Binding selectivity ethylenediaminetetraacetic and Ethylenediiminopropanedioic acid for Ni cation in aqueous solution: A density functional theory study using a continuum solvation model

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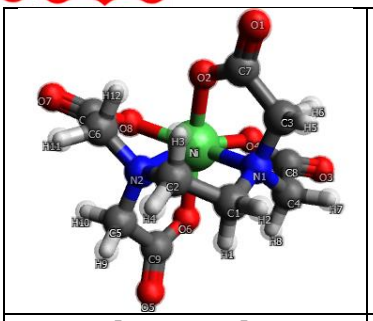
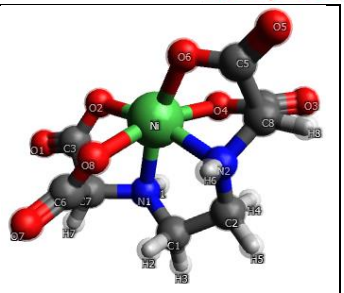
Introduction & Objectives:
Aminopolycarboxylates (APCs) [1,2] are multidentate ligands capable of coordinating with a wide range of metal cations. Chelation technology has shown its potential to develop a sustainable metal mining technology from various contaminated sites using a APCs new generation, which incites us to carry out a theoretical study on these ligands in order to find alternative ligands with a chelation capacity as effective as the EDTA. EDTA (ethylenediaminetetraacetic acid) have diverse applications in a wide variety of fields such as the removal of heavy metals from soil and water. The contamination of soils with heavy metals is a major environmental problem throughout the world. For the remediation of metal-polluted soil, the chelating agent plays an important role for its ability to extract metal ions from the soil solid phase. EDTA, forming stable and water-soluble complexes with metal ions, has been most commonly used for this purpose. The persistence of residual EDTA coupled with its high affinity for metals. The complexation is treated as a ligand substitute reaction on a hydrated metal ion with explicit water molecules.

Methodology (Material and methods):
Ehylenediaminetetraacetic acid exhibits the binding selectivity for transition metal cations in solution phase. In this study, we investigate the main forces that determine the binding selectivity of EDTA and EDDM for the Ni metal cations in aqueous solution using the density functional theory (DFT) and the conductor-like polarizable continuum model (CPCM).

Results and Discussion:
The present work demonstrates the accuracy of computational thermodynamics using density functional theory (DFT) to evaluate the extraction of metals from industrial wastes using different chelation technology

	
$[Ni\text{-}EDTA]^{-2}$	$[Ni\text{-}EDDM]^{-2}$

$[Ni\text{-}EDTA]^{-2}$	6-31G(d)/SDD		6-31G(d)/LanL2DZ	
	Gas phase	Aqueous phase	Gas phase	Aqueous phase
R (Ni-N)	2.178	2. 137	2.172	2.135
R (Ni-O2)	2.116	2.076	2.122	2.079
R (Ni-O4)	2.069	2.070	2.071	2.073
α_1(N1-Ni-N2)	85.0	86.1	85.5	86.5
α_2(N1-Ni-O2)	80.2	82.1	80.2	82.2
α_3(N1-Ni-O4)	79.5	80.7	79.6	80.8
$\Delta_{com}G$ (sol)	-87.05		-80.45	

$[Ni\text{-}EDDM]^{-2}$	6-31G(d)/SDD		6-31G(d)/LanL2DZ	
	Gas phase	Aqueous phase	Gas phase	Aqueous phase
R (Ni-N1)	2.136	2.095	2.059	2.027
R (Ni-N2)	2.136	2.095	2.023	1.975
R (Ni-O2)	2.082	2.090	2.077	2.056
R (Ni-O4)	2.126	2.105	2.198	2.172
R (Ni-O6)	2.082	2.090	2.096	2.081
R (Ni-O8)	2.126	2.105	2.135	2.102
α_1(N1-Ni-N2)	82.9	84.5	80.2	81.3
α_2(N1-Ni-O2)	79.3	80.2	79.9	81.2
α_3(N2-Ni-O4)	78	80.1	78.3	78.9
α_4(N2-Ni-O6)	79.3	80.2	80.4	81.5
α_5(N1-Ni-O8)	78	80.0	85.6	80.6
$\Delta_{com}G$ (sol)	-87.22		**722.19**	

Conclusion: Calculations of hydration free energies of metal ions indicate that first shell explicit water molecules augmented with an implicit bulk solvent model are necessary to lead to good agreement with the experimental free energies of complexation values. Inclusion of the standard state corrections for the solvation free energy calculations is considerable to remove a systematic error in the computed values. The results about the subsequent complexation reactions concluded EDTA as the most stable chelating agent among investigated ligands

Keywords: APCs, EDTA, EDDM, CPCM, DFT

Références bibliographiques

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