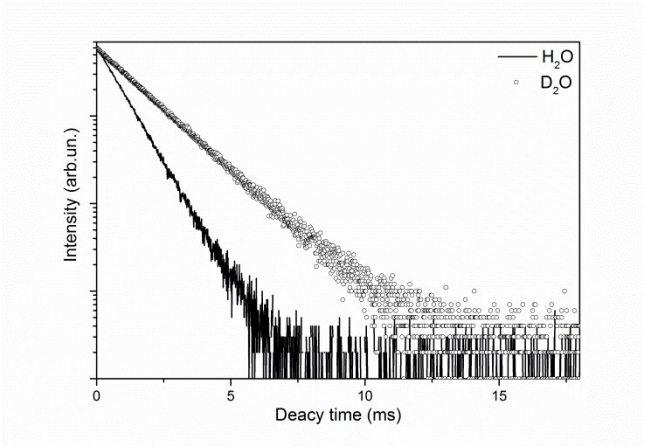


**Figure S1.** Luminescence decay curves from $^5D_4$ excited state of Tb(III) in $[Tb(bped)]^+$ complex in $H_2O$ and $D_2O$ (1mM, $\lambda_{exc}$ = 270 nm, $\lambda_{em}$ = 546 nm)

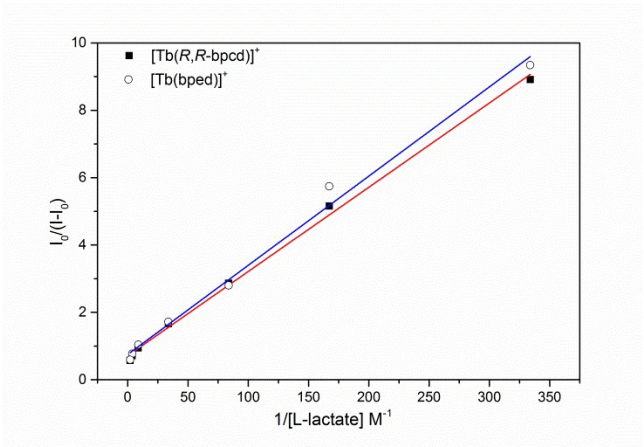


**Figure S2.** Benesi–Hildebrand plot against $[L\text{-lactate}]^{-1}$ for the $[Tb(R,R\text{-bpcd})]^+$ and $[Tb(bped)]^+$ complex. $I_0$ is the emission intensity at 546 nm of the starting complex; I is the emission intensity at 546 nm of the L-lactate:complex adduct after each addition of the analyte. Blue line: linear fit for $[Tb(bped)]^+$, red line: linear fit for $[Tb(R,R\text{-bpcd})]^+$

| Structure | $\Delta E_{gas\ phase}$ | $\Delta E_{PCM}$ |
|---|---|---|
| a | 0.0 | 0.0 |
| b | 4.3 | 4.7 |
| c | 6.3 | -0.2 |
| d | 9.7 | 1.5 |
| e | 0.0 | 0.0 |
| f | 13.6 | 9.1 |

**Table S1**. Relative energies (kcal $mol^{-1}$) of the different isomers of the $[Y(bpcd)lac]^-$ complex in gas phase and PCM ($\Delta E = E_{b-d} - E_a$). The energy difference for the solvated complex is referred to the e isomer.

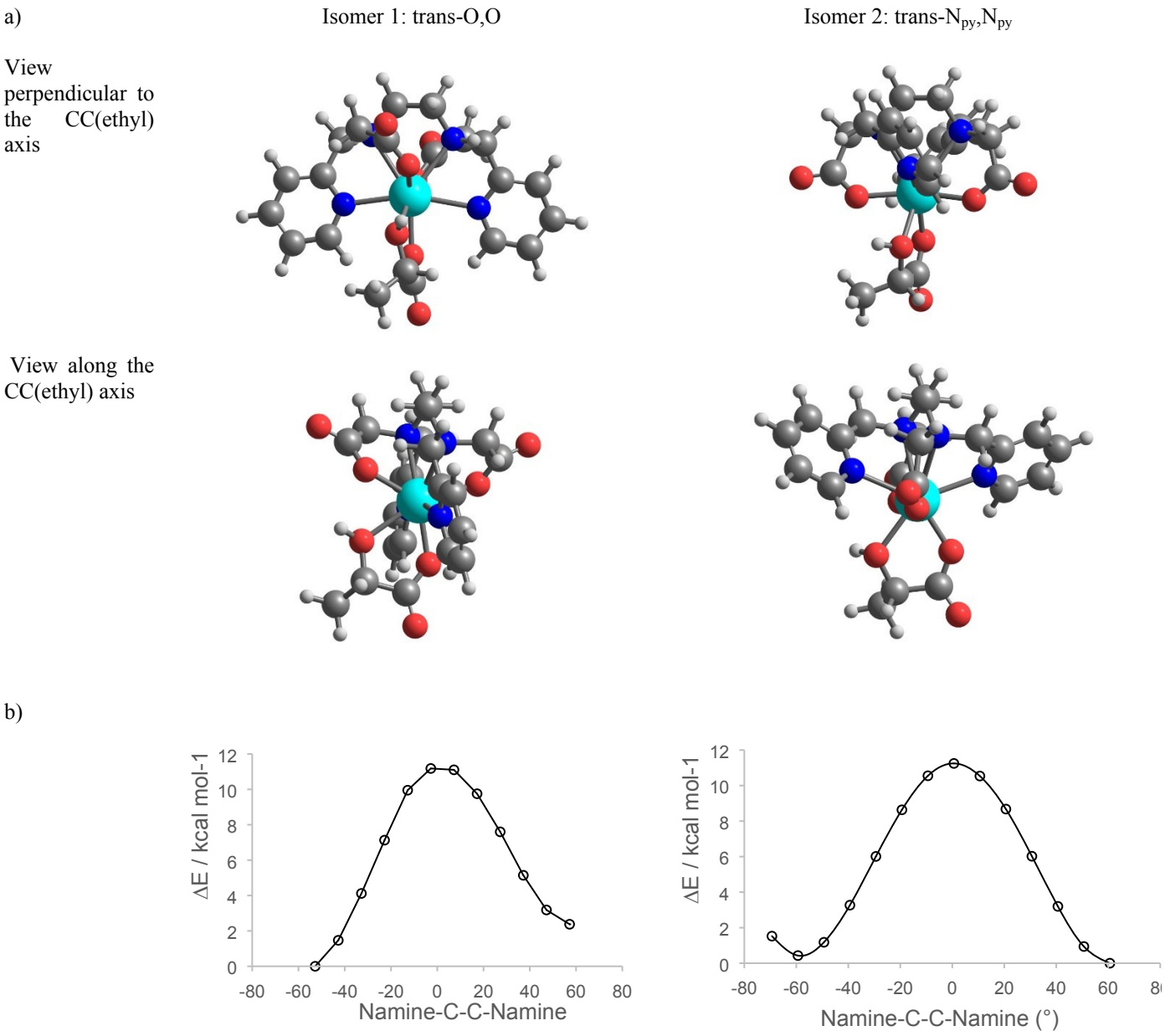


**Figure S3**. a) minimum energy structures of the coordination isomers of the [Y(bped)S-lactate] complex (*i.e.* the δ and λ forms, Chart 2); b) Energy of the [Y(bped)S-lactate] complex as a function of the $N_{amine}$-C-C-$N_{amine}$ torsional angle calculated in PCM water using the same level of theory described in the Methods section. At each angle value the geometry has been left to relax. The inversion of the dihedral angle for the isomer 1 (from ~ -60° to +60°) leads to two structures of nearly slightly different energy (ΔE = 2.4 kcal $mol^{-1}$) with a conversion energy barrier of 11.2 kcal $mol^{-1}$. For the isomer 2 (dihedral from ~ 60° to -60°) two structures of nearly equal energy (ΔE = 0.4 kcal $mol^{-1}$) are obtained. The energy barrier is of 11.2 kcal $mol^{-1}$ also in this case.

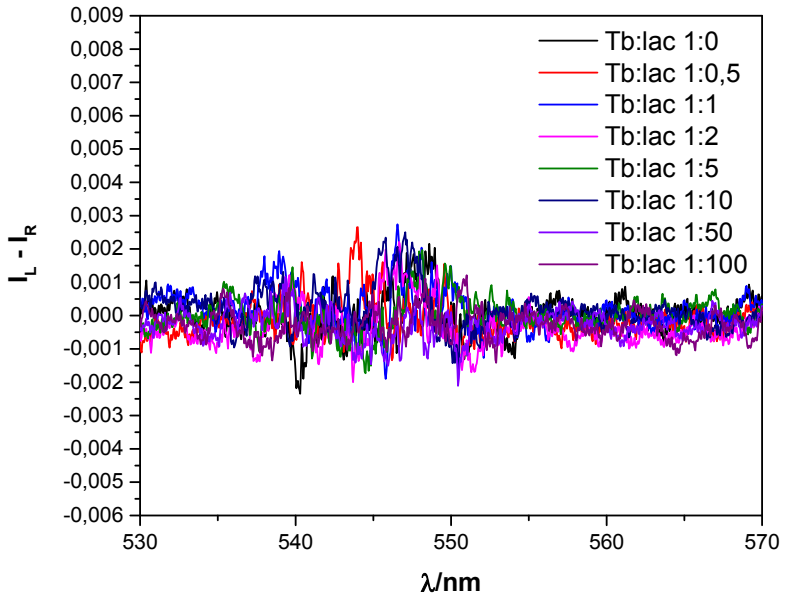


**Figure S4.** Normalized CPL spectrum of $[Tb(bped)]^{+}$ complex upon addition of L-lactate