

Enumeration and visualization of various subspaces of the octahedral complex space

Stefan O. Gugler

Massachusetts Institute of Technology
Department of Chemical Engineering

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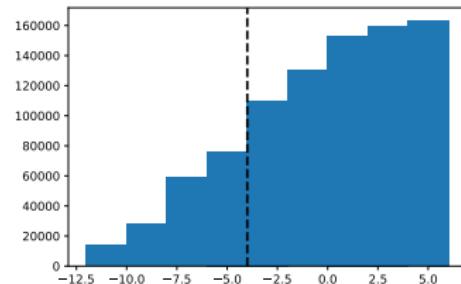
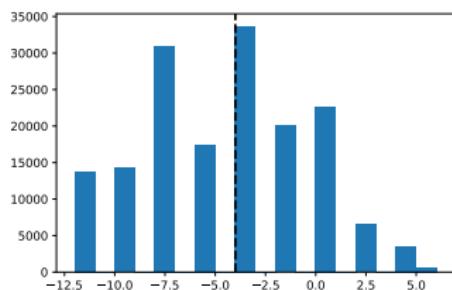
Subsets of octahedral space

The sizes of the selected subsets of octahedral space.

Set	description	size
Homoleptics	$\text{eq} = \text{ax}$	553
"5+1" symmetric	$\text{eq} = \text{ax}_1 \neq \text{ax}_2$	163,620
"4+2" symmetric	$\text{eq}_1 \neq \text{eq}_2 = \text{ax}$	185,376
Strongly symmetric	$\text{eq} \neq \text{ax}$	245,316
Equatorially asymmetric	$\text{eq}_1 \neq \text{eq}_2 \neq \text{ax}$	15,924,796
Weakly symmetric	$\text{eq} \neq \text{ax}_1 \neq \text{ax}_2$	45,077,310
Complete Heteroleptics	$L_i \neq L_j$	$\approx 5.9 \cdot 10^{12}$
Octahedral Space	all	$> 1.8 \cdot 10^{14}$

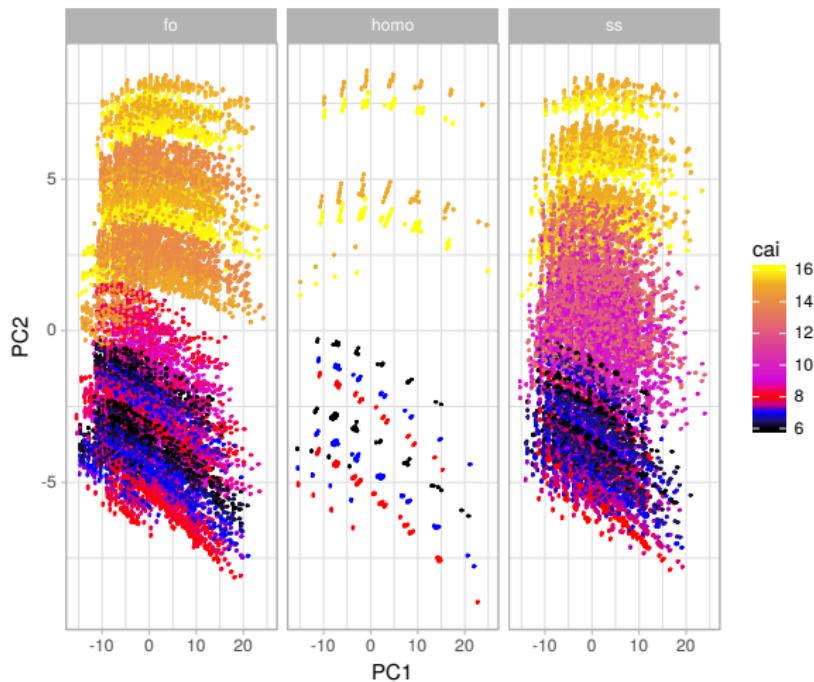
Properties of the sets

- Reduce space to facilitate sampling from non-homoleptics
- Example: strongly symmetric, monodentate ligand fields (163,620)
- Exclude all with charge smaller than -4, which results in 87,150 ligand fields (53 %).



Principal Component Analysis

The homoleptics (ho) span the strong symmetry (ss) and "5+1" (fo) set.



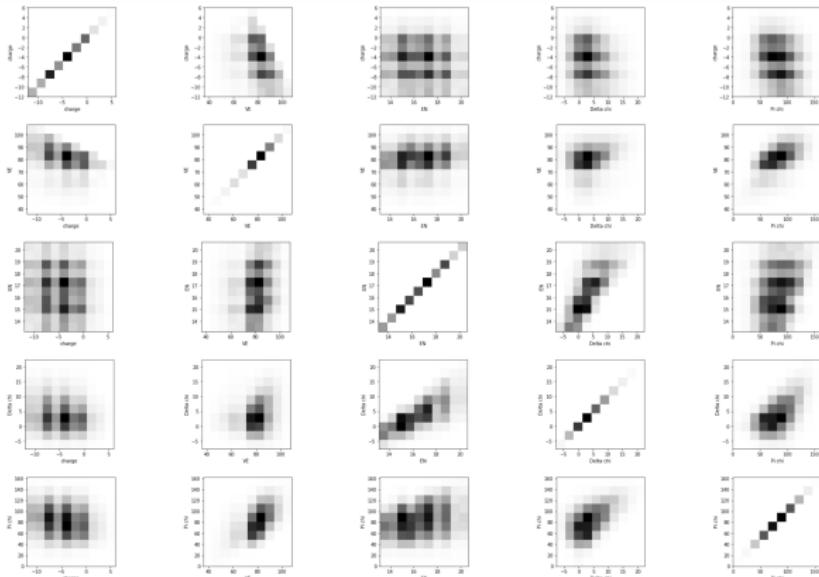
Footprint and Entropy calculation

We use five properties to characterize the ligand field and generate a five dimensional distribution:

- total charge
- total valence electrons
- electronegativity of the connecting atom
- $\chi_{\text{ax,eq}}^{\text{lc}} = \sum EN_{\text{CA}} \cdot EN_i$
- $\chi'_{\text{ax,eq}}^{\text{lc}} = \sum EN_{\text{CA}} - EN_i$

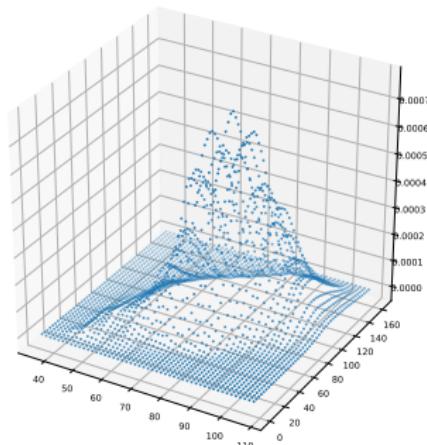
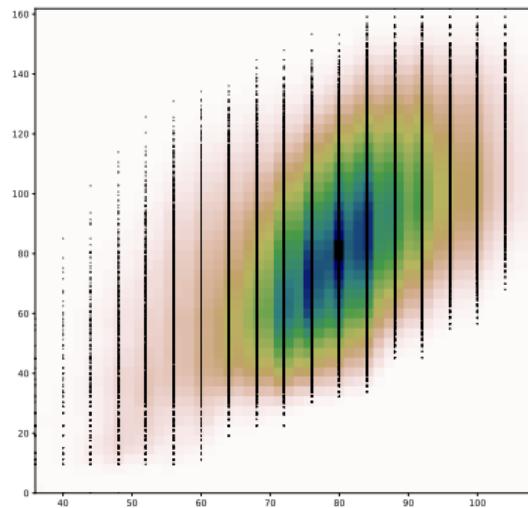
We then calculate the entropy, H_{KDE} , of the Kernel Density Estimated distribution.

Correlation analysis for strongly symmetric monodentates



Example of KDE slice

Dimensions $\frac{lc}{ax, eq} \chi_1$ vs. charge in H_{KDE} for strongly symmetric monodentates.

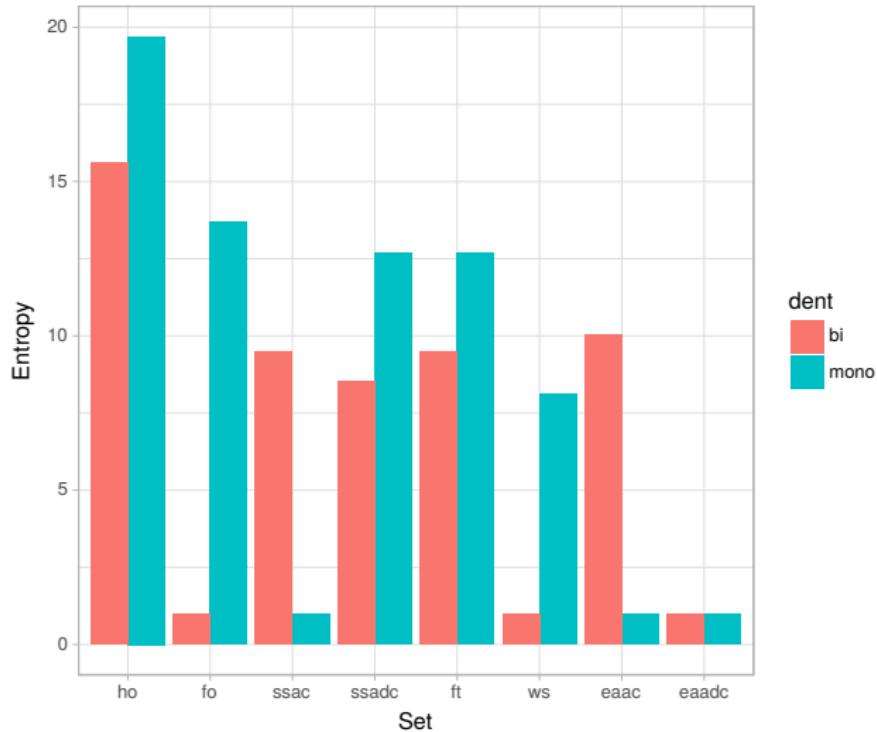


Monodentate Footprints

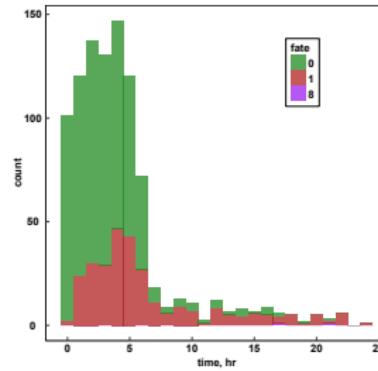
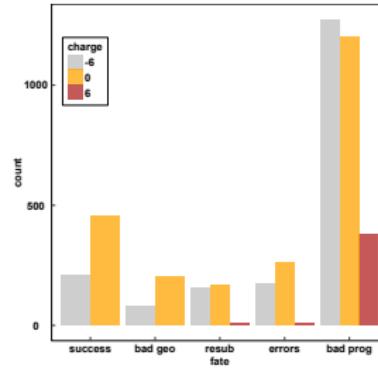
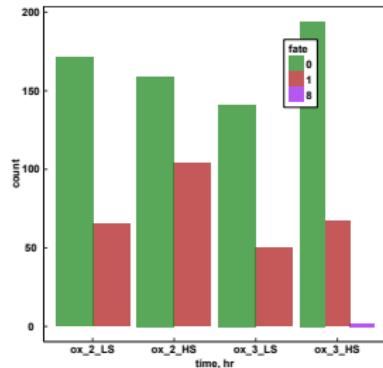
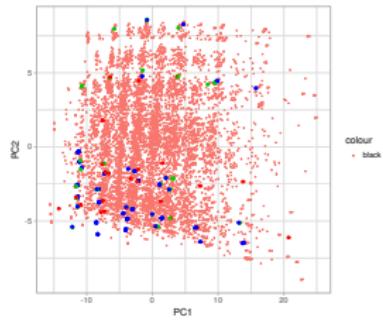
Table : Entropic footprint

Set	$H_{\text{KDE}}^{\text{monodent}}$	$H_{\text{KDE}}^{\text{bident}}$
Homoleptics	19.7	15.63
"5+1" symmetric	13.7	-
Strongly symmetric AC	-	9.47
Strongly symmetric ADC	12.70	5.53
"4+2" symmetric	12.70	9.47
Weakly symmetric	8.1	7.7
Equatorially asymmetric AC	-	10.04
Equatorially asymmetric ADC		

Entropy histogram



Actual calculations



- 0: $[NH_3]$, $[N]\#[N]$, $[C+]\#[O^-]$, $[C+]\#[NH^-]$, $[N]\#[CH]$
- 1: $[CH_+] = [CH_3^-]$, $[NH] = [O]$, $[CH_+] = [OH^-]$, $[CH_2^+] - [OH_2^-]$
- 8: $[OH_2^-] - [PH^+]$, $[P^+] = [OH^-]$, $[PH^+] - [OH_2^-]$, $[NH_2^-] = [CH^+]$