Effective and Reversible Hg(II) Uptake by Thioether-Laced, Zr(IV)-Based Metal-Organic Frameworks

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Abstract
Based on knowledge of solid-state chemistry and reticular chemistry with Hard and Soft Acids and Bases (HSAB) Principle, the rational design and synthesis of a new Zr(IV)-based metal-organic frameworks (Zr-BDBB) with a chemical formula of \([\text{Zr}_n\text{O}_{4n}\text{OH}_2\text{(BDBB)}_n]\) were achieved. One designed organic ligand H₂BDBB mainly contains two carboxyl groups (hard Lewis base) used for formation of coordination bonds with Zr(IV) (hard Lewis acid) in zirconium-oxo cluster and six free-standing accessible methylthio groups (soft Lewis base) which are potential secondary donor groups preferentially bonded to soft Lewis acids such as Pd(II), Pt(II), Hg(II). The uptake of Hg(II) by Zr-BDBB in acetonitrile and the recovery of Zr-BDBB from Zr-BDBB-Hg(II) in acetonitrile by 2-mercaptoethanol were achieved with 94.29% of Hg(II) removed, which indicates that reversible Hg(II) uptake by Zr-BDBB can be realized. The thioether-laced Zr-BDBB lowered the Hg(II) concentration in strong acid aqueous solution from 8.00 ppm to 0.137 ppm.

Synthetic Scheme of Ligand H₂BDBB

Instrumental Measurements of Zr-BDBB and Zr-BDBB-Hg(II)

UV-Visible Absorption Spectra and Standard Curve

*94.29% of Hg(II) was removed from Zr-BDBB-Hg(II)*

*Zr-BDBB lowered the Hg(II) concentration from 8 ppm to 0.137 ppm (98.29% of Hg(II) was absorbed)*