## Two Isomeric Calix(4)arene Complexes with Mercury(II)

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The X-ray structures of two isomeric complexes of partially derivatized 5,11,17,23-tetra-tert-butyl[25,27-bis(hydroxy)-26,28bis(ethylthio ethoxy)]-calix[4]arene (L) with mercury(II) were determined at 120K. The one obtained by slow evaporation from ethanol solvent,  $LHg(ClO_4)_2$ , crystallizes in the space group Pbca with a=15.568(1), b=18.696(1), c=40.322(1) Å, and Z=8. The other one, obtained from an acetonitrile solution, LHg(ClO<sub>4</sub>)<sub>2</sub>.2MeCN, crystallizes in the space group Pccn with a=21.794(1), b=45.754(1), c=12.395(1) Å, and Z=8. The structures were solved from 6870  $[LHg(ClO_4)_2]$  and 7660  $[LHg(ClO_4)_2.2MeCN]$  reflections with  $I \ge 2\sigma(I)$  and refined to R1-values of 0.053 and 0.073, respectively. The calix[4]arene ligand in both complexes shows hydrophobic cavities with a quite similar squashed cone conformation. In contrast, the hydrophilic cavities exhibit substantial differences in the conformation adopted by the opposite sulfur-containing pendant arms: in  $LHg(ClO_4)_2$  they are roughly related by a pseudo two-fold axis, while in LHg(ClO<sub>4</sub>)<sub>2</sub>.2MeCN these pendant arms are approximately related through a local mirror plane. Despite these lower rim conformational differences, the Hg(II) ion in both complexes is in a similar environment, trans coordinated to the sulfur atoms of the opposite pendant arms, conforming a nearly linear S-Hg-S bond. We thank FAPESP (Brazil) and EU (Contract ICA CT 2000-30006) for support. Keywords: calixarene complexes, environmental chemistry, supramolecules