



Schematic showing organo-aluminum compounds with different numbers of electrons added to the organic end groups. Addition of electrons changes the extent to which electrons are delocalized throughout the molecule.

Credit: Amela Arnold and Louise A. Berben

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Project Outcome - Water-stable organic MV compounds have been prepared, spanning five charge states including three that are MV states. The electronic coupling between ligand end groups is modulated by oxidation and reduction of the ligands with electron delocalization observed for  $[(12P^-)(12P2^-)M]$  and when  $M = Al$  or  $Ga$ .

These examples show us that octahedral coordination geometry provides an orbital pathway to support electron delocalization between radical ligands that are connected by metal ions with valence p orbitals, as in group 13.

Mixed-valent (MV) complexes are simple models with which to study electron delocalization and electron transfer and understand geometric and electronic effects that facilitate multielectron redox processes in biological systems,<sup>1</sup> materials,<sup>2,3</sup> and devices.<sup>4-6</sup> The degree of electron delocalization in an organic molecule is related to conductivity, so fundamental studies of electron delocalization in MV compounds can inform the design of organic molecular wires and devices.

This work was carried out by multiple graduate students as indicated in the citation: Amela Arnold, Tobias J. Sherbow, Richard I. Saylor, R. David Britt, Emily J. Thompson, Mayte T. Munoz, James C. Fettingner, Louise A. Berben: Organic Electron Delocalization Modulated by Ligand Charge State in  $[L_2M]^n$ -Complexes of Group 13 Ions. *J. Am. Chem. Soc.* **2019**, *141*, 15792–15803.

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