

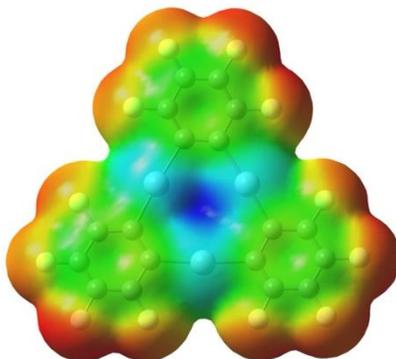
## Anion capture with Hg<sub>3</sub>-anticrowns

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The capability of Mercury-containing anticrowns as anion (and other electron-rich species) traps has been evaluated by means of a combined structural and *ab initio* study. By means of molecular electrostatic potential calculations, it has been observed that there is an electron density depleted region at the center of the three metal atoms (Fig. 1). This positively charge region can interact with anions showing interaction energies larger than 50 kcal/mol. Topological analysis of the electron density along with NBO calculations have further confirmed the involvement of Hg atoms in the interaction. Furthermore, a comprehensive search of the CSD has disclosed many experimental structures displaying short Hg<sub>3</sub>-anticrown...anion contacts. These results open the possibility to use these and other complex organometallic systems as anion capturers.



**Figure 1.** Molecular electrostatic potential of (o-C<sub>6</sub>F<sub>4</sub>Hg)<sub>3</sub> anticrown.