

# Meeting 1: Enumeration

Stefan Gugler

Massachusetts Institute of Technology

*sgugler@mit.edu*

March 16, 2018

# Mono-Heavy-Atomic Isoelectronic Ligand Distribution

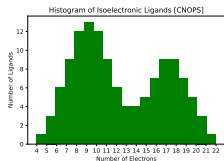


Figure: CNOPS: 15625 ligands

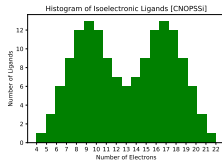


Figure: CNOPSSi: 22500 (?) ligands

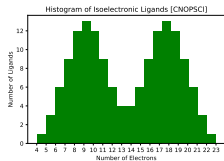


Figure: CNOPSCI: 22500 (?) ligands

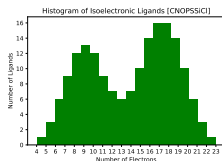


Figure: CNOPSSiCl: 30625 ligands

# Mono-Heavy-Atomic Iso-VE Ligand Distribution

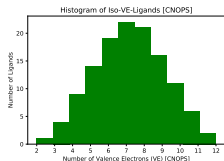


Figure: CNOPS: 15625 ligands

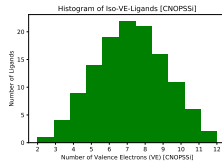


Figure: CNOPSSI: 22500 (?) ligands

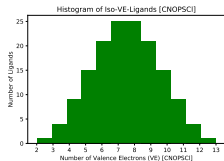


Figure: CNOPSCI: 22500 (?) ligands

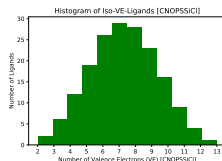


Figure: CNOPSSiCl: 30625 ligands

# Now we go to Di-Heavy-Atomic Ligands ...

- Exhaustive combinatorial combination from the Mono-Heavy-Atomic Ligands to get Di-Heavy-Ligands
- Over heavy atoms identities  $a_i \in \{\text{C, N, O, P, S, (Si, Cl)}\}$ , charges  $c_i \in \{-2, +2\}$ , number of H atoms  $h_i \in \{0, 4\}$ , with heavy atoms  $i \in 1, 2$ , where  $i = 1$  is the coordinating atom.
- Pruned by means of a health function,  $u$ , of ligand  $j$ , to encoding heuristics.

# Now we go to Di-Heavy-Atomic Ligands ...

- Only ligands with  $c_1 \leq 0 \wedge c_2 \leq 0$  are considered.

$$u_{\text{octet},i} = \begin{cases} 10 + 2 \cdot (8 - VE_i) & \text{if } 8 - VE_i < 0 \\ 10 - 1 \cdot (8 - VE_i) & \text{if } 8 - VE_i \geq 0 \end{cases} \quad (1)$$

$$u_{\text{charge}} = \begin{cases} 0 & \text{if } c_1 + c_2 > 0 \\ 3 & \text{if } 0 \geq c_1 + c_2 \geq -2 \\ 1 & \text{if } c_1 + c_2 = -3 \\ 0 & \text{if } c_1 + c_2 = -4 \end{cases} \quad (2)$$

$$u_{\text{VSEPR}} = 5 - \left| \underbrace{(VE_1 - 2 \cdot LP_1 + c_1 - 2 \cdot h_1)}_{\text{ready electrons}} - \underbrace{(VE_2 - 2 \cdot LP_2 + c_2 - 2 \cdot h_2)}_{\text{ready electrons}} \right| \quad (3)$$

## Now we go to Di-Heavy-Atomic Ligands ...

$$u_{\text{CA}} = \begin{cases} 1 & \text{if } h_1 = 4 \\ 2 & \text{if } h_1 = 3 \\ 3 & \text{if else} \end{cases} \quad (4)$$

$$u_{\text{shell}} = \begin{cases} 1 & \text{if } \neg(VE_1 + VE_2) \% 2 \\ 0 & \text{if else} \end{cases} \quad (5)$$

$$u_{\text{total}} = u_{\text{shell}} \cdot \left( \frac{1}{2} (u_{\text{octet},1} + u_{\text{octet},i}) + u_{\text{charge}} + u_{\text{VSEPR}} + u_{\text{CA}} \right) \quad (6)$$

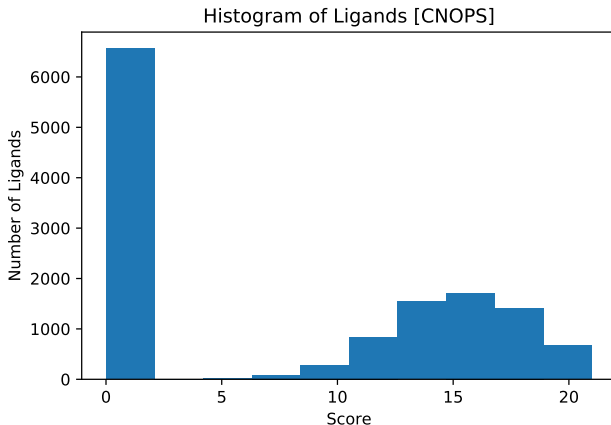
where  $VE_i$  denotes the number of valence electrons,  $LP_i$  the number of lone pairs.

# Distribution of the Score

Comparison of edge cases. Mayer B.O. with multiwfn.

1	2	Mayer B.O.	score	comment
CHHHH++	CHHHH++	$<0.05$	12	rather high
CHHHH-	CHHHH-	0.928	-	$c_{tot} > 0$
CHHH	NH	1.308	0	open shell
CH4++	-	0.577	-	Mono-Heavy-Atom
C-	O+	-	16	dummy

# Distribution of the Score



**Figure:** A histogram describing the score distribution. There are 30 ligands with score 21 and 180 ligands with score 20. CO is has a score of 16. There are 2917 ligands at least as good as CO.



```
[['[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10, '[CHHH-]', 10, 8, 0, -1, 3, 0, 1, 10], 21.0]
['[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10, '[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10], 21.0]
['[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10, '[OH-]', 10, 8, 2, -1, 1, 0, 1, 10], 21.0]
['[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10, '[PHH-]', 18, 8, 1, -1, 2, 0, 1, 10], 21.0]
['[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10, '[SH-]', 18, 8, 2, -1, 1, 0, 1, 10], 21.0]
['[OH-]', 10, 8, 2, -1, 1, 0, 1, 10, '[CHHH-]', 10, 8, 0, -1, 3, 0, 1, 10], 21.0]
['[OHH]', 10, 8, 2, 0, 2, 0, 1, 10, '[CHHHH]', 10, 8, 0, 0, 4, 0, 1, 10], 21.0]
['[OH-]', 10, 8, 2, -1, 1, 0, 1, 10, '[NHH-]', 10, 8, 1, -1, 2, 0, 1, 10], 21.0]
['[OHH]', 10, 8, 2, 0, 2, 0, 1, 10, '[NHHH]', 10, 8, 1, 0, 3, 0, 1, 10], 21.0]
['[OH-]', 10, 8, 2, -1, 1, 0, 1, 10, '[OH-]', 10, 8, 2, -1, 1, 0, 1, 10], 21.0]
['[OHH]', 10, 8, 2, 0, 2, 0, 1, 10, '[OHH]', 10, 8, 2, 0, 2, 0, 1, 10], 21.0]
```