Structural investigation of chelating agents and their mercury, lead and cadmium (II) complexes

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Mercury (Hg) is one of the most toxic heavy elements present in the environment, which is mostly ingested/inspired insidiously in small quantities, causing chronic diseases. Excretion of high doses of inorganic Hg^{2+} mostly relies on chelation therapy, which consists in administering a chelator such as DMSA (dimercapto succinic acid, FDA-approved medication) or DMPS (2,3-Dimercapto-1-propanesulfonic acid). The naturally occurring enzyme cofactor R-alpha lipoic-acid (R-α-LA) and especially its reduced form dihydrolipoic acid (DHLA) [1] have been considered potential replacement chelators for DMSA and DMPS. Yet, little is known of the complex structure formed by the various ALA:Hg and DHLA:Hg complexes and it has been long debated for a long time. In the present study, we have prepared and synthesized various [R-α-LA:Hg] and [DHLA:Hg] and investigated their solution chemistry, their propensity to chelate mercury, and the complex structure formed followed by spectroscopic techniques. Overall, several complexes are formed with various coordination number such as polydentate complexes as well as non-crystalline solid. Subsequently, synthetical approach was also considered, where two or more aggregation phases were concluded. These complex phases derive from various species of the complex and hold a different oxidation/reduction behavior as disulfides and dithiols have the capability to act as a reducing agent also depending on different synthetic performance.

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