

Computational Ligand Descriptors for Catalyst Design

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Electronic Supporting Information

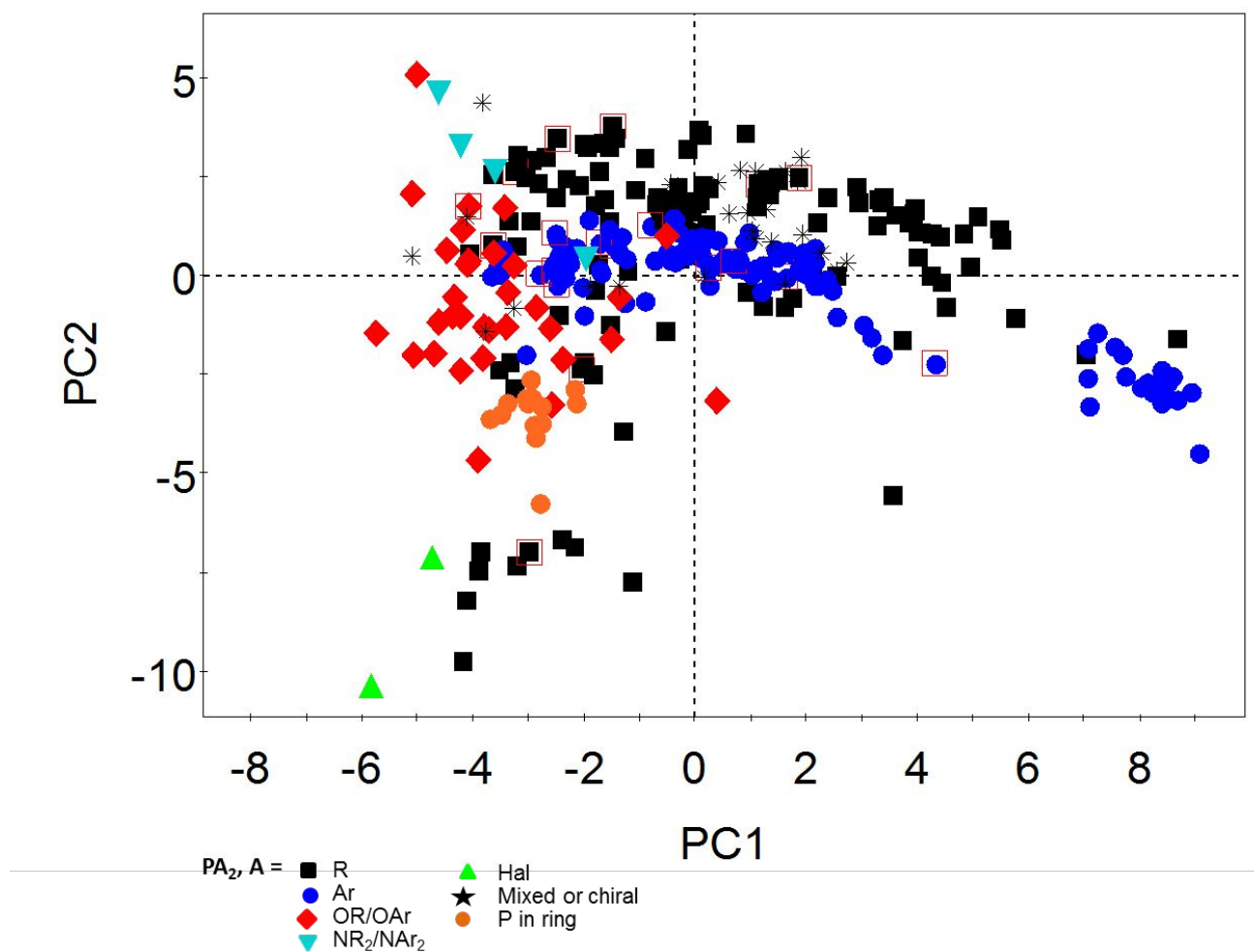


Figure S1: LKB-PP ligand map generated by principal component analysis of 28 ligand parameters capturing the structures and energies of 324 P,P-donor ligands through DFT-calculated parameters, collected in LKB-PP. The principal components are linear combinations of the original parameters derived to capture most of the variation in fewer uncorrelated parameters (58% in this case). Each symbol corresponds to a ligand, and shape and colour are determined by substituents as shown in the legend. Ligands considered here (Table 1b) are marked by red boxes.

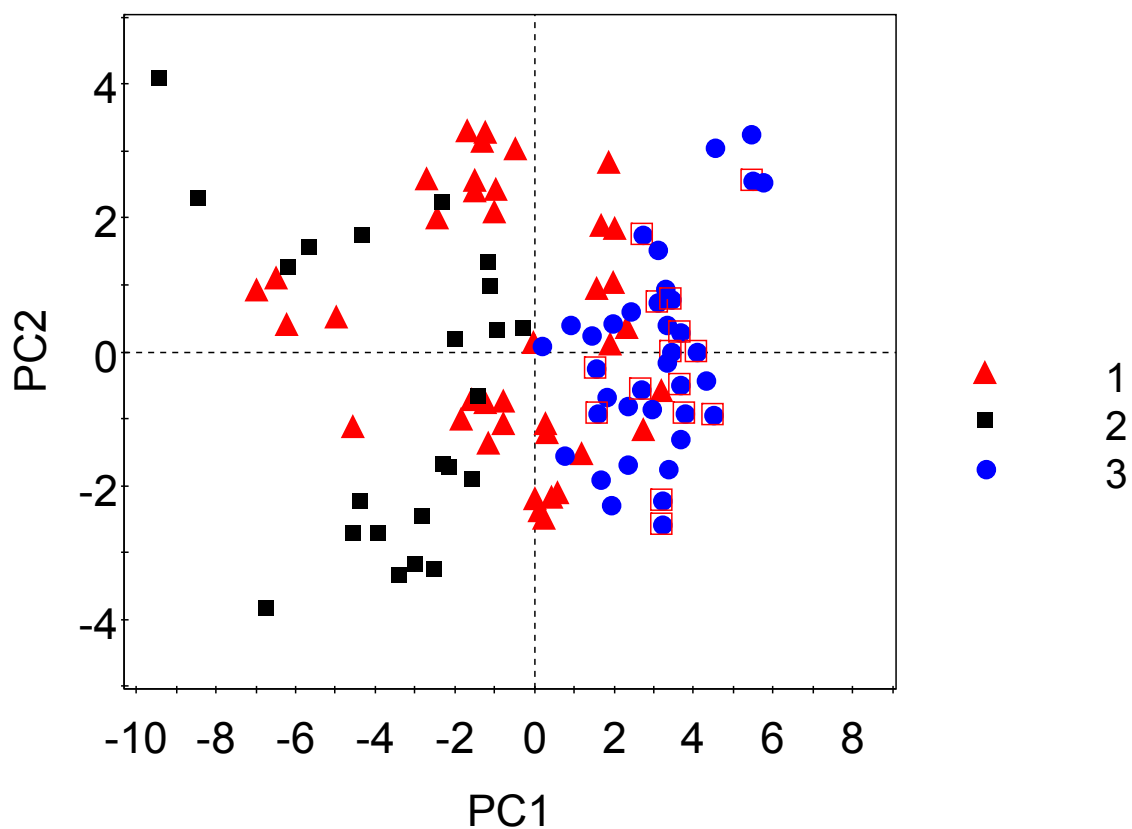


Figure S2: Principal component score plot (PC1 and PC2) for ligands in LKB-C, capturing 58 % of variation in data. Colours and shapes relate to substitution pattern, where red triangle = Schrock-type, black square = Fischer type, blue dot = NHC/Arduengo. Ligands considered here (Table 1c) are marked by red boxes.

