

## Electronic Support Information

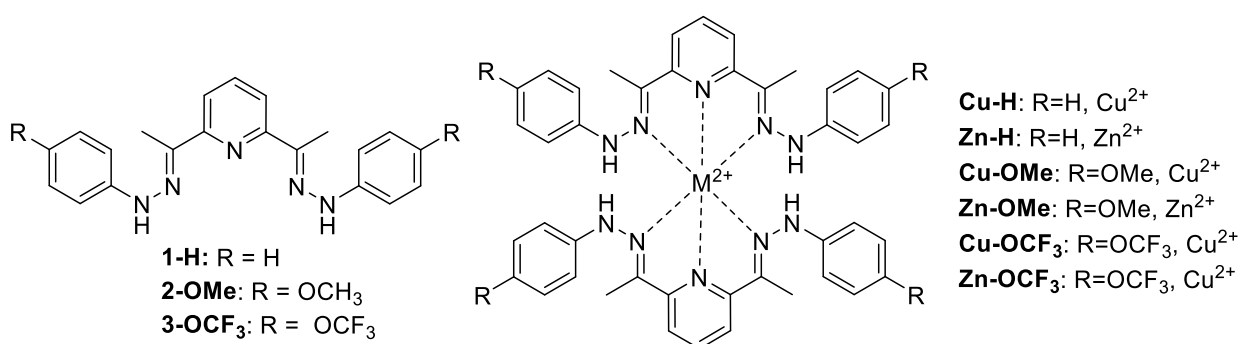
### Multipurpose made colorimetric materials for amines, pH change and metal ion detection

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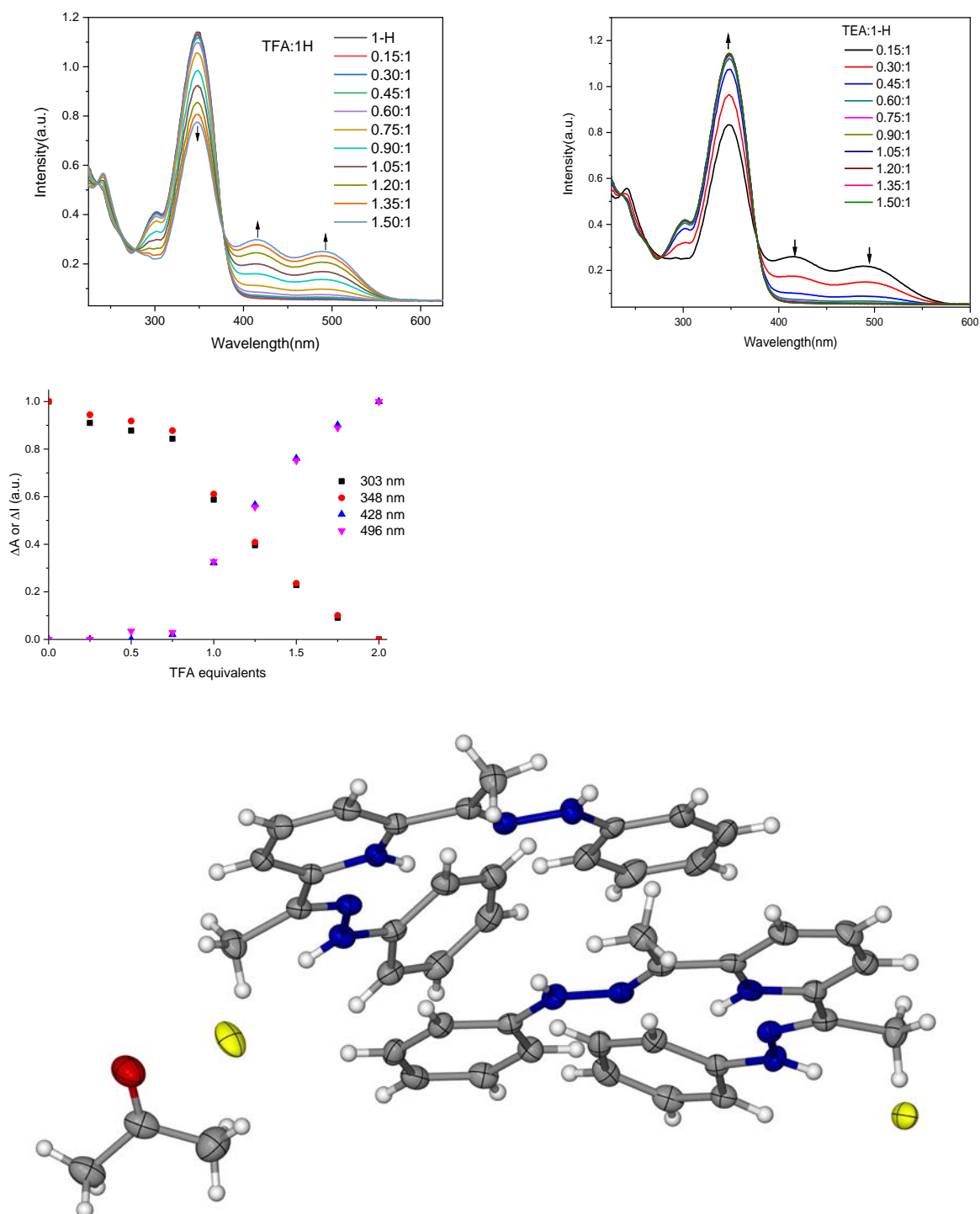
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#### CONTENT

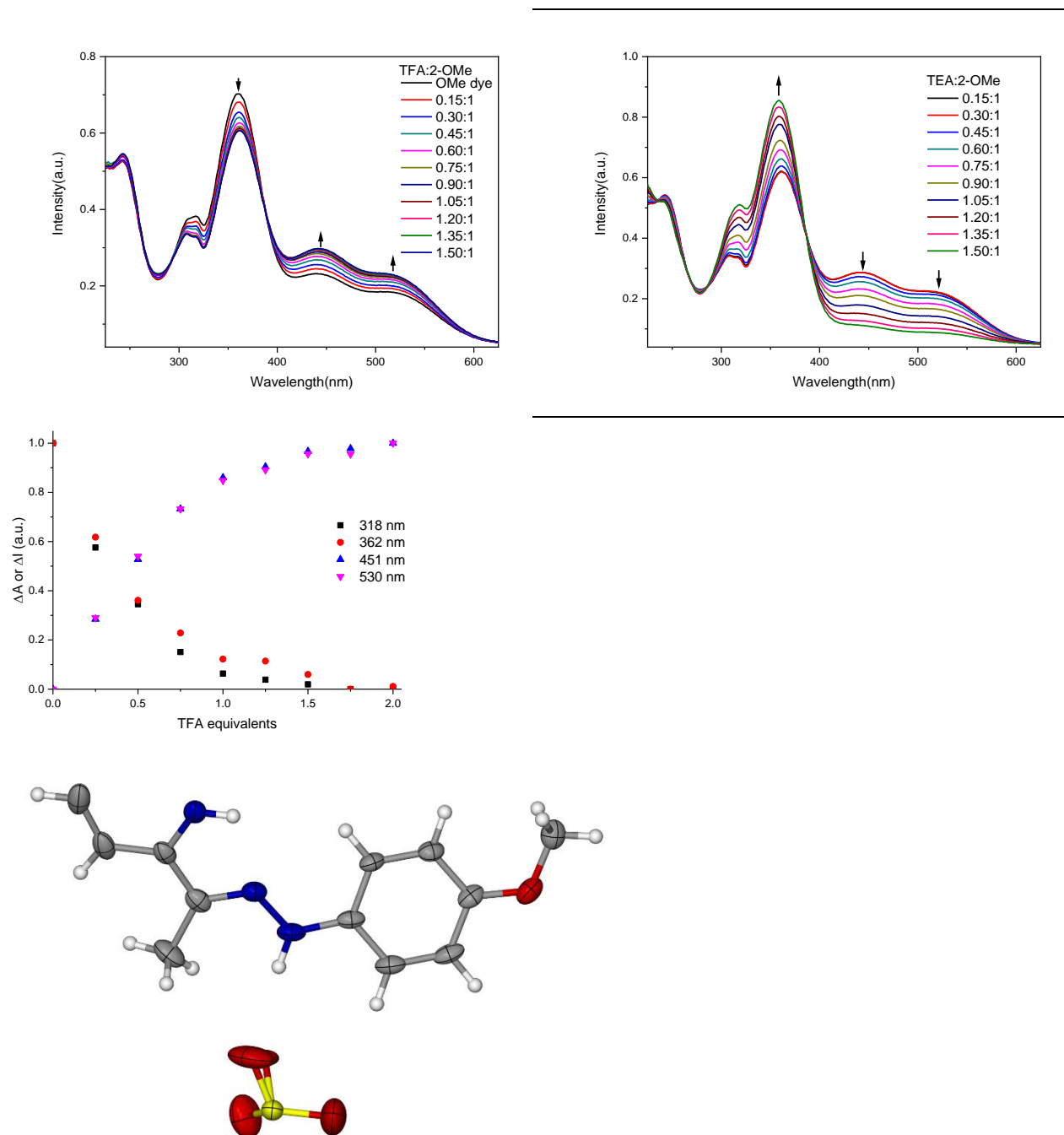
- Chemical structures of the free ligands and their metal complexes (Fig. S1)
- 1-H: X-ray structure, Spectrophotometric titrations with TFA and TEA (Fig. S2)
- 2-OMe: X-ray structure, Spectrophotometric titrations with TFA and TEA (Fig. S3)
- 3-OCF<sub>3</sub>: X-ray structure, Spectrophotometric titrations with TFA and TEA (Fig. S4)
- 1-H: Spectrophotometric titrations with Zn<sup>2+</sup> under various concentrations (Fig. S5)
- 2-OMe: Spectrophotometric titrations with Zn<sup>2+</sup> up to 2.25 eq. (Fig. S6)
- 3-OCF<sub>3</sub>: Spectrophotometric titrations with Zn<sup>2+</sup> under various concentrations (Fig. S7)
- Cu-H: Asymmetric X-ray structure (Fig. S8)
- Cu-OMe: Asymmetric X-ray structure (Fig. S9)
- Cu-OCF<sub>3</sub>: Asymmetric X-ray structure (Fig. S10)
- X-Ray structure of Zn-H. (Fig. S11)
- X-Ray structure of Zn-OCF<sub>3</sub>. (Fig. S12)
- Computational methods
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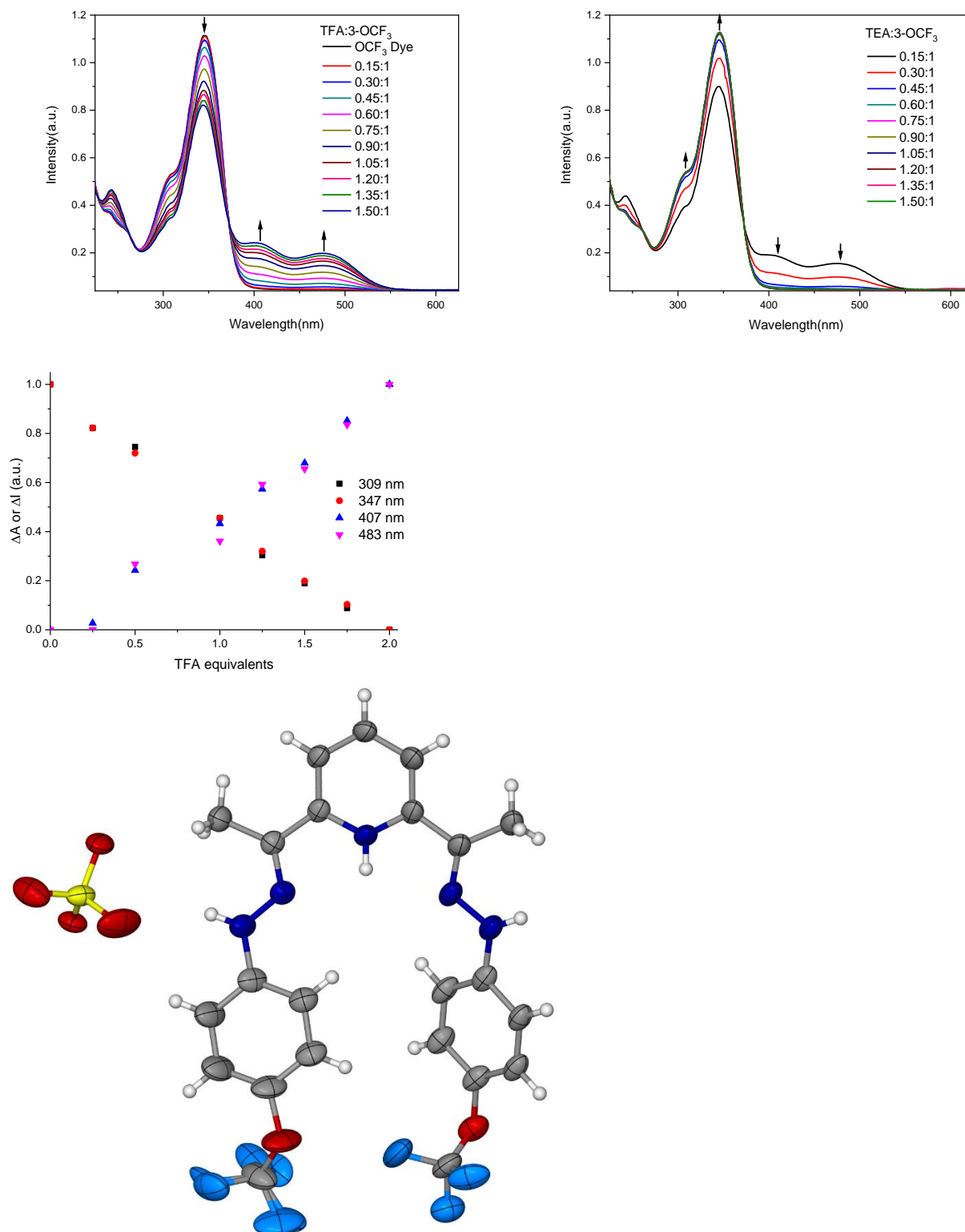
**Fig. S1** Chemical structures of the free dyes and their metal complexes



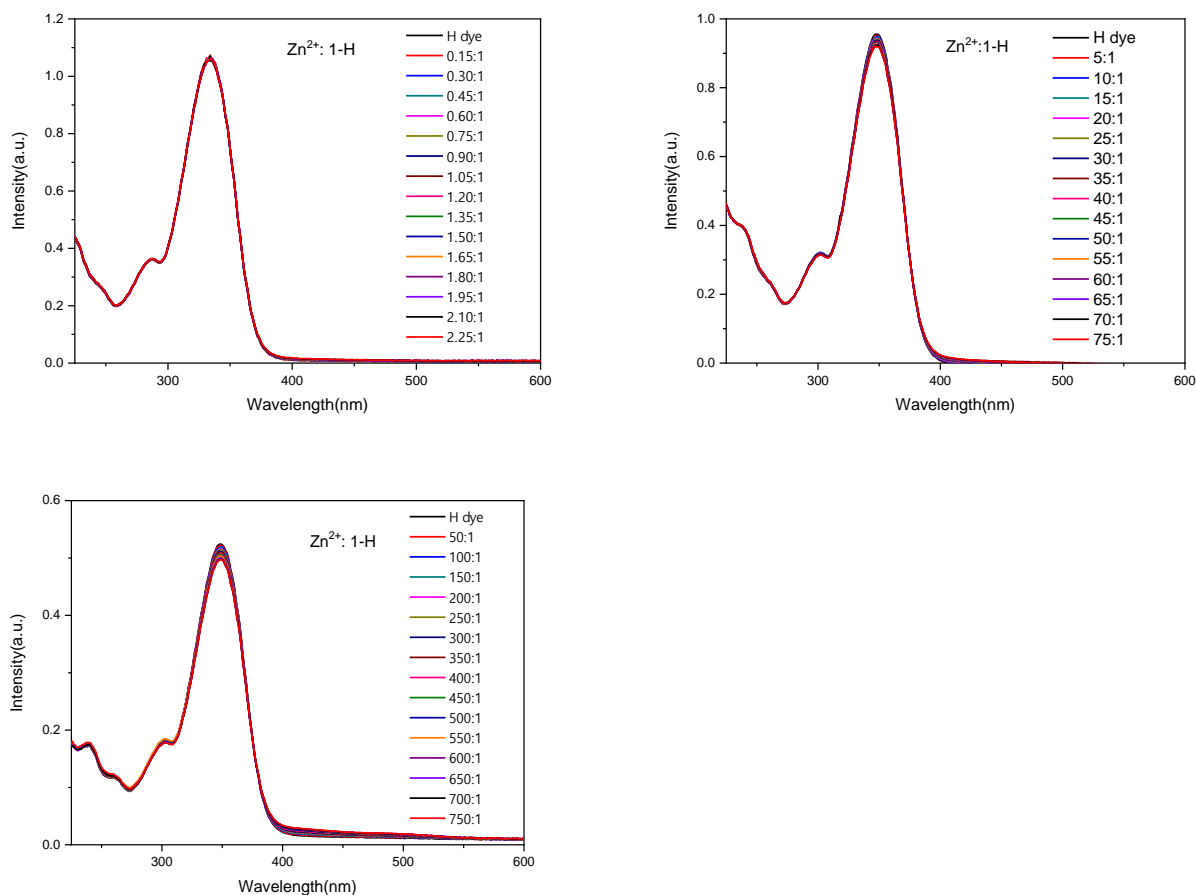
**Figure S2.** Spectrophotometric titration of compound **1-H** ( $2.3 \times 10^{-5} \text{M}$ ): (**top-left**) with TFA in EtOH; (**top-right**) with TEA in EtOH; (bottom-left) absorption differences at 303 nm, 348 nm, 428 nm and 496 nm; (bottom-right) Asymmetric X-ray crystal structure of **[1-H]H<sup>+</sup>**.



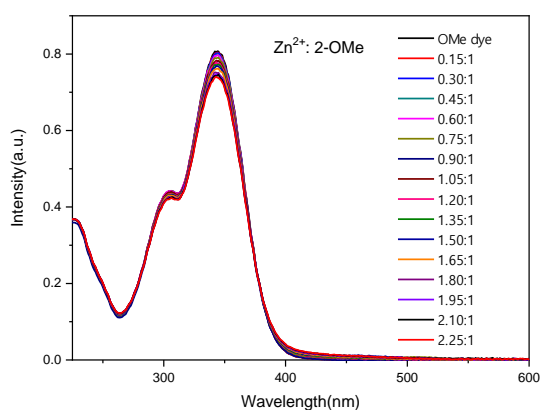
**Figure S3.** Spectrophotometric titration of compound **2-OMe** ( $2.3 \times 10^{-5}$  M): **(top-left)** with TFA in EtOH; **(top-right)** with TEA in EtOH; **(bottom-left)** absorption differences at 303 nm, 348 nm, 428 nm and 496 nm; **(bottom-right)** Asymmetric X-ray crystal structure of **[2-OMe]H<sup>+</sup>**.



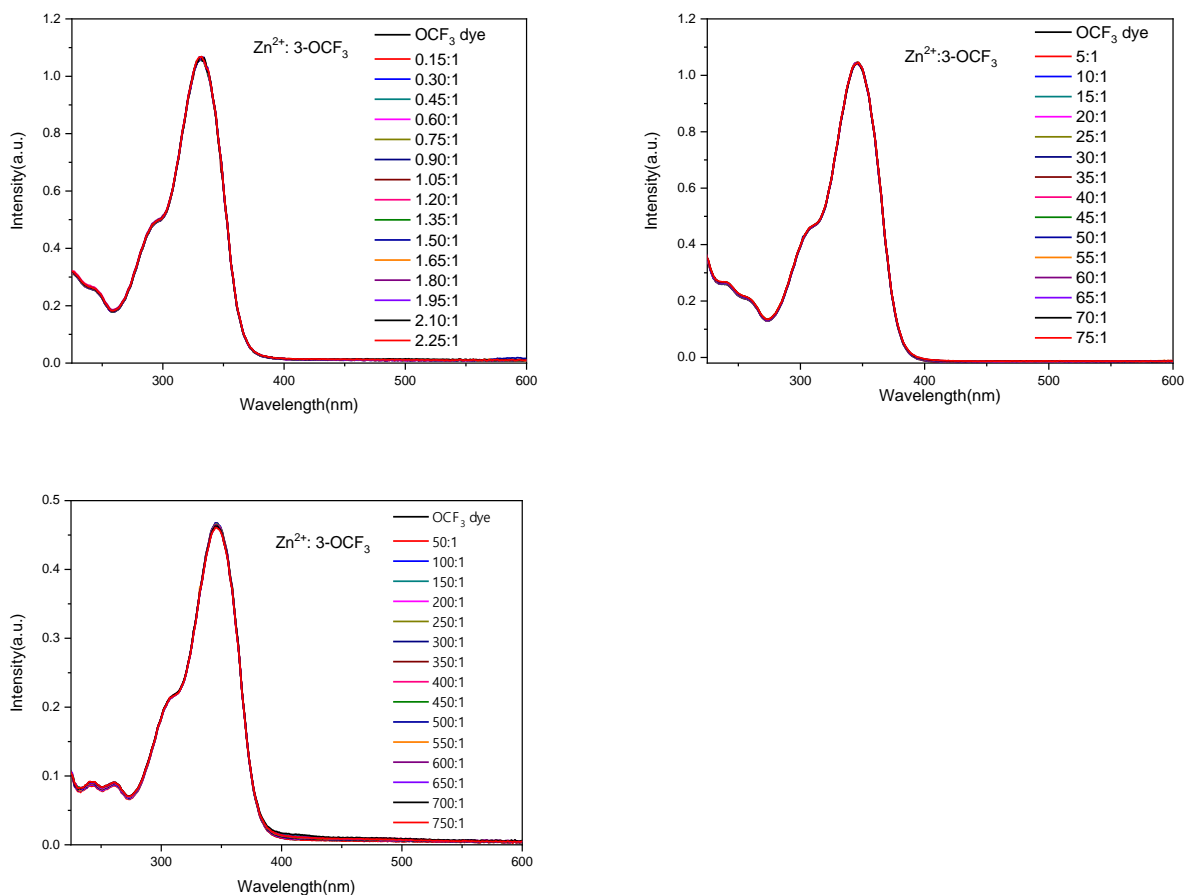
**Figure S4.** Spectrophotometric titration of compound **3-OCF<sub>3</sub>** ( $2.3 \times 10^{-5} \text{M}$ ): **(top-left)** with TFA in EtOH; **(top-right)** with TEA in EtOH; **(bottom-left)** absorption differences at 303 nm, 348 nm, 428nm and 496nm); **(bottom-right)** X-ray crystal structure of **[3-OCF<sub>3</sub>]**.



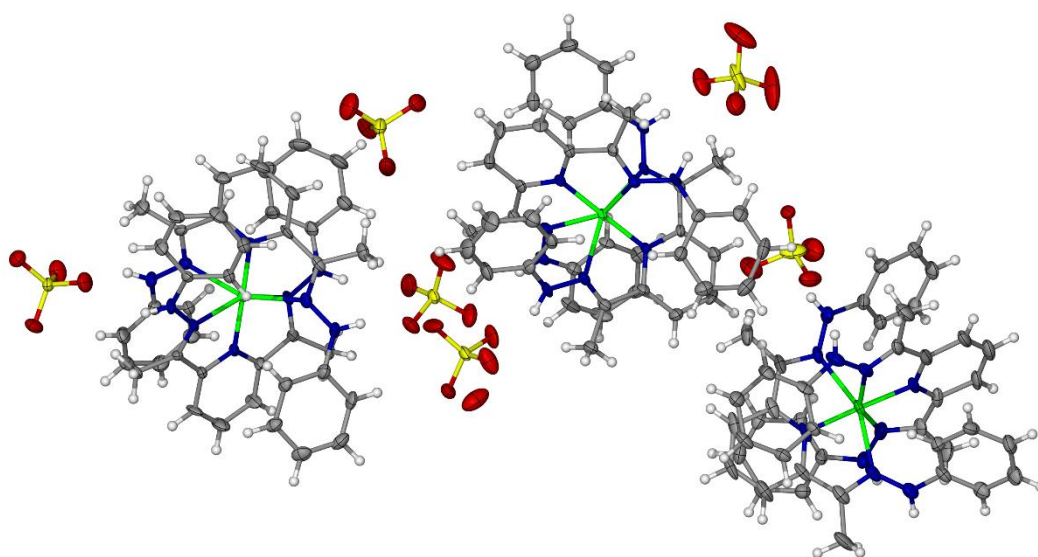
**Figure S5.** Spectrophotometric titration of compound **1-H** ( $2.3 \times 10^{-5}$  M) with  $\text{Zn}^{2+}$  ions: **(top-left)** a low concentration up to 2.25 eq of  $\text{Zn}^{2+}$ ; **(top-right)** a medium concentration up to 75 eq of  $\text{Zn}^{2+}$ ; **(bottom)** a low concentration up to 750 eq of  $\text{Zn}^{2+}$ .



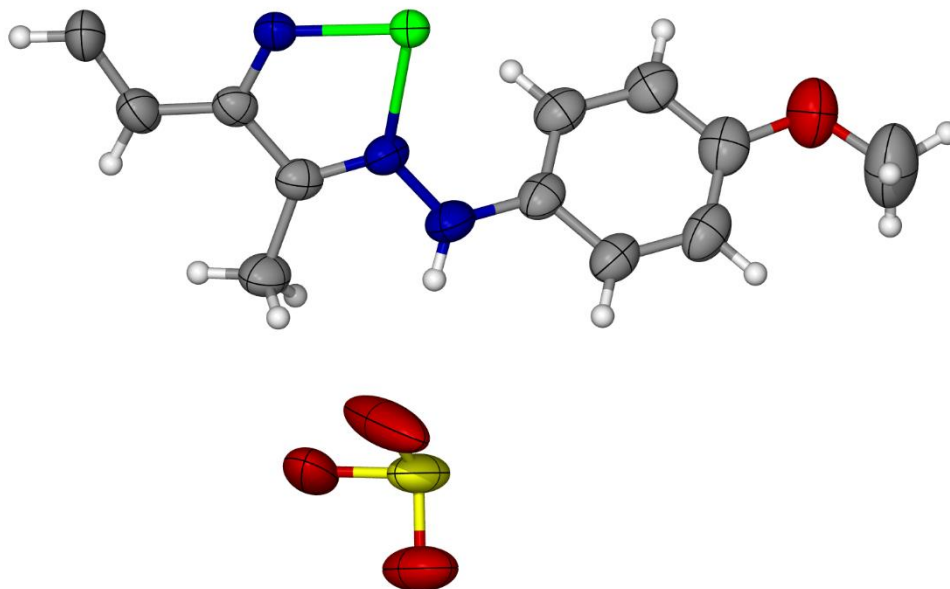
**Figure S6.** Spectrophotometric titration of compound **2-OMe** ( $2.3 \times 10^{-5}$  M) with  $\text{Zn}^{2+}$  ions: **(top-left)** a low concentration up to 2.25 eq of  $\text{Zn}^{2+}$ .



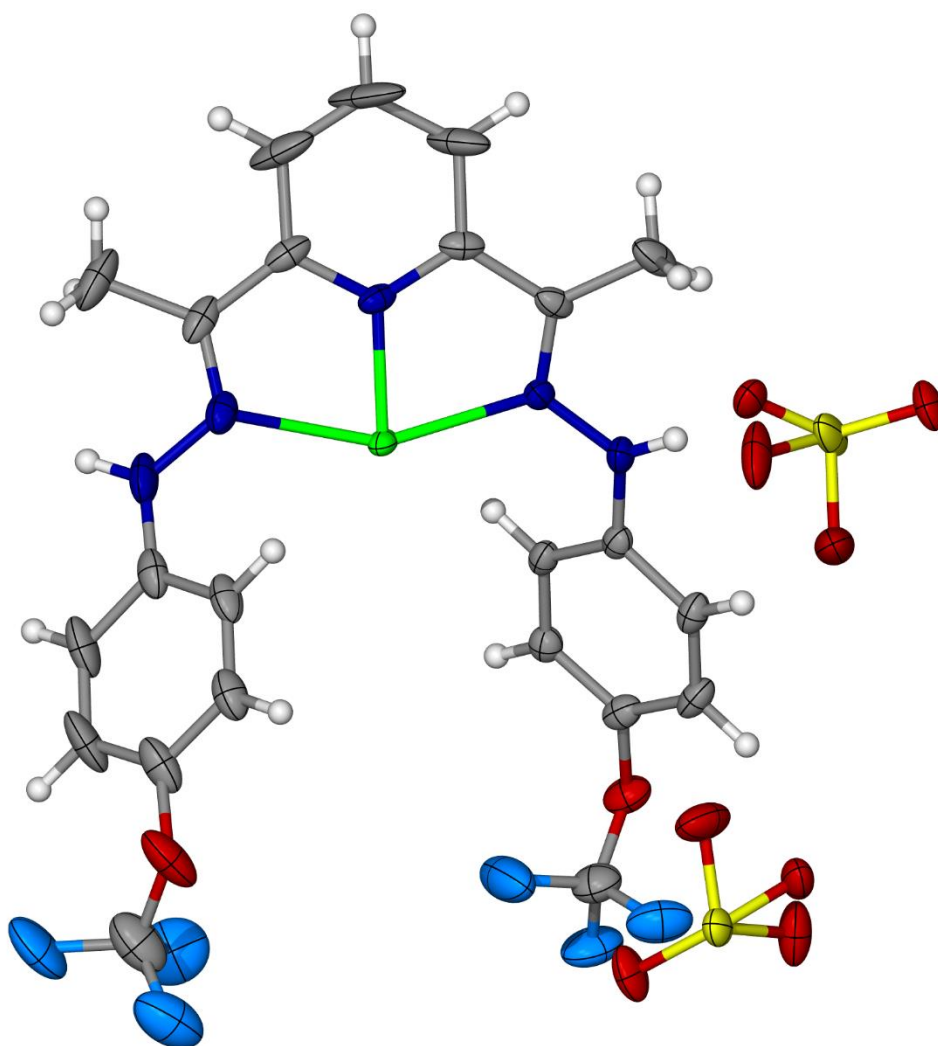
**Figure S7.** Spectrophotometric titration of compound **2-OMe** ( $2.3 \times 10^{-5} \text{M}$ ) with  $\text{Zn}^{2+}$  ions: **(top-left)** a low concentration up to 2.25 eq of  $\text{Zn}^{2+}$ ; **(top-right)** a medium concentration up to 75 eq of  $\text{Zn}^{2+}$ ; **(bottom)** a low concentration up to 750 eq of  $\text{Zn}^{2+}$ .



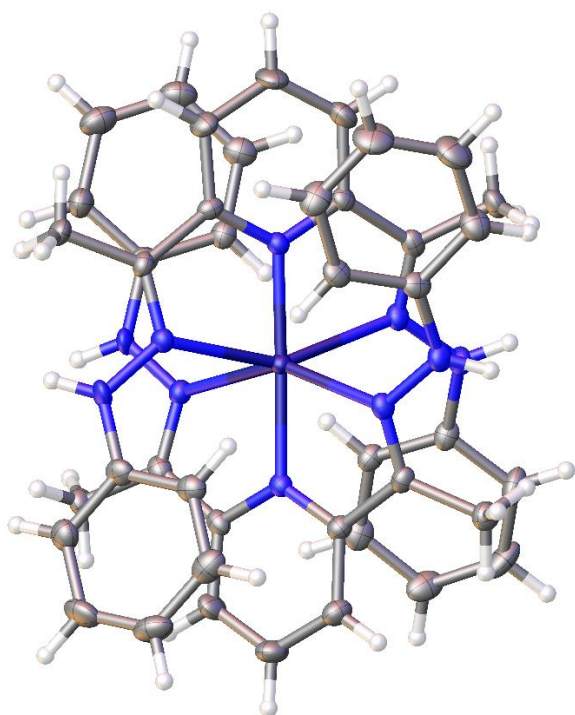
**Figure S8.** Cu-H: Asymmetric X-ray structure.



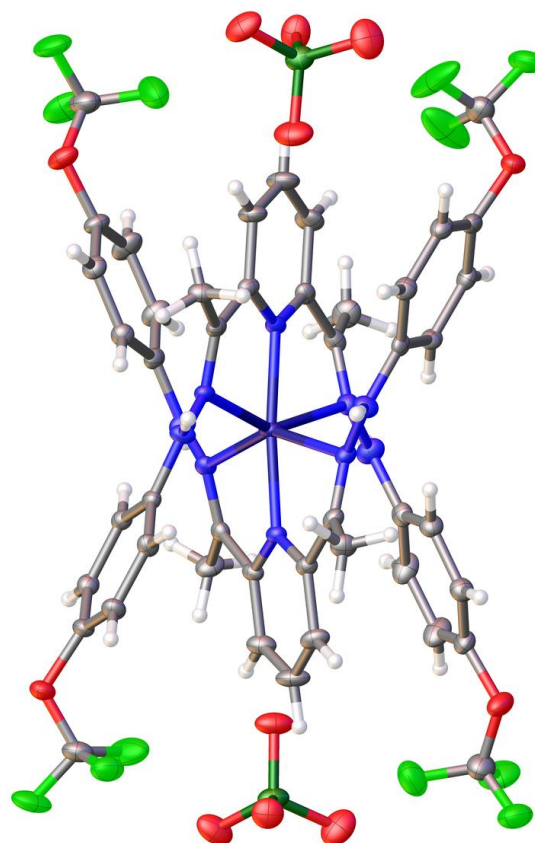
**Figure S9.** Cu-OMe: Asymmetric X-ray structure.



**Figure S10.** Cu-OCF<sub>3</sub>: Asymmetric X-ray structure.



**Figure S11.** X-ray structure of Zn-H.



**Figure S12.** X-ray structure of Zn-OCF<sub>3</sub>.

## Computational Calculations

### 3.1 Methods

The anions were removed from the single crystal structures and then the complexes were optimized in their 2+ state in the Orca program<sup>1</sup> (version 4.1.0) using the hybrid generalized gradient approximation (GGA) Becke three-parameter Lee-Yang Parr (B3LYP) functional,<sup>2</sup> the Ahlrich's triple zeta basis set<sup>3</sup> with a polarization function Def2-TZVP, and Grimme's third generation dispersion correction with Becke Johnson damping<sup>4</sup> (D3BJ); the integration grid of 2 used throughout. Kollmar's variant of the direct inversion in iterative subspace KDIIS,<sup>5</sup> was applied. To further speed up the DFT optimizations, the Coulomb integral and numerical chain-of-sphere integration for the HF exchange (RIJCOSX) method<sup>6</sup> was applied with the Def2/J auxiliary basis. All structures were optimized in

<sup>1</sup> Neese, F. (2012) The ORCA program system, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2, 73-78, <https://onlinelibrary.wiley.com/doi/full/10.1002/wcms.81>

<sup>2</sup> Becke, A. D. Density functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* 1993, 98 (7), 5648-5652, <https://aip.scitation.org/doi/10.1063/1.464913>

<sup>3</sup> F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, 7, 3297-3305, <https://pubs.rsc.org/en/content/articlelanding/cp/2005/b508541a#!divAbstract>

<sup>4</sup> S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.*, 2011, 32, 1456-1465, <https://onlinelibrary.wiley.com/doi/full/10.1002/jcc.21759>

<sup>5</sup> C. Kollmar, *J. Chem. Phys.*, 1996, 105, 8204, <https://aip.scitation.org/doi/abs/10.1063/1.472674>

<sup>6</sup> F. Neese, *J. Comp. Chem.*, 2003, 24, 1740-1747, <https://onlinelibrary.wiley.com/doi/full/10.1002/jcc.10318>; R. Izsak, F. Neese, *J. Chem. Phys.*, 2011, 135, 144105, <https://aip.scitation.org/doi/full/10.1063/1.3646921>



vacuum and then subsequently in an ethanol continuum, using Truhlar's SMD<sup>7</sup> variant of the Conductor like polarizable continuum model<sup>8</sup> (CPCM) as implemented in Orca. The orbital densities of the organic ligands were visualized according to their Frontier Molecular Orbitals (FMOs) with isosurface value  $\pm 0.03$ . The spin density difference orbitals for the copper complexes were computed at the same level of theory and visualized at the isosurface value  $\pm 0.04$ ; the Zn complexes are closed shell so no spin difference. The computed UV-Vis absorption spectra were calculated at the B3LYP/Def2-SVP level in the ethanol SMD. For the ligands, the Tamm Dancoff Approximation (TDA) was used specifying 50 roots, and for the metal complexes the simplified TDA (sTDA) scheme by Grimme<sup>9</sup> was used, using an Ethresh of 6 eV; in all cases, KDIIS, RIJCOSX, and D3BJ were applied. Due to a broad potential surface, an optimized minimum could not be found for either the Cu-OCF<sub>3</sub> or Zn-OCF<sub>3</sub> complexes in the ethanol SMD continuum, so instead the absorption spectra were computed with the continuum applied to the vacuum optimized coordinates, which should be a reasonable approximation to the continuum optimized coordinates. In Orca, the effective core potentials (ECPs) are applied only if the input has elements in the Periodic Table that either includes, or are heavier than Kr, so the C/O/N/H/Cu/Zn elements involved in the calculations here are all-electron. All spectra and surfaces were visualized in ChemCraft<sup>10</sup> (version b574b). The electrostatic potential maps were computed with B3LYP, a Slater-type triple zeta and polarization function basis set (TZP) and D3BJ in the Amsterdam Density Functional program<sup>11</sup> (ADF, version 2018.104), using Truhlar's solvent continuum model<sup>12</sup> SM12 as implemented in ADF<sup>13</sup>. The Becke grid quality was set to *good*<sup>14</sup> and large frozen cores were used to reduce the computational cost in ADF.

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<sup>7</sup> A. Marenich, C. Cramer, D. Truhlar, *J. Phys. Chem. B*, 2009, 113, 6378-6396, <https://pubs.acs.org/doi/abs/10.1021/jp810292n>

<sup>8</sup> J. Pascual-Ahuir, E. Silla, *J. Comput. Chem.*, 1990, 11, 1047-1060, <https://onlinelibrary.wiley.com/doi/abs/10.1002/jcc.540110907>

<sup>9</sup> S. Grimme, 2013, *J. Chem. Phys.* 138, 244104, <https://aip.scitation.org/doi/full/10.1063/1.4811331>

<sup>10</sup> <https://www.chemcraftprog.com>

<sup>11</sup> te Velde, G.; Bickelhaupt, F. M.; Baerends, E. J.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. Chemistry with ADF. *J. Comput. Chem.* 2001, 22 931-967, <https://doi.org/10.1002/jcc.1056>

<sup>12</sup> A.V. Marenich, C.J. Cramer, and D.G. Truhlar, *J. Chem. Theory Comput.*, 2013 9, 609-620, <https://doi.org/10.1021/ct300900e>

<sup>13</sup> C. Peeples and G. Schreckenbach, *J. Chem. Theory Comput.* 2016, 12, 4033-4041, <https://doi.org/10.1021/acs.jctc.6b00410>

<sup>14</sup> M. Franchini, P.H.T. Philipsen, L. Visscher, *J. Comp. Chem.* 2013, 34, 1818-1827, <https://doi.org/10.1002/jcc.23323>

## 3.3 Frontier Molecular Orbitals and Spin Density Plots

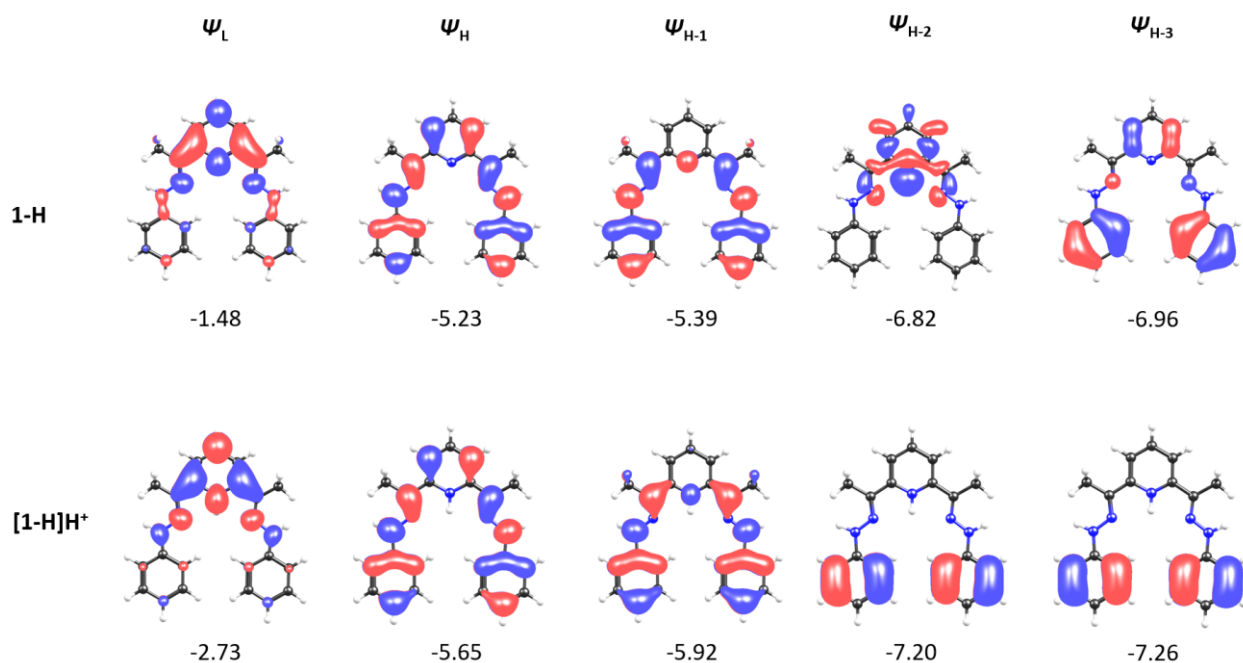


Figure S13. Frontier molecular orbitals (FMOs) and their energies (eV) for the 1-H and [1-H]H<sup>+</sup> ligands.

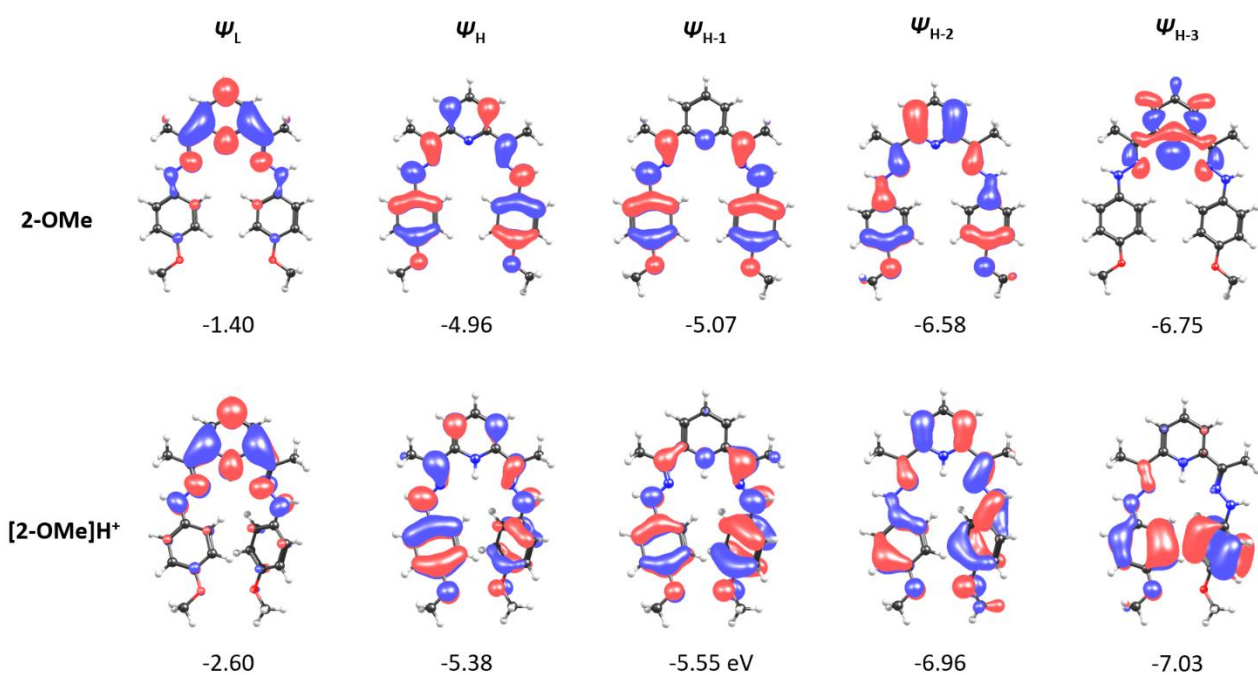


Figure S14. Frontier molecular orbitals (FMOs) and their energies (eV) for the 2-OMe and [2-OMe]H<sup>+</sup> ligands.

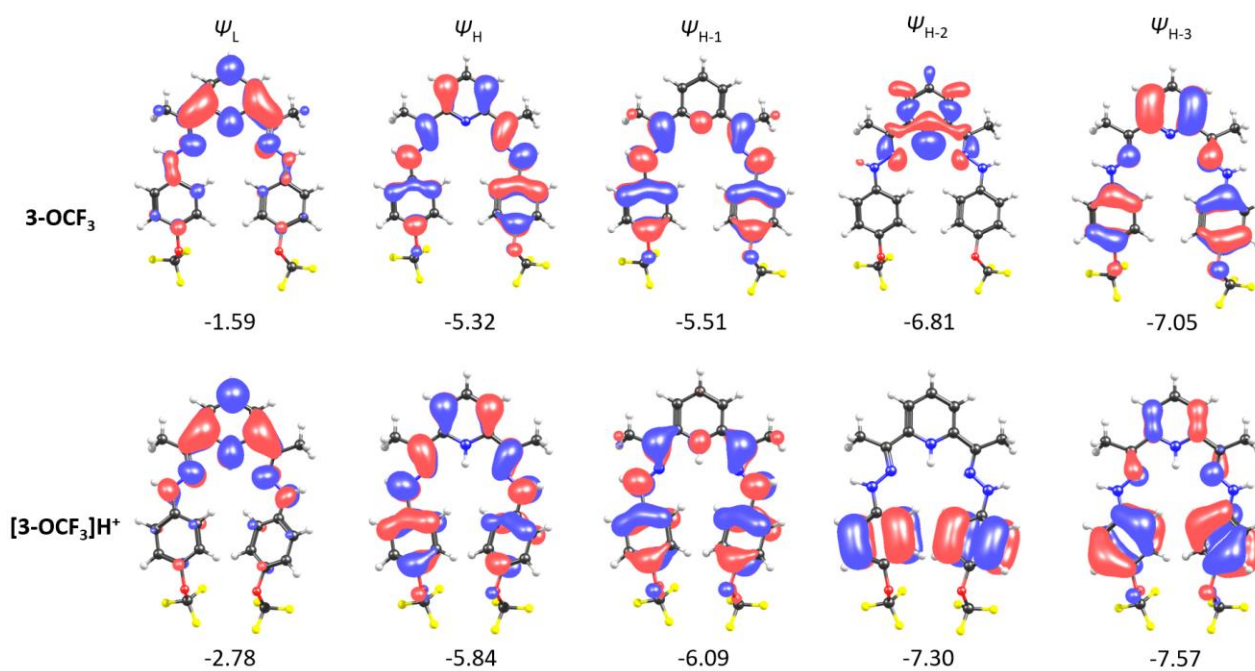


Figure S15. Frontier molecular orbitals (FMOs) and their energies (eV) for the 3-OCF<sub>3</sub> and [3-OCF<sub>3</sub>]<sup>+</sup>H<sup>+</sup> ligands.

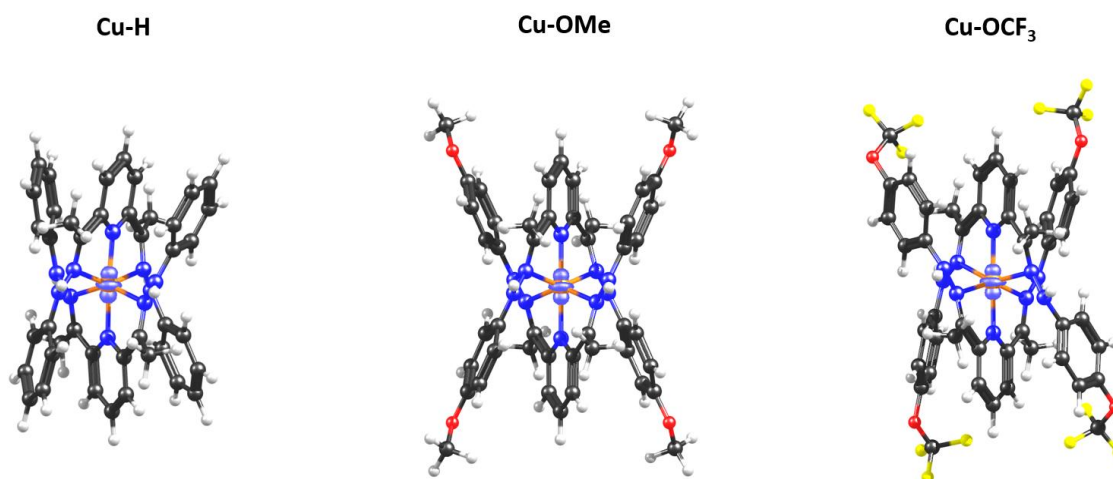


Figure S16. Spin density difference orbitals (coloured blue) for the copper complexes.

### 3.4 Bond Orders

The results are presented in the **Figure SX**, and data summarized in the **Tables SX**.

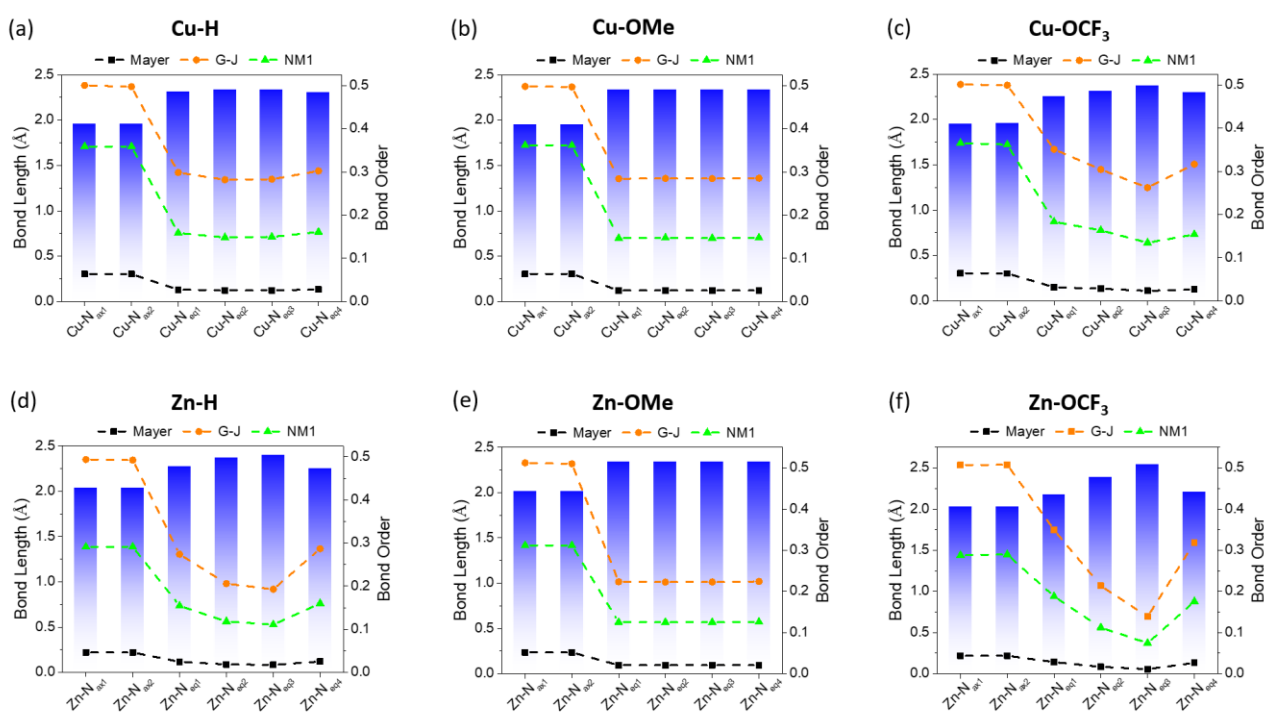


Figure S17. Bond lengths (Å) and bond orders for the metal-N interactions of all complexes; ax and eq represent axial and equatorial, respectively. For each panel, the bar graph is for the left axis and the dashed lines are for the right axis, according to the three formalisms of Mayer, Gopinathan–Jug (G-J) and first Nalewajski–Mrozek (N-M1).

Table S1. Bond lengths and bond orders with the schemes Mayer, (G-J) and (N-M1) for the **Cu-H** complex optimized in EtOH SMD continuum.

Entry	Bond Length (Å)	Mayer	G-J	N-M1
Cu-N <sub>ax1</sub>	1.958	0.500	0.302	0.359
Cu-N <sub>ax2</sub>	1.958	0.497	0.302	0.359
Cu-N <sub>eq1</sub>	2.338	0.282	0.123	0.148
Cu-N <sub>eq2</sub>	2.312	0.299	0.131	0.159
Cu-N <sub>eq3</sub>	2.305	0.302	0.133	0.161
Cu-N <sub>eq4</sub>	2.337	0.283	0.124	0.150

Table S2. Bond lengths and bond orders with the schemes Mayer, (G-J) and (N-M1) for the **Cu-OMe** complex optimized in EtOH SMD continuum.

Entry	Bond Length (Å)	Mayer	G-J	N-M1
Cu-N <sub>ax1</sub>	1.955	0.498	0.306	0.362
Cu-N <sub>ax2</sub>	1.955	0.497	0.306	0.362
Cu-N <sub>eq1</sub>	2.341	0.284	0.122	0.147
Cu-N <sub>eq2</sub>	2.339	0.285	0.123	0.148
Cu-N <sub>eq3</sub>	2.341	0.285	0.122	0.147
Cu-N <sub>eq4</sub>	2.339	0.286	0.123	0.148

Table S3. Bond lengths and bond orders with the schemes Mayer, (G-J) and (N-M1) for the **Cu-OCF<sub>3</sub>** complex optimized in vacuum and computed with a single point EtOH SMD continuum.

Entry	Bond Length (Å)	Mayer	G-J	N-M1
Cu-N <sub>ax1</sub>	1.950	0.501	0.305	0.365
Cu-N <sub>ax2</sub>	1.957	0.499	0.302	0.362
Cu-N <sub>eq1</sub>	2.258	0.351	0.151	0.183
Cu-N <sub>eq2</sub>	2.376	0.262	0.110	0.135
Cu-N <sub>eq3</sub>	2.317	0.304	0.134	0.163
Cu-N <sub>eq4</sub>	2.299	0.316	0.126	0.154

Table S4. Bond lengths and bond orders with the schemes Mayer, (G-J) and (N-M1) for the **Zn-H** complex optimized in EtOH SMD continuum.

Entry	Bond Length (Å)	Mayer	G-J	N-M1
Zn-N <sub>ax1</sub>	2.038	0.494	0.220	0.291
Zn-N <sub>ax2</sub>	2.040	0.492	0.220	0.291
Zn-N <sub>eq1</sub>	2.274	0.274	0.116	0.154
Zn-N <sub>eq2</sub>	2.376	0.206	0.089	0.118
Zn-N <sub>eq3</sub>	2.403	0.193	0.083	0.111
Zn-N <sub>eq4</sub>	2.256	0.287	0.121	0.160

Table S5. Bond lengths and bond orders with the schemes Mayer, (G-J) and (N-M1) for the **Zn-OMe** complex optimized in EtOH SMD continuum.

Entry	Bond Length (Å)	Mayer	G-J	N-M1
Zn-N <sub>ax1</sub>	2.017	0.512	0.236	0.312
Zn-N <sub>ax2</sub>	2.017	0.510	0.236	0.312
Zn-N <sub>eq1</sub>	2.345	0.223	0.094	0.125
Zn-N <sub>eq2</sub>	2.346	0.223	0.094	0.125
Zn-N <sub>eq3</sub>	2.346	0.223	0.094	0.125
Zn-N <sub>eq4</sub>	2.343	0.224	0.095	0.126

Table S6. Bond lengths and bond orders with the schemes Mayer, (G-J) and (N-M1) for the **Zn-OCF<sub>3</sub>** complex optimized in vacuum, and computed with a single point EtOH SMD continuum.

Entry	Bond Length (Å)	Mayer	G-J	N-M1
Zn-N <sub>ax1</sub>	2.031	0.507	0.217	0.288
Zn-N <sub>ax2</sub>	2.034	0.508	0.218	0.290
Zn-N <sub>eq1</sub>	2.391	0.214	0.084	0.112
Zn-N <sub>eq2</sub>	2.179	0.349	0.141	0.188
Zn-N <sub>eq3</sub>	2.209	0.319	0.132	0.175
Zn-N <sub>eq4</sub>	2.546	0.139	0.055	0.074

## 3.5 Electrostatic Potential Energy Maps

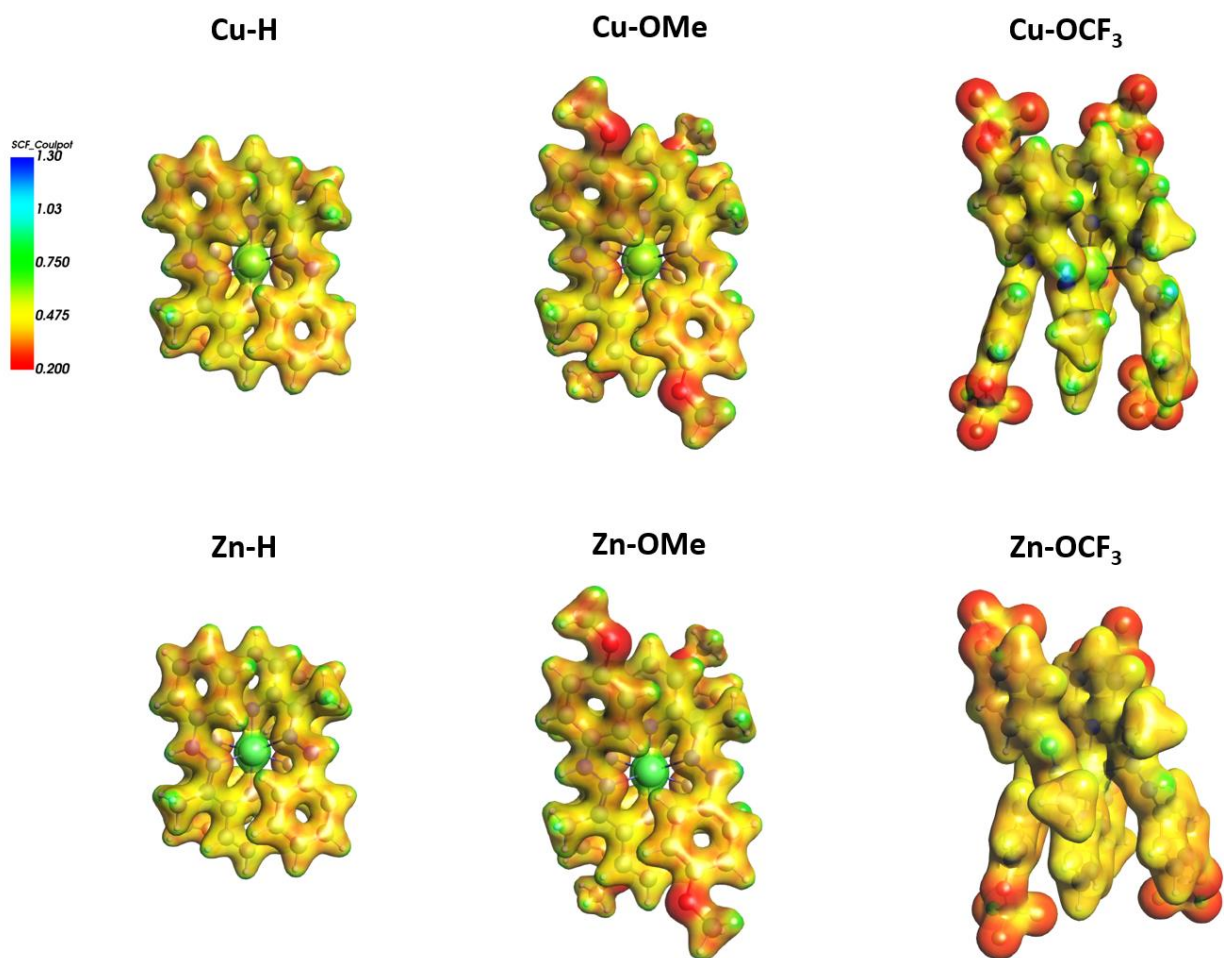


Figure S18. Electrostatic potential energy maps for the metal complexes.



### 3.6 Absorption Calculations

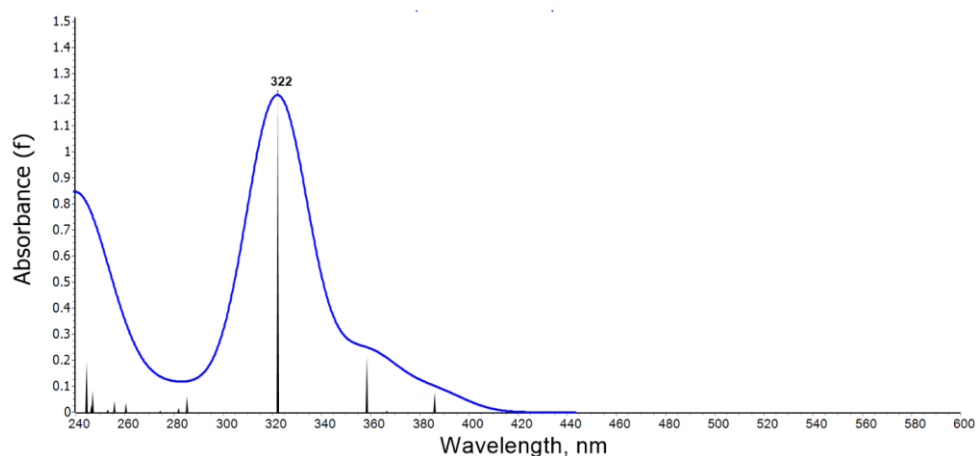


Figure S19. Calculated UV-Vis absorption spectrum for the **1-H** ligand in an ethanol SMD continuum.

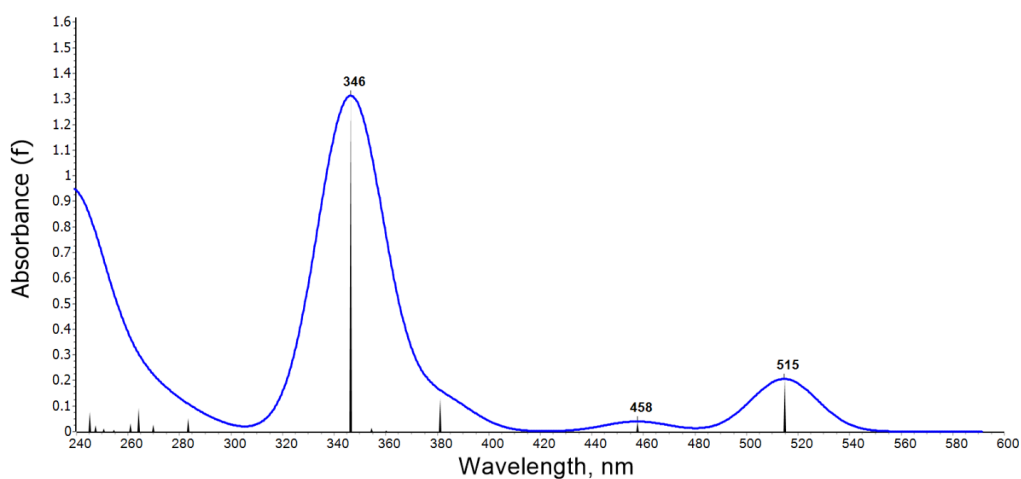


Figure S20. Calculated UV-Vis absorption spectrum for the **[1-H]H<sup>+</sup>** ligand in an ethanol SMD continuum.

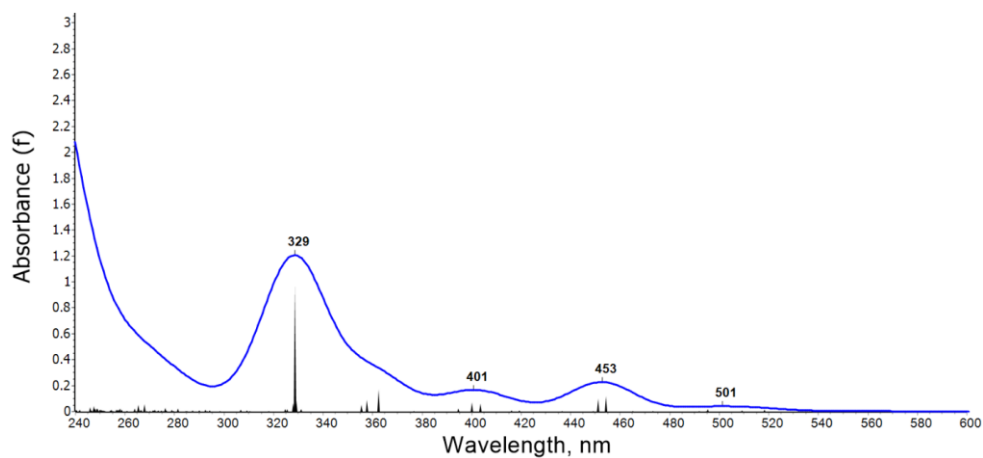


Figure S21. Calculated UV-Vis absorption spectrum for the **Cu-H** complex in an ethanol SMD continuum.

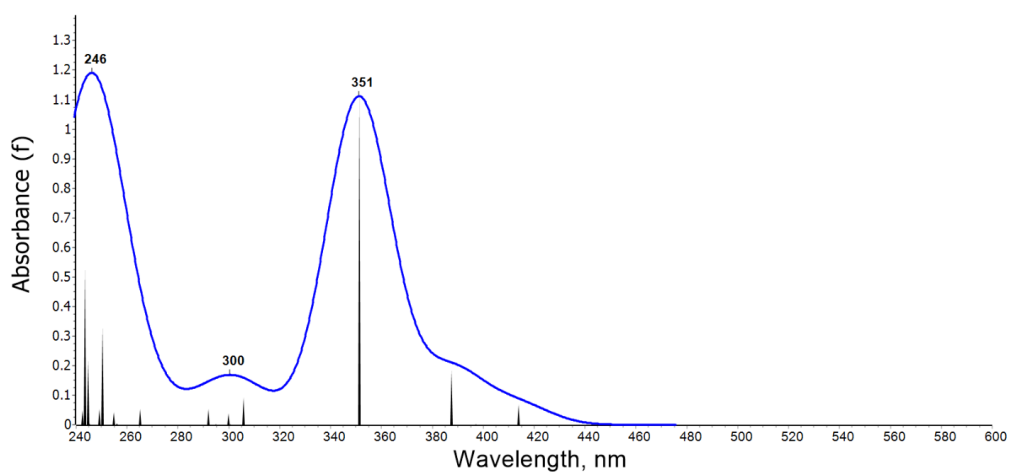


Figure S22. Calculated UV-Vis absorption spectrum for the **2-OMe** ligand in an ethanol SMD continuum.

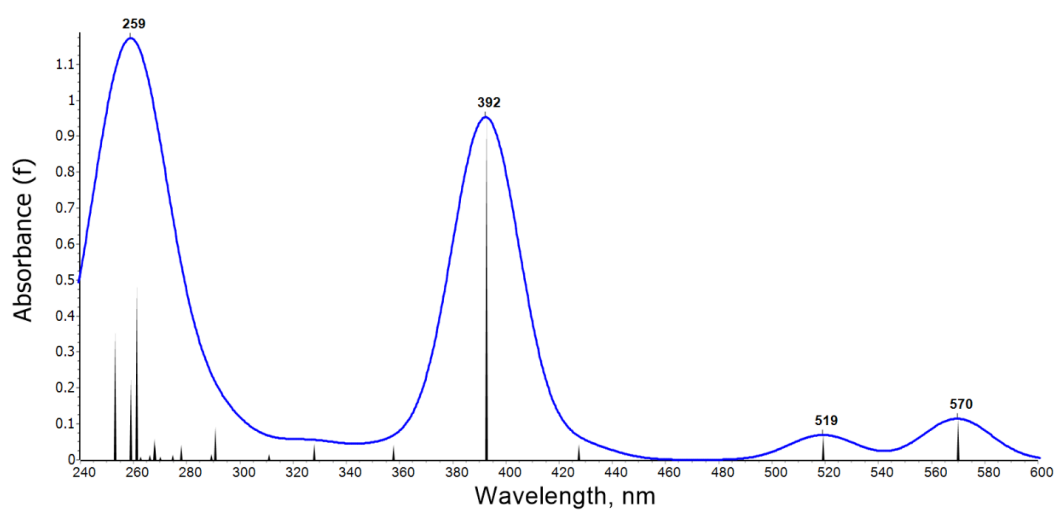


Figure S23. Calculated UV-Vis absorption spectrum for the **[2-OMe]H<sup>+</sup>** ligand in an ethanol SMD continuum.

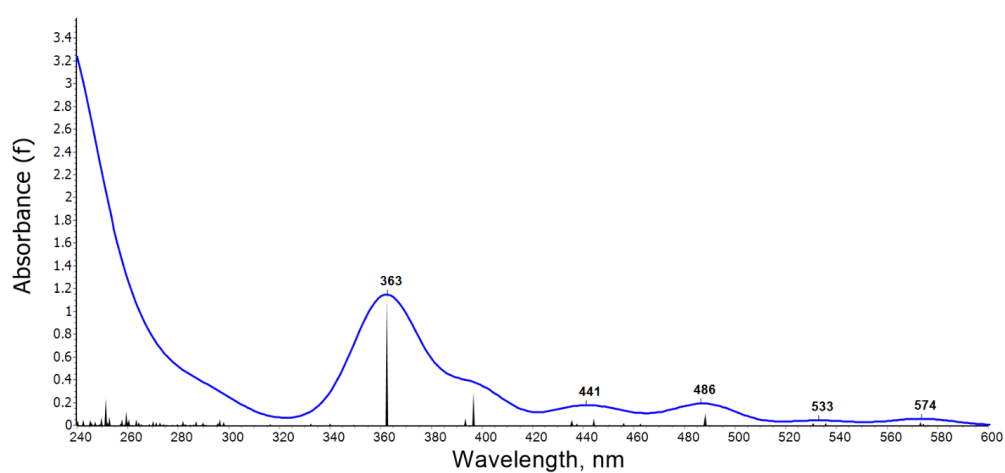


Figure S24. Calculated UV-Vis absorption spectrum for the **Cu-OMe** complex in an ethanol SMD continuum.



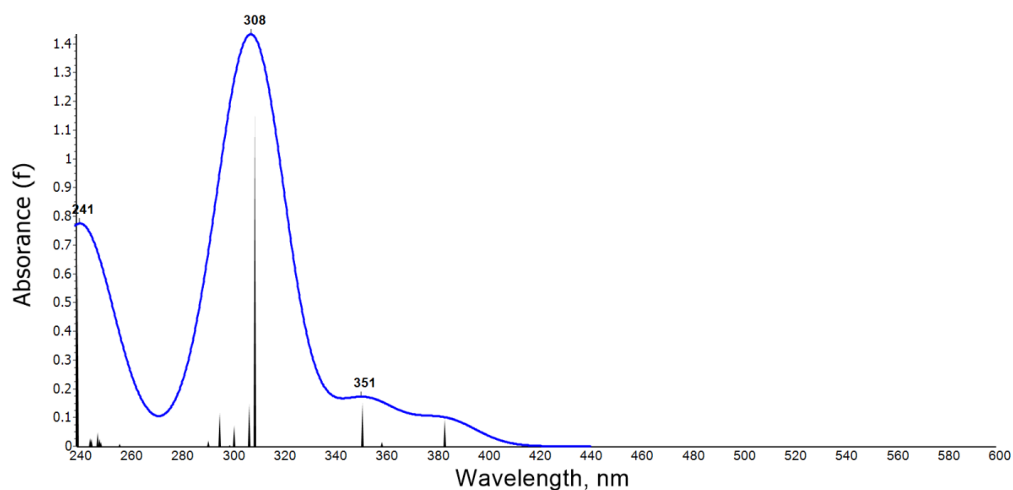


Figure S25. Calculated UV-Vis absorption spectrum for the **3-OCF<sub>3</sub>** ligand in an ethanol SMD continuum.

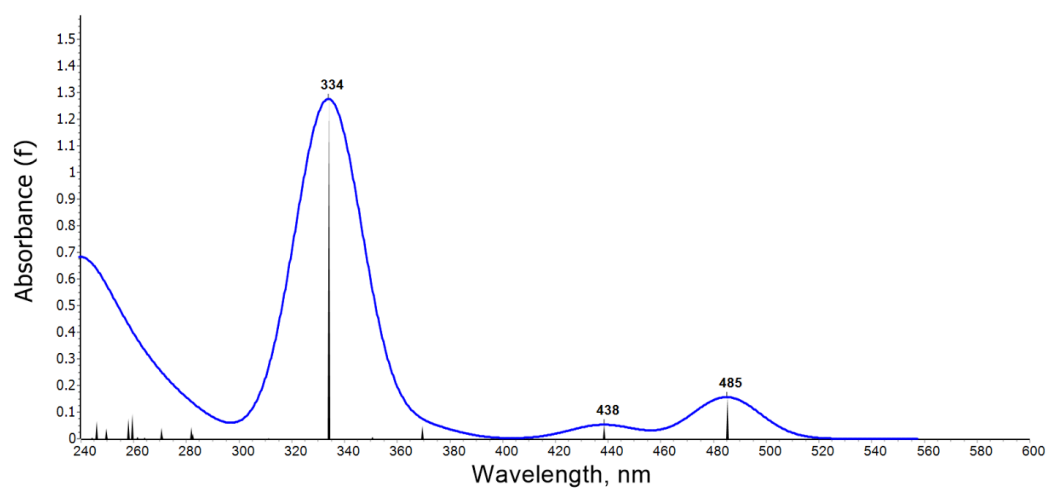


Figure S26. Calculated UV-Vis absorption spectrum for the **[3-OCF<sub>3</sub>]<sup>H+</sup>** ligand in an ethanol SMD continuum.

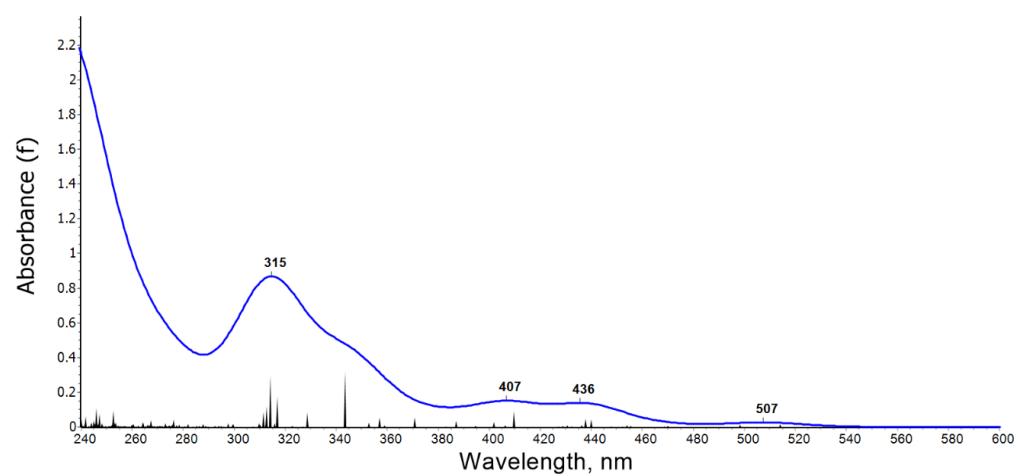


Figure S27. Calculated UV-Vis absorption spectrum for the **Cu-OCF<sub>3</sub>** complex in an ethanol SMD continuum.

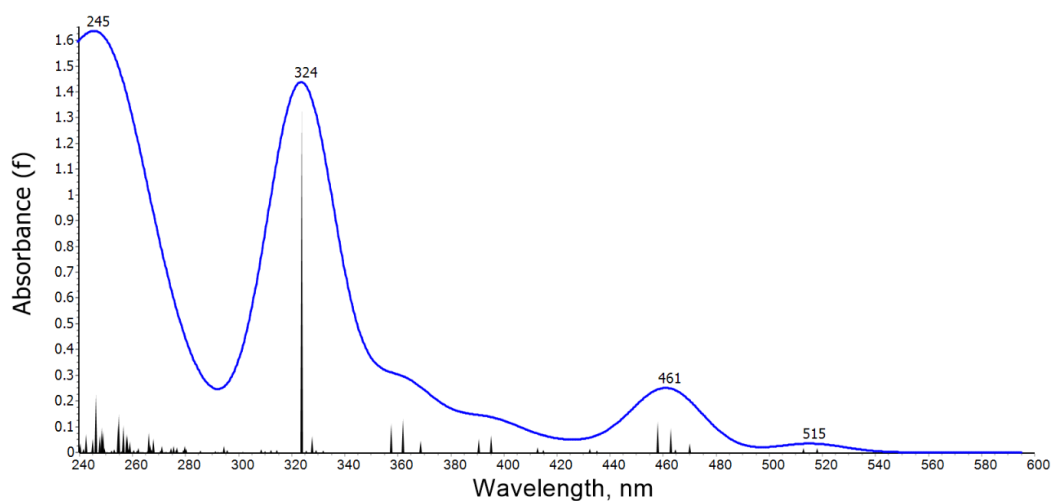


Figure S28. Calculated UV-Vis absorption spectrum for the **Zn-H** complex in an ethanol SMD continuum.

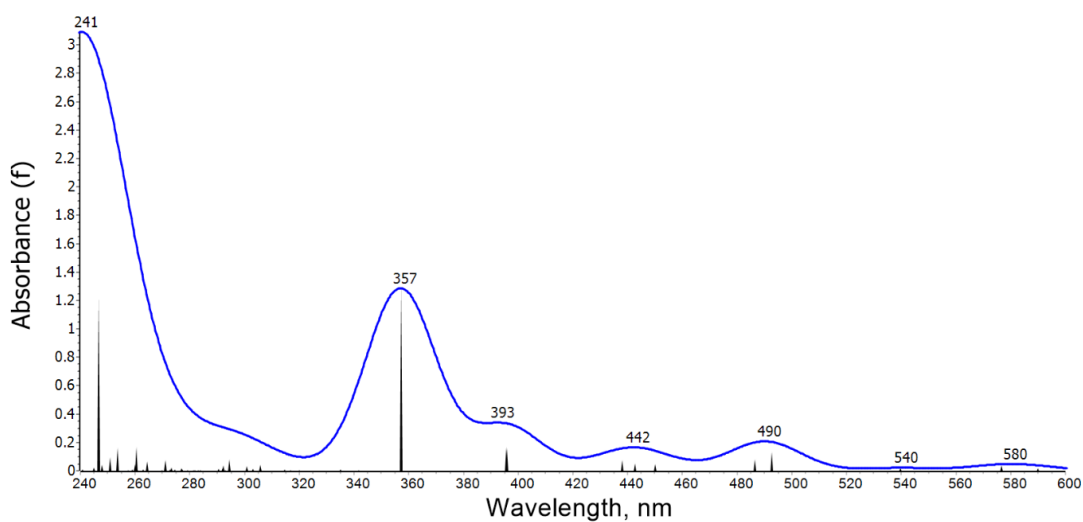


Figure S29. Calculated UV-Vis absorption spectrum for the **Zn-OMe** complex in an ethanol SMD continuum.

## 3.7 Cartesian Coordinates

**1-H (vacuum)**

H	-6.40141696493727	-1.13847696543479	-0.91366036754484
H	-1.57509209195617	-8.58553036557375	0.16935824484790
H	0.50895725215950	-9.92300655786829	0.14248802895114
C	-0.61572461302254	-8.08624833496181	0.13198393957988
H	-1.48129619274151	-6.10671888656554	0.11652462275710
C	0.55359477892473	-8.84200945603778	0.12308419684078
H	-6.96678489877272	-4.20475573262461	-0.05222683110303
C	-0.57842610740586	-6.69943152745281	0.10775344009184
H	-8.09555485201038	-6.21813325062276	-0.04276675936666
H	1.17526294727021	-1.19602644700069	-0.85890706913604
H	-7.21954365181013	-2.40634522287211	-0.02380268050848
C	-6.33171301443960	-1.77737471466140	-0.03022153593359
N	-6.03994174756389	-4.60884310117858	-0.04902683478944
C	-5.04069713899734	-2.55779241579110	-0.02956447154951
H	-4.73089213485208	0.15794981928628	-0.03390186917270
C	1.78047446598375	-8.18823402868023	0.09018998384520
N	-4.95499762902212	-3.84220103133970	-0.03994758541439
C	-3.79939421454960	-0.38626375089213	-0.02025607151331
C	-7.14240642626402	-6.73532803865567	-0.06402310318700
C	-3.77143228997072	-1.79154989629455	-0.01691447949676
C	0.65812838601134	-6.05001810865874	0.07405607887746
H	2.70092757258993	-8.75829694133997	0.08430827367699
H	-2.59082711751100	1.38606320880821	-0.00910479487176
C	-2.59953870793340	0.30279709162235	-0.00699922215779
N	-2.62138218174792	-2.46809708342144	-0.00210687690284
H	-8.03073408303785	-8.67970488413042	-0.07692084751291
C	-5.95423131114752	-5.99732373206125	-0.06996387593243
C	-1.46082671788231	-1.81008679967071	0.01023743150853
C	-1.41067901615196	-0.40527829048306	0.00866215163165
C	1.83687517388187	-6.80310211726015	0.06786670957017
N	-0.31062428021602	-3.88007239776880	0.03915179176886
C	-7.10319935635179	-8.12117999206617	-0.08258039290900
H	-0.47077299007203	0.12443847089058	0.01988074309162
C	-0.20426620940255	-2.59704361598856	0.02483481470520
N	0.76268833176565	-4.66291223069790	0.04913785629149
C	1.09903510660137	-1.83732653321271	0.02201967907810
H	1.97686609545856	-2.48023118061259	0.02141684785370
H	-6.39634221268100	-1.12893292510200	0.84640442149724
H	2.79636592521568	-6.29801735583615	0.04333265426791
C	-4.72583987727197	-6.66245020091816	-0.09922367223227
H	1.69532480901697	-4.27233074263204	0.04786944488566
C	-5.88454331543406	-8.79053739774925	-0.11113761988150
H	-3.81556608778402	-6.08119860931319	-0.10768806919044
C	-4.70582129954635	-8.04962652379575	-0.11969279876853
H	-5.85368329884846	-9.87205073742540	-0.12739808171428
H	-3.75282137510108	-8.56112860225919	-0.15381724392289
H	1.17784505755766	-1.19388324939552	0.90129174939397

**1-H (EtOH)**

H	-6.40615253762754	-1.15829009083315	-0.93680848741574
H	-1.53445458432889	-8.60878845002969	0.10367215854324
H	0.56349114382357	-9.92495318008129	0.10278280031120
C	-0.57933811906555	-8.09845843969892	0.09036308777655
H	-1.46602944144151	-6.13331800855907	0.07705518715009
C	0.59741393865614	-8.84294681272337	0.09240631119942
H	-6.97508808979186	-4.19073988212574	-0.07241797514656
C	-0.55217917303485	-6.70947198298364	0.07779609509611
H	-8.11711346926386	-6.19214568844896	-0.06977891345883
H	1.18791994682614	-1.21245154982419	-0.84826256481874
H	-7.22124786345980	-2.40904581590817	-0.01727227750412
C	-6.33360159482713	-1.78089986124677	-0.04182671180377
N	-6.05247163806533	-4.60507912812415	-0.05777259623279
C	-5.04660810838552	-2.55775500257455	-0.03405005636880
H	-4.73137069965904	0.15497190396977	-0.03993584022737
C	1.81927589677749	-8.17339077314243	0.08193923977581
N	-4.95603277910523	-3.84389185209929	-0.04170928061846
C	-3.80051326382407	-0.38994762451493	-0.02330083820786
C	-7.17011446217996	-6.71980726871292	-0.07142932499121
C	-3.77461744570426	-1.79335021350716	-0.01837680643291
C	0.67812415952584	-6.04206803975474	0.06599983929872
H	2.74587809621654	-8.73443058656882	0.08493619929854
H	-2.59016768129754	1.38141931114611	-0.01101223384253
C	-2.59914845402982	0.29826647926199	-0.00761895827633
N	-2.62197790723040	-2.47175990891915	-0.00035336753050
H	-8.07436588466604	-8.65569378409954	-0.08088807454918
C	-5.97402983739817	-5.98884658274437	-0.06611370148645
C	-1.45838744430088	-1.81259508291544	0.01489745525201
C	-1.40924140701287	-0.40963457021099	0.01225792507595
C	1.86521139549102	-6.78776659703350	0.06985771001838
N	-0.31087697194450	-3.88282900535279	0.04043542824940
C	-7.14097093269011	-8.10599245824864	-0.07713623523260
H	-0.46913272294896	0.11946449114487	0.02628700615675
C	-0.19941108607502	-2.59807254099787	0.03307991744616
N	0.77464363896248	-4.65969039864385	0.05126592682297
C	1.10010003757643	-1.84236368352689	0.04001758538319
H	1.97690954065123	-2.48570309112291	0.06343995101840
H	-6.39022425583304	-1.11579078418783	0.82266338259016
H	2.81847499268018	-6.27159001726687	0.06229906760065
C	-4.75191518009711	-6.67134630257161	-0.06935461321301
H	1.70267416361425	-4.25747465056710	0.05099415307525
C	-5.92736950692226	-8.79057679597516	-0.07953584673642
H	-3.83078481330470	-6.10694599440941	-0.06734363826446
C	-4.74172441001290	-8.06054520179628	-0.07597639946335
H	-5.90685958368943	-9.87294054457351	-0.08426887656090
H	-3.79295616338258	-8.58265900589992	-0.08280197763006
H	1.16169305779942	-1.18592631869716	0.91089911917397

**1-H protonated (vacuum)**

H	-6.44420861029251	-1.15598725660591	-0.92059164493197
H	1.21934355770493	-1.21246347427842	-0.85599668578682
H	-3.70531725082673	-8.62104652921028	-0.20149861501712
H	-5.82960929286422	-9.88072716378938	-0.13028168163259
C	-4.64342998280439	-8.08740282284048	-0.14696395744270
C	-5.83811962773315	-8.79931477213882	-0.11358658940043
H	-3.71133223727632	-6.14675540709656	-0.16393901862411
C	-4.63691315430481	-6.69996871873424	-0.12741318447366
C	-7.04413520219859	-8.10929142052099	-0.06429296117717
H	-7.98068221319814	-8.65011013023405	-0.04138640064229
C	-5.84972986786767	-6.01808069263681	-0.07530236688139
C	-7.05428030069467	-6.72345168361754	-0.04700685686025
H	-6.86322647361154	-4.22779695106566	-0.04852548946581
N	-5.92926600407438	-4.61869940902518	-0.05635998228552
H	-7.99562042988557	-6.18682792462515	-0.00963791908210
N	-4.89230083328685	-3.82211160682918	-0.04487355174147
H	-4.73766874279405	0.19157396842982	-0.03136018405782
C	-6.35144767886648	-1.78665302696580	-0.03405443724652
C	-5.04265613604799	-2.52822932226579	-0.03247601429460
H	-7.21746666399757	-2.44394794449590	-0.02682405351520
C	-3.80911319926597	-0.35388963133923	-0.01910954620920
C	-3.82035537960154	-1.74834555930325	-0.01817243846940
H	-2.59051446262327	1.40376000488389	-0.00804437015767
C	-2.59928062748858	0.32144142338392	-0.00665872827285
N	-2.62083205357927	-2.38647473970231	-0.00355604450968
H	-2.62916957204336	-3.40335238832054	-0.00228854887608
C	-1.40031787824520	-0.37326612037379	0.00747974476786
C	-1.41126419472754	-1.76786208182825	0.00986239278717
H	-0.46329587687921	0.15767758273880	0.01825963150027
H	1.97393610017885	-2.51838994413537	0.02671474642043
C	1.11847789189891	-1.84737424782628	0.02635667719450
C	-0.20202549342089	-2.56771333337776	0.02643553256464
N	-0.37369607607344	-3.85913670090951	0.04198623982929
H	2.69622207483949	-6.26448094642689	0.01401550530437
H	1.59055060684389	-4.29471196665185	0.04559207562681
N	0.65083530909408	-4.67164412115997	0.05505404161116
C	1.74859540257911	-6.78974899499626	0.05297317229215
C	0.55251152137965	-6.06977877861076	0.07863277771991
H	2.65230384524344	-8.72715062814884	0.05416895204916
C	1.72223586316010	-8.17522126877720	0.07494015651858
C	-0.66838378294260	-6.73680837357810	0.13297291485494
H	-1.58726840018156	-6.17232488033804	0.16744222740862
C	0.50809612957220	-8.85051207197147	0.12651428657655
C	-0.67811181083391	-8.12428021807816	0.15718724472326
H	0.48651103396075	-9.93168470548378	0.14716024224676
H	-1.62242178541148	-8.64678829891716	0.21338092340967
H	-6.43952219558205	-1.14398004624920	0.84403857979406
H	1.21900962987012	-1.21213957545632	0.90869446375426

**1-H protonated (EtOH)**

H	-6.42852198813021	-1.17323337969294	-0.93869049239510
H	1.20887129166143	-1.21980048545891	-0.84970044643246
H	-3.72117951671997	-8.61417053090890	-0.11093474268720
H	-5.84406036314292	-9.87903649064136	-0.09506976590120
C	-4.66179868955439	-8.08047444060623	-0.09197817413411
C	-5.85527274198865	-8.79669738981343	-0.08654964707491
H	-3.73216926281210	-6.13745405808084	-0.08901681982477
C	-4.65868077231186	-6.69150989707414	-0.08159404971541
C	-7.06318976461960	-8.10407913903314	-0.07179454869976
H	-8.00088571339311	-8.64558988666746	-0.06887562202655
C	-5.87371072009366	-6.00481084006461	-0.06613638778907
C	-7.07781422162939	-6.71782634538275	-0.06270843118416
H	-6.88382794569054	-4.21324729288198	-0.06144605410048
N	-5.95426025038829	-4.61510729759983	-0.05679896869004
H	-8.01800379690346	-6.17874917868998	-0.05204623779934
N	-4.89625372634875	-3.82803535704960	-0.04132140320695
H	-4.73675646246972	0.17934201742381	-0.03187395693879
C	-6.34508361835851	-1.79502870576403	-0.04471120039058
C	-5.04361374531747	-2.53923284856401	-0.03429789194700
H	-7.21121068815710	-2.45149733391980	-0.02950719304588
C	-3.80794606224630	-0.36590277551371	-0.01907938672316
C	-3.81518832876421	-1.75774173874209	-0.01817508302381
H	-2.59046069940112	1.39271656514468	-0.00479905772730
C	-2.59902980156432	0.31066109197780	-0.00427970343061
N	-2.62034311397311	-2.39620642163569	-0.00273518108072
H	-2.62849616318273	-3.41382460454645	-0.00189737631214
C	-1.40078039871768	-0.38491480808988	0.01144092848298
C	-1.41570924407802	-1.77675755795358	0.01236395929118
H	-0.46312325753648	0.14523014787850	0.02574844027854
H	1.96982432881091	-2.52113347450369	0.04357738842040
C	1.11233068630307	-1.85320607671233	0.03443288812995
C	-0.20002497379255	-2.57791622792489	0.02910125849166
N	-0.36834991506056	-3.86422400799327	0.03889226812078
H	2.71910378976090	-6.25799997899130	0.05448457182197
H	1.61269579781766	-4.28045955860654	0.05501836306010
N	0.67713731119516	-4.66784005110591	0.05294666600765
C	1.77206245925631	-6.78477446144700	0.06741228331099
C	0.57721104573295	-6.05625467660473	0.06848197579963
H	2.67071381878408	-8.72396138027915	0.08033311685780
C	1.73997517141413	-8.17062100797586	0.08143748459464
C	-0.64646427630151	-6.72701480484734	0.08762006200848
H	-1.56592700786203	-6.16123741524784	0.09434873807285
C	0.52332717342200	-8.84750277775570	0.09922965697498
C	-0.66090512503172	-8.11592034648230	0.10293969133774
H	0.49805387146270	-9.92957737523674	0.11183821602543
H	-1.60849031403189	-8.63701322100101	0.12476476573173
H	-6.42392078841431	-1.14020006986805	0.82529116878672
H	1.19579218716692	-1.21163700496580	0.91397518857529

**2-OMe (vacuum)**

H	1.92575789383746	-10.51142241547951	-1.60060542793943
H	-6.64593128912638	-1.89874504616203	-1.54316063461739
H	-1.79466539437956	-8.21896679113464	-0.92093943025726
H	0.76106851905551	-11.79572649248416	-1.19288175127759
O	0.05090718043076	-9.94139228646882	-0.90309944638227
C	1.15263935565317	-10.82621920283784	-0.89234204797940
C	-0.84148028489124	-7.79223980801226	-0.64203704825007
H	-1.58751171788555	-5.79039584343007	-0.41857482470135
C	0.27519050548564	-8.62983291140976	-0.59161426036317
H	-6.83403149183028	-4.21979434791954	-0.43314809051389
C	-0.73187197296355	-6.44551626537875	-0.36121475640383
H	-7.81768847745391	-6.37597659754415	-0.26569382933377
H	1.12265501031296	-0.76179363992736	0.23624255294860
H	-7.14727541848543	-2.33459044928582	0.09128026857731
C	-6.36746665008106	-1.83022999776934	-0.48570569949786
H	-6.73526385875008	-10.94298457381189	-0.17295532830642
N	-5.90251068509138	-4.55726798328923	-0.22806253587190
C	-5.02168533591044	-2.45552602577174	-0.23080526371848
H	-4.75785890321900	0.31038904370575	-0.22639192285837
C	1.51264655617252	-8.09440852925647	-0.24818629991737
C	-6.83657590830437	-6.77349499098406	-0.03140707483014
N	-4.87189069050200	-3.72978190776780	-0.11372822188290
C	-3.78974684581028	-1.63599479761784	-0.11558595131029
C	-3.83028088379485	-0.23163576930784	-0.12591146528245
C	0.51161283667483	-5.90181351758646	-0.02179126003687
H	2.39597060960975	-8.71392174178504	-0.19861032477218
H	-7.57014201101990	-8.76875069359259	0.18793041056452
N	-2.63373714133677	-2.29213200202690	0.00083744335039
C	-2.63947286926895	0.46535830193604	-0.00149169827802
H	-2.64143679075189	1.54881696921632	-0.00358118080061
C	-5.73677211671199	-5.92369455388642	0.01362760106475
C	1.62404178935649	-6.73455135536993	0.03452354047702
C	-1.48081739711451	-1.63106468159749	0.11915016651639
C	-1.44608881434626	-0.22649273310253	0.12606449430356
N	-0.38476085476479	-3.71920925045460	0.11818440668837
C	-6.69637100010330	-8.13523421005951	0.22773138952385
H	1.59615403019264	-10.90628732336851	0.10606667896155
H	-0.52087871036035	0.31947388292478	0.22685289327261
C	-0.24578628205790	-2.44425227702779	0.24314363376050
N	0.65099359446821	-4.53795364974347	0.24864253568101
C	1.09140866860846	-1.80961490095550	0.52085979861892
H	1.88413293278809	-2.30795296819209	-0.04382751130090
H	-6.40102930371627	-0.78212252345888	-0.20245066713493
H	2.59299862871047	-6.32487549015313	0.29685223991270
C	-4.47663414172517	-6.45145407578581	0.31592971528491
H	1.57817540386352	-4.18894412060754	0.45459139577977
C	-5.44261865627042	-8.65445998064224	0.53605859658671
H	-3.63112895439451	-5.78262415854955	0.36350186144272
C	-6.27705821209005	-10.86927357585579	0.81941757482238
C	-4.33850284343795	-7.79970855970751	0.57383581728030
O	-5.19034495742603	-9.96606834730225	0.82442529296552
H	-5.86474144419424	-11.83604992965146	1.10035511815597
H	-3.37235058425444	-8.21475211149812	0.82437803737231
H	1.35348296494974	-1.87602430806597	1.58249492056573
H	-7.04386420834517	-10.57725665550491	1.54391900834077

**2-OMe (EtOH)**

H	2.15591845614454	-10.64983700997905	-1.16050038517153
H	-6.43103118834837	-1.08241419810748	-0.84300609957127
H	-1.56947536158996	-8.43053027472401	-0.24101100178189
H	1.17080271047387	-11.88919332900995	-0.34751997675797
O	0.37467117827413	-10.04184199552854	-0.25611617684686
C	1.53598987777549	-10.86583729460360	-0.28609735186342
C	-0.61824651608205	-7.91711237161432	-0.20543655262943
H	-1.47185065122671	-5.94858635147931	-0.16725988815954
C	0.54788334197216	-8.68344728047721	-0.21213121154611
H	-6.93939020170910	-4.15546637916313	0.05718703813292
C	-0.56481459081347	-6.53483602406999	-0.16677897154318
H	-8.01012157387499	-6.22605626036434	0.07173214344460
H	1.17694437015756	-1.04058731604719	-0.91255505295805
H	-7.22244343892530	-2.36725862929033	0.04919609865807
C	-6.34909024476601	-1.71842150872696	0.04158068196983
H	-7.28849575605886	-10.80370237494062	-0.68226005019743
N	-6.00479158251504	-4.54214936610842	0.06839091691850
C	-5.04653893093637	-2.46906579219731	0.04422028204493
H	-4.77419899075166	0.25193709658615	0.05616921290874
C	1.78310523449273	-8.04081384650686	-0.17786166562940
C	-7.03974742946030	-6.70817226964373	0.09833408041156
N	-4.93171964482787	-3.75448436525508	0.05876594438750
C	-3.78921245776186	-1.68330191074137	0.03001354138233
C	-3.83549034593730	-0.27971466400273	0.03796709869465
C	0.67363024193981	-5.88314920602685	-0.13308712028311
H	2.70595550376162	-8.60261725617169	-0.18109548114850
H	-7.88709909262527	-8.66891066424829	0.13042905153448
N	-2.62592613321916	-2.34333480498082	0.00827839874965
C	-2.64346189626317	0.42546989204143	0.02418156936194
H	-2.65064972178682	1.50876615757053	0.03067332015204
C	-5.88219361865641	-5.92867666007177	0.09863648364263
C	1.83914590480841	-6.65055409094150	-0.13991733705317
C	-1.47112889120827	-1.66785089177473	-0.00540273804537
C	-1.44254134235690	-0.26393725405837	0.00239807699167
N	-0.30214705740822	-3.72246397003083	-0.06710200133740
C	-6.96994067855114	-8.09789445928377	0.13131053990282
H	2.13219068999243	-10.74681311857477	0.62284147852263
H	-0.51005740725244	0.27881224865548	-0.00891168949361
C	-0.20367278792962	-2.43626453014349	-0.03238512940062
N	0.78080892917332	-4.49577946254384	-0.09755534562872
C	1.08985776640381	-1.67024657617333	-0.02358517754412
H	1.96958559835030	-2.31012873416780	0.00271307158111
H	-6.42663616945583	-1.06937065694505	0.91699912350510
H	2.80453786058884	-6.15845139187287	-0.11365934912834
C	-4.63752876518679	-6.56799034387757	0.13422220344321
H	1.71032129423770	-4.09692420414811	-0.08750499761515
C	-5.72850654655943	-8.72824215810501	0.16752808298449
H	-3.73616713731606	-5.97312259261726	0.14113462595785
C	-6.69520714424674	-10.92065460731029	0.22889741459146
C	-4.57024776182716	-7.94993416318163	0.16786221549895
O	-5.54189730634390	-10.08511563261562	0.20739875958721
H	-6.32028505409342	-11.94065034393300	0.28738832944778



H	-3.61366781028332	-8.45315332608940	0.20561215165542
H	1.14674081071216	-1.01221958234490	0.84642518993017
H	-7.32090516310355	-10.71414207083946	1.10134706434000

### 2-OMe protonated (vacuum)

H	-6.72303425916258	-1.85272798652304	-1.39688312839790
H	-2.92888075276343	-7.98426023930887	-0.66192558784999
H	0.36255442743565	-10.87457256125025	-1.42332074337595
H	-0.96836914059439	-11.92355660623598	-0.87894604482186
O	-1.35192751949840	-9.96062488053321	-0.66952508430645
C	-1.90191643735247	-7.70018611761867	-0.48024998108938
C	-0.40424751415982	-11.02124708575293	-0.65837008921242
H	-2.33387738774832	-5.61985973868821	-0.31879786478704
C	-0.92116963281856	-8.69806794203378	-0.44638362208636
C	-1.56706535771451	-6.37782778448826	-0.28583746991751
C	-6.46440134884594	-1.72375839598479	-0.34087798653464
H	-4.76802072346985	0.53072663361566	-0.09858028569735
H	-6.54001867323327	-0.66352687527128	-0.10838108608224
H	-6.71898254710150	-4.22176294687186	-0.22596134137171
C	-5.10519964849304	-2.27249166593870	-0.03459082390954
C	-3.86191760320378	-0.04893480420908	-0.03047633792183
C	-3.91259975346389	-1.43979559194336	0.00698366160057
N	-4.86386447586030	-3.53099903234292	0.19181177213787
H	-2.57992922756915	1.66216026430555	0.02100798465565
C	-2.62356011296515	0.58062850441331	0.03757923445359
N	-2.73035796923885	-2.09528738493969	0.08819643261882
H	-2.77341197285662	-3.11214359979792	0.11261275801212
C	0.40511079956270	-8.34279456240668	-0.19725622670105
N	-5.79513502234452	-4.44747718000354	0.12342334452352
H	-6.90537736290487	-6.65575883295715	-0.84112421928130
N	-0.72735383162978	-3.71066599094848	0.10362137871182
H	1.68295400150786	-2.55976252896794	-0.40584502426838
C	-0.23796990656833	-6.02216162565981	-0.04589582460959
C	-1.44004827940731	-0.14282386808946	0.12229362391338
C	-1.49726915544896	-1.53625147469133	0.13674570016096
H	-7.22572311781880	-2.23461427546299	0.25317445439436
H	1.18333646446872	-9.08948095321596	-0.15708013865012
H	0.07188657929246	-11.11513908252948	0.32170078170319
N	0.14274266345763	-4.68034638530883	0.13499919841906
H	-0.49119795820548	0.36697928626964	0.16350609747949
C	-0.37595570274001	-2.45705162152919	0.17562348307256
C	0.73970205308610	-7.00929475522905	0.00151385254635
H	1.16691782942426	-0.95023148473663	0.04853157888552
C	-6.19983213247711	-6.83228832062815	-0.03796515569561
C	-5.53328369536154	-5.76490027284544	0.55254688457862
H	1.13080248365542	-4.48285487025544	0.25045723115008
C	1.04610652349280	-2.00363899937327	0.28735829400608
H	-5.10830009032395	-10.83210622592141	0.26267059166437
H	-6.48155253029476	-8.94773057404836	-0.09120380775009
C	-5.95445882487575	-8.13494476507011	0.38375749824478
C	-4.60777501419748	-6.00215990737821	1.57150335989257
H	1.77247757382418	-6.74488462224741	0.19727877609013
H	-4.09909315250593	-5.17015915959952	2.03574982100870
C	-5.02576669064069	-8.37239537044547	1.39983207741373

C	-4.35561684551446	-7.29193454687270	1.98560276929208
H	-3.64302876540392	-7.49334545495756	2.77330787225636
H	1.43677576386936	-2.16566577353665	1.29744969738115
O	-4.70429871130601	-9.59130229041961	1.88543676367952
C	-5.33055387043088	-10.74217988185934	1.32966333252594
H	-4.90967878564553	-11.59135015477084	1.86006527965279
H	-6.41285108751728	-10.71669828300536	1.48484746099259

## 2-OMe protonated (EtOH)

H	0.95274875566825	-10.86078845408894	-1.03370343104477
H	-6.61275457538839	-2.11580303216390	-1.59459031476809
H	-0.55630325889481	-11.73552214337603	-1.38396480480842
H	-1.78775056518737	-7.61622995040492	-2.38750338831055
O	-0.74898395144034	-9.73084517269687	-1.46788179353164
C	-0.12967545971579	-10.87257691066633	-0.87813575105676
C	-1.07040911841440	-7.41889678946383	-1.60142433264442
C	-0.41508117485843	-8.49491613082258	-0.99788553272947
C	-6.35465628984699	-1.95715066856740	-0.54226378585090
H	-6.53728565275524	-4.42151270476633	-0.35904602121671
H	-1.31317943345129	-5.29689160205283	-1.67937367787874
C	-0.80921693465676	-6.12372822717569	-1.20123508849948
H	-7.25101969072063	-6.65964687739608	-0.16387809175025
C	0.51245343233295	-8.25456020506277	0.01579913057747
C	-4.97105926188645	-2.44289908762466	-0.25480535115247
N	-5.57222582502145	-4.63912754377558	-0.13656969954967
H	-4.77942064378529	0.37678836158427	-0.31138669142007
H	-6.47287910145653	-0.89895660864185	-0.31960207956713
H	1.03146459529989	-9.06496737373619	0.50490419009908
H	-5.66506794476927	-11.06165694548185	-0.01253115471380
C	-3.84891197888974	-0.15463040181088	-0.19287601569589
C	-3.82535242969285	-1.54574608497677	-0.16461116908303
N	-4.66584892493819	-3.69221712570087	-0.07568810227409
H	1.86794058630215	-2.40670069899446	0.20257411040007
C	-6.23633464610517	-6.94060977027980	0.09169637260874
C	0.11123442643625	-5.87820647786661	-0.17845689547440
H	-2.66826361140729	1.62335160893626	-0.06599886214937
C	-2.65346048533304	0.54122196090550	-0.04862348502669
N	-2.61763269016050	-2.13374137803573	-0.01449218259724
H	-2.60210172874103	-3.15144378886593	0.00407975816371
C	-5.23794623878067	-5.97132065252464	0.13351532077962
C	0.76755754403414	-6.94797216962625	0.42430755989211
H	-7.08676897826792	-2.49907442316141	0.06093473239653
H	-0.35178016253600	-10.93426526876276	0.19070306169950
N	-0.52670157603700	-3.62691551008201	0.06321893466876
C	-1.42845097936249	-1.50837947912691	0.13025080625274
C	-1.44024211182188	-0.11724025813447	0.12048978225587
H	-6.73984029829434	-8.99875188995905	0.33619025978708
H	-0.52465293216570	0.44103186143804	0.23279117532858
C	-5.94327670894901	-8.27046605550760	0.37313453515140
H	1.19194358703636	-0.80391749322857	0.46124024929233
C	-0.26647970181235	-2.37577159182286	0.28888326277477
N	0.37568632076005	-4.56651274593822	0.24186042006242
H	1.47391947450597	-6.76657806293147	1.22554677353663
C	-3.93053267615168	-6.34929394473335	0.45096144518579

H	-3.14604393174480	-5.60943307265480	0.48148736988258
H	1.25767777663637	-4.36438262248890	0.69842229864051
C	1.07043799545443	-1.85708661069864	0.70742664443595
C	-4.63962931107983	-8.64200305268828	0.69947136557289
C	-3.63715051607340	-7.66997215076464	0.72671266618215
C	-5.23715330287197	-10.94325589693128	0.98687511296600
H	-2.62438291138074	-7.96464407414013	0.96682264768114
O	-4.25219840243748	-9.91227021362487	1.00918536876026
H	-4.71688103983819	-11.85611155913904	1.26936760022350
H	-6.03598798155732	-10.74395009767811	1.70515856560768
H	1.21891102191322	-1.97285781562017	1.78618294572819

### 3-OCF<sub>3</sub> (vacuum)

F	-0.32483151611539	-10.18665349557557	-2.27054161802164
H	-6.11619882164276	-0.90775597169473	-1.36669422760613
F	-0.07517132970179	-12.01559573682147	-1.12329400432485
H	-1.93597020088859	-8.39622325508799	-0.20919533731417
O	0.00070321923726	-10.13236892553198	-0.04924874984724
C	0.29809725968575	-10.74005703039104	-1.21426010581767
C	-0.96911660672788	-7.93622353817270	-0.06332484963451
H	-1.71498986598995	-5.91631523191452	-0.02568749259200
C	0.16099957346134	-8.73468548879813	0.00858830507213
H	-6.87626866874276	-4.18724949445751	-0.42115477753258
C	-0.85014424940986	-6.55907917350617	0.03959037602729
F	-3.67393149687731	-10.22067147707603	-0.15493295070649
H	-7.87356817321673	-6.33354882589242	-0.27664051751011
H	1.10304590318059	-0.85502532535754	-0.05202819521156
H	-6.71526752851078	-2.52695635578191	-1.65094973902486
C	-6.29996997996174	-1.86414962159164	-0.88510679745568
N	-6.02573712836929	-4.47730125358930	0.04489980711369
C	-5.04473576521081	-2.45322623412218	-0.29895568874906
H	-4.76649433287838	0.29721244146112	-0.23049457088438
C	1.41854621235410	-8.18394882411677	0.19224031232895
C	-6.93726209317077	-6.70685133299805	0.12048099883837
N	-4.96733172661113	-3.66760089110103	0.11255230554309
C	-3.80370289552428	-1.64914639897809	-0.17689902532698
C	-3.83525554909303	-0.24655630232879	-0.16232827199415
C	0.41449351671017	-5.98633825328268	0.20692111999974
H	2.28658656772993	-8.82410605517533	0.25636480204507
H	-7.60532424131511	-8.75126241971856	0.19857500753527
N	-2.66081983526516	-2.32408509707646	-0.07349108971050
C	-2.63737580280971	0.43571384012649	-0.02528798072695
H	-2.62630404075412	1.51841973017577	0.00374296940664
C	-5.87488775189681	-5.82778113655176	0.34467872262833
C	1.54347127560699	-6.80661777084940	0.28395265861443
C	-1.50098424724831	-1.67679625354799	0.05529349812663
C	-1.45136836408877	-0.27439110557534	0.08327794542874
C	-6.79480424738044	-8.06059004945769	0.38527144902101
N	-0.45774710620540	-3.78679801259818	0.17817790980304
H	-0.51961610036922	0.25848329368486	0.19518504166208
C	-0.27947220372638	-2.51089809652464	0.16387142676167
N	0.58238762835276	-4.60810647619142	0.29427105854046
C	1.08868249713027	-1.89266801890104	0.26662960609932
H	1.80279607132193	-2.42419923063212	-0.36891488619633

F	1.62267800152254	-10.71138616265510	-1.48962397894158
H	-7.07235001065085	-1.71877909436397	-0.12273235211114
H	2.52399953142063	-6.36531454368965	0.41777459846423
C	-4.67659366004259	-6.31501494941107	0.87455116289973
H	1.52732468644314	-4.25412318491736	0.36812837806712
C	-5.59287862827380	-8.53026497546576	0.88302737853164
H	-3.86698554490706	-5.62557805500783	1.05937591452906
C	-4.88886081295136	-10.66924294664294	0.21994498371962
C	-4.54283322697675	-7.66532370336910	1.14710141424620
O	-5.45645468252004	-9.90207398504355	1.17215706524664
H	-3.62157155889966	-8.05148459035233	1.55925509188924
F	-4.74866433592097	-11.89926162376153	0.70839057310534
H	1.46876060105737	-1.93422724130959	1.29300311548596
F	-5.62916483616907	-10.74236425899062	-0.90439435014039

### 3-OCF<sub>3</sub> (EtOH)

F	2.10126548455082	-10.55389308658001	1.26936472929287
H	-6.96668254418120	-1.77651662071566	0.01989252433709
F	0.43648611686282	-11.90220111642765	0.91504611257724
H	-1.55786690764822	-8.37359020638384	0.06617931492076
O	0.45138829875723	-10.01348214918449	-0.15325688868754
C	0.77784673132258	-10.61312981164179	1.00345531055901
C	-0.61709427601213	-7.86323937124202	-0.08598786134782
H	-1.45832335386024	-5.88513388347697	-0.06576183880599
C	0.54821039081291	-8.60130457383129	-0.19621313719282
H	-6.83653738229463	-4.19749270236396	0.31558487453946
C	-0.56251093906735	-6.48003139004546	-0.15724263419935
F	-7.50749872091721	-11.05756281140514	-0.76545267185858
H	-7.94500917443634	-6.23617608200969	0.01404625907595
H	1.45280740963650	-1.74524355393131	-1.41111870244078
H	-6.73592551914004	-2.61921814938130	1.55308085159724
C	-6.25807063293591	-1.94390544219832	0.83742292385830
N	-5.93908903827011	-4.55363384550091	0.01118894625965
C	-4.96781202107670	-2.53066141835712	0.34192873882734
H	-4.75844683586481	0.21653569968483	0.41111033632043
C	1.77630306510500	-7.99038114794139	-0.39280473925811
C	-6.98647161849625	-6.70150602798576	-0.18000779340458
N	-4.85830999248377	-3.76354581430733	-0.02147525197951
C	-3.74329803972546	-1.69715628937310	0.24573580604301
C	-3.81516338635039	-0.29691270998555	0.29983561464580
C	0.67130657900654	-5.83952928078542	-0.32790959852724
H	2.67405592659085	-8.58355397600693	-0.49775833207349
H	-7.83659802719569	-8.65013000361351	-0.39847443033561
N	-2.57655739686447	-2.32895715647274	0.09370996372114
C	-2.64137339689731	0.43039701101972	0.18623136836223
H	-2.66594152645255	1.51278900424032	0.21859362979688
C	-5.82721735204008	-5.91739152819944	-0.20696083286971
C	1.83663354260407	-6.60693333785051	-0.45083444786180
C	-1.43769896269591	-1.63449996776566	-0.01309760620569
C	-1.43403003145156	-0.23293946860488	0.02933780649493
C	-6.92636812148999	-8.06838919901638	-0.40841862978213
N	-0.30648096423398	-3.69393160280005	-0.19964546746675
H	-0.52163315826225	0.33529470281311	-0.05985231282221
C	-0.18333292105732	-2.41032161793223	-0.18480716469817

N	0.77353579003539	-4.46047969096833	-0.37610188224544
C	1.14419343599604	-1.73082954264805	-0.36049752950664
H	1.92218963254665	-2.23930358082704	0.21424312129584
F	0.15030326035607	-10.08500085429389	2.07278686531907
H	-6.10908635335212	-0.99838326909243	1.35091635906006
H	2.79098695745688	-6.11516907161872	-0.59358007069965
C	-4.59321843053874	-6.52944120407713	-0.45341395009494
H	1.69344092752604	-4.05517201260546	-0.49534301155524
C	-5.69205290760292	-8.65375714280833	-0.64954497324580
H	-3.69701534050688	-5.92819034453677	-0.47374920528007
C	-6.23543467000044	-10.95934835348596	-0.31660866631848
C	-4.53311933777823	-7.89703235986153	-0.67126921812319
O	-5.52726452453101	-10.02200496273879	-0.95945490142388
H	-3.58969896776384	-8.38506119105656	-0.87153167464280
F	-5.64772823735332	-12.14257617399654	-0.53190118213840
H	1.13380648850639	-0.69683939452665	-0.03051538702253
F	-6.30723564864334	-10.76037009579800	1.01199397661052

### 3-OCF<sub>3</sub> protonated (vacuum)

F	0.55794137369567	-10.13394514274452	-2.29653265792550
H	-6.85434637224176	-2.45128506343150	-1.30164043893384
F	1.72609882020891	-10.84016952091814	-0.62276328487862
C	0.47033305698261	-10.71360574443565	-1.08880045560161
F	-0.05556267943507	-11.92094067406322	-1.22316494832989
H	-6.38260216879466	-0.85041715971154	-0.78045595081537
C	-6.37987297539459	-1.89551779143302	-0.48692448060611
H	-1.81479005325006	-8.17683311269438	-1.29968065837974
H	-6.67895230055164	-4.27105654526885	-0.20561959186121
H	-1.49546832858636	-5.71949805445321	-1.10015603642307
C	-0.98957130308849	-7.77077725011783	-0.73286191783831
F	-5.63273021584887	-10.77418098403268	-0.98003084381821
C	-5.00094021285189	-2.42459094816709	-0.23034323946986
O	-0.32409118491028	-10.00314141295766	-0.24241420444564
C	-0.81527849305333	-6.40231025234121	-0.61506340411385
C	-3.83009100414107	-1.56680610247391	-0.17865316552139
C	-0.08328333711079	-8.63403670687376	-0.13702189359427
H	-4.77432996961762	0.36243172044640	-0.27642224574309
H	-7.01409851931070	-1.99714669060029	0.39937402143186
N	-5.72485035131765	-4.56481420980193	-0.03032312467799
H	-2.61132328745389	-3.18790065352799	-0.03758334325323
H	-7.57613205674735	-6.41826406905888	-0.10817345007226
C	-3.84197758492719	-0.17297295760648	-0.20468586164881
N	-2.62019823433304	-2.17070365388308	-0.07079039529220
N	-4.75410348069506	-3.68681829439908	-0.02577887275290
H	1.85604827846654	-2.34931890071770	-0.31084618095090
C	-2.64252195740306	0.51802039879035	-0.10738779768577
C	-1.42108209983775	-1.54298570462298	0.01825571525508
C	-6.59143253098341	-6.79793505732147	0.13632994013790
C	-5.50416357676710	-5.92899135829003	0.21067239359535
H	-2.65175294179273	1.60033412281395	-0.11347327354381
N	-0.47797218762777	-3.65979748786306	0.08027257234957
C	0.27333491772768	-5.90994693241232	0.10129332312550
C	-1.42984827902822	-0.15121762625248	0.00391475266551
C	-0.23798655761959	-2.38268666411708	0.12924751904697

C	0.99994468967119	-8.15441893633220	0.58558797315380
H	1.19346577146647	-0.76564837131489	0.02610915248451
H	-0.50823449927329	0.40132556787339	0.08077396950050
N	0.49374485805445	-4.53025985333509	0.22229155613188
C	1.17999848409163	-6.78495112688863	0.69886607319328
H	-3.39659459026336	-5.75289108522235	0.59731727336714
C	-4.24029048280315	-6.42109475299144	0.52894941551975
C	-6.42744606145096	-8.15406940205413	0.37276860666801
H	1.68619506918942	-8.84380082018044	1.05499173092670
H	-7.27816548555791	-8.81566044899526	0.31724525475028
C	1.13563181295839	-1.81237168447265	0.31094083617546
H	1.42032842439014	-4.22292239765658	0.49110699696664
C	-4.07553667094275	-7.77362394871742	0.76180176052563
H	2.01597184449143	-6.39801343581266	1.26877800434561
C	-5.54965714502720	-10.96633456302343	0.34610530969817
C	-5.16051651497574	-8.63551109655165	0.67814653529652
H	-3.10519541934449	-8.17688057668680	1.01156477897736
F	-6.80662941719322	-11.10030973927956	0.80813761296930
O	-4.87818071270587	-9.96296645738940	0.96861463619193
F	-4.89291667891640	-12.09262106577626	0.57997894458309
H	1.46680949388083	-1.89271265505022	1.35141846474418

### 3-OCF<sub>3</sub> protonated (EtOH)

F	-0.69536714043454	-10.67137284493113	-1.79686888386732
H	-6.88052564890957	-2.49915911899173	-1.04163963779238
F	1.03570319543966	-10.89083916966102	-0.52279448400736
C	-0.31218495106642	-10.86727236441506	-0.51861904843548
F	-0.75015715628742	-12.06727615127831	-0.13635064538989
H	-6.37748997527799	-0.87748412985907	-0.60640554833174
C	-6.37102938553637	-1.91053000139049	-0.27225163962383
H	-2.08142526264560	-8.15429845799151	-1.09594340442389
H	-6.66628051482769	-4.27077267173157	-0.00006161866026
H	-1.53763907371897	-5.73956557246926	-1.18876656938813
C	-1.22201843923467	-7.76634892047740	-0.57040805500089
F	-3.74811977833647	-10.03123957484952	-1.35468443751017
C	-4.98937144276935	-2.43653865308645	-0.05117631212249
O	-0.81660891968489	-9.95790990342460	0.33064913121637
C	-0.91874825729422	-6.41566554456187	-0.61819858741595
C	-3.81070952793872	-1.57918751659684	-0.12079700284586
C	-0.42131503985343	-8.61186457895904	0.17637418447046
H	-4.75865650603388	0.34673859837963	-0.21756685038550
H	-6.96446602255372	-1.98092191121009	0.64385930728214
N	-5.73035041507666	-4.55054635850121	0.27090881621972
H	-2.59368492917509	-3.20356495638531	-0.02656081050484
H	-7.42167720561369	-6.44123129441875	-0.35422125014965
C	-3.82478996551713	-0.19067800692702	-0.19579632529483
N	-2.60427682654616	-2.18692075301086	-0.09059759842470
N	-4.73521812475050	-3.68108148485995	0.20657676193384
H	1.85264262063252	-2.42289759660191	-0.56726861131917
C	-2.61877213111436	0.49730437591504	-0.21450347217452
C	-1.40429410431602	-1.56401589952287	-0.11215120378900
C	-6.48109234916401	-6.81395105435631	0.03120841613605
C	-5.48330198755362	-5.91476749042160	0.41747594195398
H	-2.62490257414226	1.57830825143199	-0.26224613576595

N	-0.47860417336201	-3.68076196118245	-0.06435555942035
C	0.19028482084674	-5.92952366920742	0.07480999147551
C	-1.40475014341963	-0.17538454547803	-0.16889386293995
C	-0.21826138338142	-2.41265982708550	-0.05379701315952
C	0.69517922265486	-8.15131135327757	0.85494990154877
H	1.20794660874354	-0.81313691355491	-0.28164393398771
H	-0.47648748940333	0.37188224215519	-0.18249564124884
N	0.49484699168049	-4.56757597480058	0.06228564697863
C	1.00681436888781	-6.80139657923713	0.79847628907070
H	-3.51824109585179	-5.69887029951262	1.26594091840915
C	-4.27893750477914	-6.39068035085557	0.93703232873534
C	-6.26015701241826	-8.18004917267760	0.10793384573166
H	1.29688457199973	-8.83228026297740	1.44083302140629
H	-7.02519891081686	-8.87595552978854	-0.20513218096644
C	1.15997766426663	-1.84694678424614	0.05030208301121
H	1.41034970859595	-4.27847589807948	0.38713042052408
C	-4.05966590849920	-7.75695615644226	1.01206034376694
H	1.86202669906653	-6.41848049663160	1.34087460783671
C	-4.56536050784975	-10.67931812643208	-0.50293710003936
C	-5.03674400695510	-8.63291146819392	0.57363926584368
H	-3.13070017289656	-8.14278823896517	1.40504250990733
F	-5.71516898593034	-10.90764482840033	-1.17476419948219
O	-4.75580011665423	-10.01611265792170	0.65272206900956
F	-4.02215457175163	-11.86561486728981	-0.21998877401546
H	1.52317813862825	-1.88705885915332	1.08206400101550

### Cu-H (vacuum)

H	5.30868794974515	6.53228745060349	0.98728889291941
H	4.22624503803352	7.83783523264900	1.47464699728296
C	4.65234757876677	6.89067624101576	1.78557208122316
H	3.81444273993417	6.19233211178751	1.87819669793961
H	5.36958264645003	4.69683684248847	2.16785397702324
H	5.60320048860585	2.24747666284436	2.56464598839187
H	8.39494301015328	9.40031210692770	2.01187557451068
H	4.69590543179979	9.56512004897872	2.38429628936812
N	5.99793545329256	4.80038041061746	2.95232573062103
C	6.61975556244057	2.48382921606016	2.85531891324310
H	8.85437585375565	11.75556545003062	2.61642951769985
H	7.29396233321864	0.45916234476673	2.71875934144248
C	5.39675061492120	6.98603276363423	3.07976839807713
C	6.97815075791156	3.80579851512105	3.12032463565025
C	7.57152396927817	1.47974394013034	2.94625910890648
C	8.64348701625323	9.65876740914735	3.03288995106753
C	8.90324930913298	10.98203570980516	3.37049791645635
C	5.01374462913737	9.44811994033974	3.40762469764369
N	6.06215920520559	5.98115526179564	3.56578893154256
H	1.64755590034946	5.77794040506782	3.43828920480823
C	8.28254937435759	4.11990759130339	3.49170479286375
H	0.53514355552407	7.96607278170356	3.19589736128048
C	8.87629573837058	1.78566332404411	3.31895509714532
C	5.38913028923441	8.20016829232883	3.89800384704911
H	8.57822675678647	7.61913267056868	3.71447895979962
H	8.56129723689074	5.14913858408195	3.66524262381391
H	9.62197894836033	1.00431157565464	3.37238341726341

H	4.81074143308005	11.52786446897868	3.87216939507729
C	8.73953960249010	8.65235552748991	3.98519700698109
C	9.22312176379916	3.10349583774872	3.59477120522599
C	1.85330376688832	6.57285316839163	4.14591973138138
H	3.83659646671848	2.40028584863103	4.66757841485457
C	5.08260774261073	10.54924237493917	4.24373429891079
H	2.84984274983493	4.31015221950054	4.88807676402391
C	1.22831838031874	7.80351284848266	4.01046282855726
C	9.25515387635849	11.30354128350387	4.67745060204605
H	10.24262139484321	3.34951461765037	3.86100803594773
H	9.47223982520875	12.32829900935194	4.94790765942137
N	3.33220607677368	5.08802782267841	5.31592025331334
N	5.78645029452778	8.06922271294129	5.17588266593144
C	2.74012153454575	6.35475487693505	5.20112375919673
C	9.08763875564516	8.98267009392456	5.29167685771577
C	4.07007332304571	2.50278996556149	5.73330626249796
C	9.33839524147807	10.30988973736424	5.64073595641965
C	5.49531612850944	10.39332381527223	5.55649378857638
H	4.50063971400987	1.56134563267544	6.05160306862391
C	1.48632633371056	8.82202242869059	4.92220312906918
H	3.12598616337345	2.63572192600335	6.26844421955886
N	4.55219130267665	4.89135995890889	5.81076587196346
C	4.96960505868270	3.67253558588098	5.98019141357492
H	0.99501378395848	9.77947381857571	4.81684486419336
Cu	6.40540899407862	6.33246418041040	5.82405345780815
C	5.83089302492143	9.12087872972297	6.01411790747566
H	5.54204268536203	11.24684241556852	6.21276192554925
N	8.67885919898044	6.79669857522230	6.19984523334798
N	9.24337562668106	8.00187616065216	6.28976376513541
C	6.36363337328201	3.51223404267176	6.40014016531397
H	9.61268012243949	10.55882695028419	6.65885189445141
C	2.98087774283989	7.36125097339242	6.13277328221753
N	7.13258199855967	4.61943859380694	6.45325068769239
H	6.30282621894810	1.37836214889737	6.68798790625621
C	2.35781028553921	8.59236237452658	5.98095534171285
C	6.90169024547713	2.27168038068890	6.74061453982432
H	10.02573452950923	8.12130580237718	6.91857569397452
C	8.41413938760210	4.56064821507888	6.86489758655207
C	9.17674902153208	5.81265618830818	6.88327906649921
H	3.63506483542968	7.17449687099327	6.97133272686206
C	8.21625048617835	2.19383660551150	7.16261303923152
C	6.22833839266986	8.83905504309413	7.39576980269923
H	2.53664250161936	9.37117199001079	6.71066232525419
H	11.24960948689812	6.34098411757929	7.04459501977345
C	8.97934884853209	3.34467762492517	7.23941147326982
H	8.64518319916973	1.23878821396505	7.43375835758854
N	6.29151178022889	7.58016457755097	7.71494121947460
H	6.29811688995800	10.90522944080526	8.01280088051913
C	10.44008352618700	5.96036765168538	7.67454010524489
H	10.00568068552679	3.29208278472102	7.56363518482697
C	6.58411786715561	9.92019839138544	8.36411046554246
H	10.77214828784116	5.03026119354208	8.12086516761900
H	7.66481163666710	9.94390715721958	8.54128683215243
H	4.63197929992691	5.68047332141997	8.53188994391841
H	10.29708388926765	6.66740268092599	8.49884963914453
N	6.78544371375483	7.21500131936301	8.89515126932352
H	6.09038150633545	9.75285847876135	9.32505243942872



C	5.39572848919024	5.22911978231908	9.14748907567012
H	7.20916150973199	7.91384832257730	9.48867115274738
H	4.30406321458115	3.41852089029994	9.47251089725579
C	6.56594409197865	5.92904815149963	9.42593086226885
C	5.21813518543077	3.95952611965157	9.67917574971421
C	7.54066684777297	5.37342866164618	10.25462325035360
C	6.18688438210710	3.39551420139833	10.50098977708813
H	8.44511197836819	5.92688753312331	10.47548905733059
H	6.03143668976684	2.41482227577170	10.92905179623469
C	7.34551735589444	4.10924207065493	10.79234110089339
H	8.09861686508057	3.68087133241281	11.44017893666306

### Cu-H (EtOH)

H	5.29870714424331	6.41708123765137	0.98217248285558
H	4.14556083492573	7.66860725895241	1.46679512884232
C	4.61928629360774	6.74290585645285	1.77520867251431
H	3.82655583103899	5.99345475476691	1.85940444595215
H	5.26423632382783	4.53908811997687	2.28036364686955
H	5.63652553698496	2.15691259641451	2.52921852896636
H	8.37588573200376	9.41195188618897	2.17633229819220
H	4.72414873518678	9.42694723642107	2.25891729497925
N	5.97569857211673	4.69993506491626	2.98094392423055
C	6.64670436616999	2.40776078291769	2.82764881573184
H	8.86644984175308	11.75022505966024	2.84151847246207
H	7.35837316357821	0.39880388019638	2.68279776475469
C	5.36246705658016	6.87730056060638	3.06315770037236
C	6.97290851367901	3.73429048593955	3.12139927336484
C	7.61801267725132	1.42331145577686	2.91789647037674
C	8.63080623363418	9.64358621866336	3.20265352058760
C	8.90773347821352	10.95515855860826	3.57447639468703
C	5.01617241466514	9.34879721065090	3.29373787538588
N	6.04485357228520	5.89620924103779	3.56980346082805
H	1.68850402168135	6.02417492613854	3.36380176799984
C	8.26865047768426	4.06658496988758	3.51502844704559
H	0.75199213598195	8.29917240451368	3.15046016097559
C	8.91244593032654	1.74644603801253	3.31555520261451
C	5.35653004087690	8.11675493596503	3.84361569593740
H	8.51070946513958	7.59244180607878	3.83149557225143
H	8.52495841377239	5.09620410186010	3.71832015950825
H	9.66926944031668	0.97612169852775	3.38624199892816
H	4.85344752558599	11.44986691778904	3.67025944934324
C	8.69453889200454	8.61370476172927	4.13181403535600
C	9.22760342410929	3.06722027950415	3.61647655225705
C	1.88752718386869	6.76957554042181	4.12389321622795
H	3.69796897359081	2.54595907993714	4.43907107359618
C	5.09317173568423	10.48102316929890	4.08639486223642
H	2.78909811651807	4.44293906686378	4.71934470017150
C	1.36448656529082	8.04841892877018	4.00716954079423
C	9.24654355861436	11.23641918709878	4.89513449115211
H	10.23231001446360	3.33009000833509	3.92199273799746
H	9.46605487544425	12.25238780674835	5.19843046613160
N	3.22580781068230	5.15574543795101	5.28942829966864
N	5.72594739286234	8.02505265144608	5.13432294143577
C	2.69660774120646	6.44647629809007	5.21537436712520

C	9.02454778265873	8.90488825253730	5.45539485871311
C	3.92795246636521	2.54307681751552	5.51017555228720
C	9.29943711157933	10.22095956057745	5.83696818294957
C	5.46973001991493	10.36910696001257	5.41335196834571
H	4.35261021882431	1.57434556253684	5.74751955427398
C	1.64245457069244	9.01160965521453	4.97241641401513
H	2.97997272083588	2.63884495867184	6.04634603068914
N	4.43740205638845	4.91015366720870	5.79636263240338
C	4.83166136062082	3.67466743199841	5.87001341710215
H	1.24874572805600	10.01415695714297	4.86947773573615
Cu	6.32277279911732	6.29224203374189	5.82384080338775
C	5.76343552765463	9.10904927303683	5.93197854227046
H	5.51518280005372	11.24673237139973	6.03646626899888
N	8.55119068222746	6.70872240276181	6.27889564303827
N	9.11909365375750	7.90825514557225	6.42543858463363
C	6.21478830031346	3.46333247913098	6.30070628675276
H	9.55560889624912	10.43745731860309	6.86672508910264
C	2.94629988642665	7.39492894961080	6.20587681625892
N	6.99602271091824	4.55330827942658	6.42113775817293
H	6.11919884851606	1.31858663097257	6.48637816217547
C	2.42382878648922	8.67414572459887	6.07249147498147
C	6.72707866255060	2.20100051123968	6.59540518901375
H	9.76130647363451	8.05958230137738	7.19261627934213
C	8.26017245167257	4.46306217841697	6.87271093797261
C	9.02407477353050	5.70945417095225	6.95909792756212
H	3.54484373246492	7.13250880134634	7.06609636913049
C	8.02687313471466	2.09048318953565	7.05620400614170
C	6.10955500236003	8.89134372568641	7.33751351965190
H	2.62818137978840	9.41236303046056	6.83716775145714
H	11.08364161835621	6.21439711498555	7.18313969235403
C	8.80005881563996	3.22713890844785	7.21516406757076
H	8.43600203113039	1.11949372651979	7.29949535738324
N	6.18974642376951	7.65253770502242	7.71944678724346
H	6.13239146989583	10.98557266811864	7.85357046308702
C	10.25800718738248	5.83027983592810	7.78939715858482
H	9.81297346468957	3.15157286072239	7.57566406097262
C	6.37983433738534	10.01859854306705	8.27691695181881
H	10.55982039507663	4.88658837277835	8.23072454893476
H	7.43598687741143	10.04803389292460	8.56607468192900
H	4.92917678827947	5.39636236117672	8.44491979804158
H	10.09980530644551	6.53052228959140	8.61533060163610
N	6.62444034345736	7.39839796592620	8.95672190982312
H	5.79614703029619	9.88816522860091	9.19203789883785
C	5.74175288348525	5.13623574122023	9.10690146075079
H	7.15162556265588	8.11392698881599	9.44070075230591
H	5.14481919504428	3.09300912823116	9.30328899868760
C	6.68386989140817	6.09931783768896	9.46578314936744
C	5.86814926862218	3.84338073560691	9.59553279288928
C	7.71058671308112	5.77868901909137	10.35733797083827
C	6.90841935466169	3.50782520582090	10.45601094548286
H	8.42974849119439	6.53660251107014	10.64139663914078
H	7.00876342122022	2.49496142507503	10.82322297696544
C	7.81813683099943	4.48630694235785	10.84795789512034
H	8.62585770258468	4.23797816915832	11.52478977296587

**Cu-OMe (vacuum)**

H	-0.54750479250386	21.64242535650486	7.58109110333828
H	10.78586555289514	15.09296484012104	7.57888064638937
H	1.85206495440143	18.26799777025520	8.88916334835111
H	8.38907789555817	18.46873161380303	8.88772953758571
H	-1.79829588008043	20.38379843668259	7.73565922989078
H	12.03741870903704	16.35100887219176	7.73205558888623
O	-0.04207571216196	19.89381803036522	8.59210777114546
O	10.28220508336452	16.84203474239596	8.58997122103725
C	-0.99298327286066	20.90127129764573	8.24905147395240
C	11.23231169025996	15.83404431192906	8.24628051278104
C	2.09252579330074	19.25344874305798	9.26434127295325
C	8.14832050323185	17.48353669863906	9.26339114724060
C	1.12943477319752	20.26149381053187	9.14686558239416
C	9.11089815398901	16.47503716225632	9.14561601340776
H	4.08188881354844	18.74543604754338	9.84125679225825
H	6.15947894354263	17.99250951967357	9.84138861083344
C	3.33685597486500	19.52400992364597	9.79450165020483
C	6.90420429214903	17.21366763143818	9.79438306038693
C	1.43635512864544	21.55234393425477	9.58426567271630
C	8.80373102764981	15.18444555259233	9.58361015228651
H	0.71970167139747	22.35483403165377	9.49291542387033
H	9.51999974087018	14.38163565507943	9.49205883383993
H	-1.38714796771953	21.39673964443070	9.13983895029721
H	11.62703299168549	15.33857046975475	9.13681740110608
C	3.63256780730509	20.80617392619749	10.25782098805925
C	6.60824306719332	15.93176229347921	10.25825123911270
H	7.41309983344837	22.19334739127059	10.35031152761926
H	2.82772446828605	14.54522549508114	10.35202221613561
C	2.68008035602979	21.81288658316706	10.14385524141309
C	7.56022989617584	14.92460232849665	10.14401443499335
N	4.87677154612536	21.12446792237261	10.83204340590853
N	5.36414133308111	15.61402634792619	10.83300233926139
H	2.90637847734144	22.81345825570753	10.49270211010143
H	7.33367056532084	13.92422227039259	10.49324453948085
H	5.21972501234562	22.06616334733523	10.70070813765598
H	5.02094784622807	14.67236664546455	10.70202906002440
H	8.48852026323979	22.00012501012242	11.73587903665751
H	1.75259940447978	14.73898974387289	11.73773243052360
C	7.46173608541729	21.89644115387845	11.40269218204454
C	2.77931927004227	14.84252808903517	11.40430222828954
N	5.69958449714417	20.20013227372880	11.30962707694939
N	4.54156218647132	16.53867776777729	11.31036518732114
C	6.92592550428487	20.51511514098705	11.60912542969140
C	3.31522958553963	16.22391953781676	11.61009983765303
H	9.66301537440483	20.32406260014894	11.80914960789586
H	0.57821602634575	16.41489547554675	11.81055439778409
H	6.86908165326423	22.61549419870222	11.97771610446982
H	3.37204739673833	14.12365723089863	11.97947812171109
C	7.73470260937386	19.44053270380281	12.18223321951316
C	2.50654064699610	17.29878056659890	12.18276592974890
C	9.12831471425662	19.47155045664250	12.19576670923326
C	1.11292250358761	17.26765156293932	12.19662338895970
H	10.90353848126562	18.36989854175796	12.66665325800987
H	-0.66232362527846	18.36930264105184	12.66740997117939
C	9.82179044608955	18.36993633278008	12.66694611924001

N	7.07748151546656	18.36997850985728	12.66762342906053
C	0.41942511036611	18.36939621919672	12.66743745875301
N	3.16377604376259	18.36964565465119	12.66746076302497
Cu	5.12070156964410	18.36995946358293	12.66741109452562
C	9.12850445380315	17.26836282978568	13.13846522752023
C	1.11271021416936	19.47123999206790	13.13833656049143
C	7.73487796516942	17.29937605555216	13.15269962715356
C	2.50633317707351	19.44033485965516	13.15227879978437
H	6.86990913726154	14.12424561251981	13.35785506029664
H	3.37149032984711	22.61551648895441	13.35667479281964
H	9.66339404350691	16.41582851281481	13.52476701410833
H	0.57783882681149	20.32387346789752	13.52444837485271
C	6.92638074770776	16.22473028600088	13.72602874688806
C	3.31485459556028	20.51512452923578	13.72531620456231
N	5.69995487061564	16.53942991026122	14.02555239618188
N	4.54116340702833	20.20029062688748	14.02507751985759
C	7.46251059608132	14.84354179966656	13.93262877371136
C	2.77882849947009	21.89639336507233	13.93159999809001
H	8.48925480327839	14.73997262355634	13.59929516869463
H	1.75209004101408	21.99994608868365	13.59823578930325
H	5.22068600314066	14.67347609519764	14.63515275026893
H	5.02080119039744	22.06616631116172	14.63463223354386
H	2.90896399503208	13.92448874120590	14.84543837699199
H	7.33378374893340	22.81356400882833	14.84470988866820
N	4.87746028370084	15.61501812940698	14.50341077580427
N	5.36383466132398	21.12454283537176	14.50295740781888
C	2.68159335225684	14.92535636054269	15.19275488624286
C	7.56002604555677	21.81274729410785	15.19289694945148
H	7.41413192573005	14.54683530230582	14.98507911854531
H	2.82722527320268	22.19332570414036	14.98398499568862
C	3.63299374329573	15.93293932742592	15.07720807286032
C	6.60774786370728	20.80598378169291	15.07762664471164
H	-1.38619022583795	15.33861045635028	16.19695011930284
H	11.62670761556278	21.39661182392523	16.19963873624568
H	0.72183599525696	14.38229221090873	15.84464057897103
H	9.51990465172680	22.35447949042612	15.84547735331391
C	1.43765094243162	15.18539147036085	15.75207592726313
C	8.80341340327883	21.55196233864086	15.75310037296459
C	3.33588543974330	17.21552382515031	15.53845781826525
C	6.90339253665402	19.52347861987670	15.54002633040777
H	4.08001716182903	17.99487217634515	15.49012508258441
H	6.15854135334093	18.74478770079480	15.49207501515754
C	1.12938682019181	16.47657718735616	16.18756300366489
C	9.11026333457425	20.26080933402472	16.18968793222069
C	2.09134051724548	17.48552781036355	16.06840036635425
C	8.14742463358448	19.25268605150705	16.07077334505941
C	-0.99212566163653	15.83577296196669	17.08683536532333
C	11.23182948949927	20.90035428724124	17.08967044631101
O	-0.04249913613021	16.84378073405741	16.74184445702158
O	10.28148942087745	19.89293607759258	16.74491469884941
H	-1.79774800476731	16.35309871932926	17.59989099903110
H	12.03678642303384	20.38267008099604	17.60340826198368
H	1.84969461506163	18.47127578795634	16.44203712343574
H	8.38782701453564	18.26696509904901	16.44527957293425
H	-0.54549395595538	15.09606949489421	17.75563529849014
H	10.78553828117722	21.64086954217272	17.75779442077328

**Cu-OMe (EtOH)**

H	-0.58153669873543	21.72098027329012	7.61805115696874
H	10.84677477451253	15.01127318233929	7.65438477738977
H	1.87986615604468	18.26954977492152	8.85988710768353
H	8.35796315358681	18.47037682860712	8.85550870838969
H	-1.81483260779002	20.44574387478202	7.76649003473661
H	12.06818106954612	16.29800583056748	7.80056810953608
O	-0.01221354154785	19.91930392621692	8.50103686123249
O	10.25267800387733	16.82106480392819	8.50489575937286
C	-0.98324437082934	20.93767349224106	8.26623320578583
C	11.23396742866454	15.80665179169709	8.29650539027072
C	2.11438699372613	19.26094867285115	9.22554695997594
C	8.12321983837419	17.47929165221781	9.22174178329422
C	1.16274127480925	20.27340670960098	9.09318987132036
C	9.07606612562063	16.46729624009613	9.09400736368130
H	4.08233000838718	18.73677916347328	9.85601127944071
H	6.15305897321062	18.00314247750575	9.84578826014518
C	3.34945226586052	19.52492672942741	9.78672684660176
C	6.88700634814225	17.21557058334859	9.78053386518743
C	1.46133284876896	21.55920747924866	9.54245987446287
C	8.77685981921294	15.18187624518151	9.54402784271594
H	0.74744124100913	22.36432709479924	9.45010740426437
H	9.49130726669867	14.37701346151640	9.45377107835391
H	-1.33354662509791	21.37957398228492	9.20249791441763
H	11.57491788229273	15.38030571075822	9.24344943128757
C	3.64237757346088	20.80571413585502	10.25968556042676
C	6.59413464351688	15.93566602609379	10.25597087085013
H	7.36687487912693	22.23638385826697	10.43577203937668
H	2.87613131460297	14.50444079799989	10.43360235417034
C	2.69395680619620	21.81569634123980	10.12822559802022
C	7.54311680640048	14.92569881008784	10.12761422761094
N	4.86327811952705	21.11974387793717	10.86450832065455
N	5.37274401494899	15.62250406844768	10.86007152478579
H	2.91645418781420	22.81151367486235	10.49006467717303
H	7.32074841509657	13.92986225599591	10.48996673518484
H	5.15256702304489	22.08929601288792	10.86210420721096
H	5.08471730467684	14.65275270286440	10.86100952866270
H	8.44990846732658	22.02129710100105	11.81617641356056
H	1.78901977092831	14.71571434704012	11.81127923412143
C	7.42355153427901	21.91491850869291	11.48022578197362
C	2.81620244216428	14.82388676751275	11.47853186127879
N	5.69645596589679	20.18900669698736	11.31437298803918
N	4.54056256975265	16.55220915505864	11.31375940736630
C	6.91029149862537	20.52329597543003	11.63973775266776
C	3.32754910012654	16.21587407434543	11.64102871553771
H	9.65358915911916	20.33790171820171	11.82719198716517
H	0.58397468677210	16.39409277788664	11.84562490668734
H	6.81658149343952	22.61044810107254	12.06855091016191
H	3.42239848603917	14.12774387530925	12.06715410308383
C	7.72847483776306	19.44529112646547	12.19273509628446
C	2.50946329683105	17.29125818678817	12.19908397245683
C	9.12146866693303	19.47766364432199	12.20125204711912
C	1.11654302433435	17.25560025752249	12.21601104004745
H	10.89626680695788	18.36177168732715	12.63894307403958

H	-0.65822380309751	18.36589078219057	12.66871352419643
C	9.81441339685026	18.36457766674054	12.64818272376331
N	7.07356180520899	18.36940136176120	12.66542753159525
C	0.42366373135014	18.36642808482664	12.66869038055574
N	3.16440863836941	18.36810188895226	12.66969928981453
Cu	5.11894103479441	18.36937007332891	12.66849502360208
C	9.12304722188416	17.25499443735306	13.10626434153296
C	1.11502653804205	19.47783749669396	13.12240000606654
C	7.73023716516595	17.29179720646683	13.13222418668758
C	2.50796159515351	19.44394952164735	13.14070758764599
H	6.82840418875269	14.12846187953607	13.27060599761653
H	3.40842403109012	22.60817058155311	13.28002888060005
H	9.65713350130508	16.39297755486340	13.47301344580178
H	0.58110756058545	20.33840806263067	13.49285885604719
C	6.91484948059232	16.21694173580122	13.69539680405608
C	3.32417647413420	20.51930723651725	13.70166610342028
N	5.70134867045892	16.55138855045967	14.02262675056262
N	4.53914656592040	20.18534089720726	14.02383935445639
C	7.42891736166769	14.82654547460396	13.86258814262491
C	2.80933253710535	21.90912798507107	13.87226164096505
H	8.45847779013548	14.72002850524241	13.53685102793595
H	1.77927317691776	22.01508982775105	13.54787262999842
H	5.16713440694341	14.65440910258725	14.49781980551007
H	5.07374541291021	22.08210434175647	14.49807946228053
H	2.92449682511544	13.92872003419042	14.85708661642749
H	7.31769280600643	22.80819718849951	14.85277847948608
N	4.87117510283254	15.62170378366909	14.47998818100063
N	5.37050663205871	21.11517491945269	14.47882336929135
C	2.70127998772349	14.92582469114995	15.21546169089526
C	7.54146443204071	21.81114275765178	15.21085905803535
H	7.36214821492556	14.50827162920102	14.90729995614599
H	2.87751591546049	22.22619504888896	14.91734002770305
C	3.64947323540269	15.93609814578583	15.08363045298488
C	6.59330243550540	20.80076539375774	15.08009370630565
H	-1.33185679976128	15.37932449333417	16.10064756538681
H	11.57155159684121	21.36884728471887	16.10364252269330
H	0.75307137184573	14.37822860371493	15.89026839452609
H	9.49039436905107	22.35887632941913	15.88334148330807
C	1.46701866753481	15.18323250163818	15.79739841782744
C	8.77652608797886	21.55374946998752	15.79100234523862
C	3.35509984422065	17.21743944089771	15.55401772604561
C	6.88861342657786	19.51923212642667	15.54932953290119
H	4.08796122935771	18.00563765781778	15.48587338005103
H	6.15551977013469	18.73118220671202	15.48223284982301
C	1.16661125049528	16.47005665212910	16.24270628525748
C	9.07779418961706	20.26677148618883	16.23517225980029
C	2.11861964703791	17.48235640601779	16.11160036295989
C	8.12594553930730	19.25426402367951	16.10487083097526
C	-0.98976701237724	15.81016009330516	17.04509780619781
C	11.23105560116981	20.92855722795129	17.04424938858052
O	-0.01027046071516	16.82501036549789	16.83027862842081
O	10.25557319784220	19.91171710169072	16.82084122244538
H	-1.82364167414167	16.30262312245741	17.54052121343538
H	12.06694622064678	20.43543651967929	17.53557442315884
H	1.88314575620259	18.47454685677755	16.47435750739055
H	8.36218015458903	18.26219221574163	16.46757582439856
H	-0.60013797188214	15.01822737854800	17.68999929285838

H 10.83776940506853 21.71328204347624 17.69576387847395

### Cu-OCF<sub>3</sub> (vacuum)

F	12.26310479015844	9.22479931121157	0.99796589520065
F	11.26688457838384	11.14519676517737	0.85891846055168
O	10.11546956577813	9.22538429255506	0.72753085698104
F	-1.96355869103750	8.28549039462899	0.29396827285678
O	-0.20025931121307	7.02222661709274	0.23074996132839
C	11.15893813869018	9.88652941877546	1.29640729952296
H	8.35526088193278	7.42824556794349	0.79124152790855
H	2.25210082985129	7.88034358971542	-0.03125236863079
C	8.81360721453541	9.48080871777915	1.13199859347232
C	7.96772406998109	8.38169468291934	1.11987843427539
C	-0.93364663821412	7.86448533742721	0.99370997232672
C	0.92371219724156	6.43660104847031	0.81850017787701
C	2.16881778728502	6.99604424576780	0.58441043161800
H	8.98007673354832	11.60499601558641	1.45066500846119
C	8.33867456204600	10.73723782081602	1.48822962856793
C	6.64973874836402	8.51868312485924	1.51691317570675
H	5.99196677674466	7.66589338389671	1.50171255446433
H	-0.19890617029448	4.84746741551430	1.71100809870721
C	0.78279697629856	5.27339430554294	1.56217743306674
F	-1.38125981467988	7.27792980680477	2.12497378782319
C	3.29434372523321	6.39078777257352	1.12377208751789
H	4.27133845083191	6.79854270151222	0.92017218716375
F	11.04203857395605	9.94230569121980	2.64456414190492
F	-0.20751798981573	8.94201137677032	1.39328859897508
C	7.02293689100906	10.86426446102328	1.91100779610314
C	6.18064050034766	9.75327773731584	1.95733535866411
C	1.90758039039795	4.68653232794383	2.12094034857385
C	3.16336312150886	5.25248732405822	1.91286428920253
H	6.67211924799638	3.34227306146595	1.62425840393030
H	6.65414466571380	11.83735167583716	2.21091278723786
H	2.20341199150459	10.58278523164751	1.99940273067773
H	1.81008868672554	3.79669857858435	2.72846133318326
N	4.86686060849771	9.91734404154761	2.42615662118885
N	4.29644697986147	4.64594882964958	2.52060331237284
H	4.43239154133898	10.82300528967215	2.31442295131861
H	7.93393626469717	3.35708597226822	2.85665198592413
H	4.51436122070642	3.69765344005880	2.24024085756127
C	6.88551950402243	3.56846950844066	2.67326058034147
N	5.31237886452813	5.43558281331497	2.90239332623274
N	4.20465343380888	8.94808876779221	3.05268938842369
H	1.21758300721901	10.40238428463480	3.44427605386893
C	2.23687434009149	10.40187193441711	3.07788532002466
C	6.51778840905914	4.97703518915945	3.01592508381245
H	9.28934137639255	4.94439384936663	2.87130463838824
C	2.96434048901591	9.13147993333064	3.39039973619787
C	8.87398140938776	5.80405198910711	3.37403555870763
H	6.30668245312375	2.87042820298623	3.28551657241129
C	7.49960926820219	5.94326872026412	3.53394722543119
H	0.29106512151963	8.71860082149126	3.93940954686364
H	2.74252997784992	11.25211319980053	3.54596328137165
H	10.77861780133928	6.72665021256383	3.71880904814890

C	2.32388590865038	8.02690704680564	4.11325489622825
C	9.70712960589291	6.81018589889573	3.84117997907339
C	0.94575435876898	7.95279185500687	4.31871245202184
N	6.99753016883552	7.02883888796943	4.14810080372234
Cu	5.06175202664240	7.15063504219225	4.34879518611982
N	3.12116998753041	7.04787612250889	4.58058306615124
C	9.16750220367751	7.92272340213093	4.46413854426768
C	0.41698637958527	6.86132250142516	4.98524092829430
C	7.78408499244529	8.01346939559576	4.61532634256289
H	-0.65023611387844	6.79207232860825	5.14735881604733
H	7.33341482343099	11.24819643422515	4.99174568712730
H	9.81625259028171	8.69464428356552	4.84097307470799
C	2.62616799135216	5.98054131246813	5.23437832056862
H	3.815644445394025	2.90234447993956	5.46034755962486
C	1.25697082127395	5.85765937676224	5.44283437172739
C	7.11110757158799	9.14095392593462	5.26795376341214
H	0.85343558727528	5.01314874152094	5.97961073042129
C	3.60302298990081	5.00554772294131	5.74995119506499
C	7.81377952799542	10.43282429584279	5.54137281104054
H	8.85222402107552	10.41442541294740	5.23146628103314
N	5.85925051665454	8.9522028372662	5.56399206354967
N	4.80816029612543	5.45653292414358	5.88139716869024
C	3.22322780990353	3.59338331456736	6.06763454734254
H	5.59655652105079	3.70928551791473	6.53821719185412
H	2.17926939672554	3.38689661290550	5.85526581339735
H	5.58096419002937	10.85145501590945	6.22026120829161
N	5.81707835404304	4.65869160551440	6.26336798558563
N	5.14787109853682	9.94668429550916	6.09627549009977
H	8.28672500594344	3.74705244298522	6.11137691195390
H	7.78593068707803	10.68130042163848	6.60642695507144
H	3.25321632346432	11.76279921018817	6.29025051537817
H	3.41043992320142	3.35227985716202	7.11829047930429
C	6.95597390624424	5.25553351101697	6.86773115216724
C	8.20107495533618	4.65520780838290	6.69321853751235
C	3.87771568801871	9.74016819300612	6.66609637911233
C	2.97445155811483	10.79988547069929	6.70031852899634
F	10.34489321615080	8.91539843875495	7.40050443393369
F	-1.27572652639183	10.02336388743250	6.87337138624277
H	5.87359598572905	6.85584681963006	7.80117241168241
C	6.84231709131385	6.41950934758081	7.62211648620843
F	11.50258869139764	7.24874182562105	6.64968853903616
C	9.33121462988794	5.23063232619950	7.25378437764082
H	10.30523933385664	4.77902240847477	7.13135059646626
H	4.21247432998296	7.69621091788356	7.22223243472518
C	3.51325197219471	8.51515589224085	7.21894132760221
C	1.71243463112322	10.64098554072694	7.25831828611133
H	1.03533791726942	11.48041012724233	7.28999092643241
C	7.97329329510823	7.01192159680067	8.16327722621917
C	9.20730451041831	6.41555666096865	7.96470399012816
C	11.06853992791367	7.83263797077930	7.78826461318456
C	2.24961989337079	8.34283209384052	7.75172312769827
C	1.34799134635391	9.39932929603877	7.76781680360539
H	7.90255944657029	7.91435243230292	8.75363570446053
H	1.95270438240152	7.39729697066820	8.18239075462850
C	-0.96827870682453	9.88362208833625	8.17929457030524
O	10.33819178804865	6.98833609352659	8.55168426112047
F	12.10689823562926	8.24315978122472	8.48168780321697



O	0.13031067944252	9.09690739931605	8.34942170721978
F	-0.80365017078193	11.11022730474873	8.68990644176510
F	-1.97615457837114	9.29053302480210	8.79163269903126

### Zn-H (vacuum)

H	5.40155241516282	6.95083583048134	0.97522537735546
H	4.32663813595603	8.23974256070128	1.51760665026882
C	4.71509599747863	7.25966787283394	1.76924454009321
H	3.85976082858463	6.57729572079466	1.76354009567867
H	5.33692796889730	5.00614602103762	2.01645291387226
H	5.30889181513354	2.47444056155949	2.54184736239829
H	8.37419781244307	9.23485543222005	1.79796027803799
H	4.82303650279622	9.88991520206050	2.54779462969570
N	5.86786393378178	5.01169738173110	2.87594885174107
C	6.33148874096657	2.64931649979169	2.85358256074918
H	8.82100874512981	11.62227982519476	2.27007467597028
H	6.86674809861604	0.57989824559165	2.79972723408955
C	5.39963849346797	7.23148035639815	3.09752759335010
C	6.77229722537523	3.95173464623639	3.08780364285027
C	7.20948419290382	1.58610434786889	3.00108370263869
C	8.62845793763036	9.55053240662627	2.80149487410752
C	8.88034433938787	10.89130106305201	3.06475735859300
C	5.10265987485135	9.68915045796967	3.56918573207049
N	5.97249726158288	6.16093913020735	3.55208584064822
H	1.92799104657610	5.48567592657167	3.34021995378057
C	8.08712636921937	4.18583569564073	3.48104781750525
H	0.77757829631742	7.63146439231159	2.92388566260139
C	8.52336430380912	1.81373354760975	3.39785451571087
C	5.42844912428337	8.40165432551603	3.98632925775098
H	8.58708355326060	7.55004869632149	3.59346843689588
H	8.43374460717120	5.19790717013483	3.63263418558149
H	9.21040772367201	0.98469647467594	3.49758112320483
H	4.92345974946375	11.73338506609222	4.17982931744237
C	8.73864851666431	8.59787051871862	3.80644499393704
C	8.95434590079103	3.11343767013510	3.63984156556864
C	2.05766606625343	6.31559191703796	4.02526053887533
H	4.01176766617337	2.20324298129284	4.92782072947889
C	5.16901561190827	10.72553113577991	4.48600820805562
H	3.02864466894334	4.11035244357853	4.95911025867772
C	1.41237105277930	7.52178967599973	3.79306169469965
C	9.23738837532229	11.28512955402353	4.35075394391755
H	9.98142679394677	3.29851353153514	3.92486098807810
H	9.44914516376525	12.32457510255258	4.56351606626227
N	3.46533601622682	4.91622622346794	5.38233245439918
N	5.80523081355405	8.17800958050780	5.25334904615502
C	2.86632123659227	6.16534042240050	5.15242193328763
C	9.08922349009701	9.00020869930262	5.09164590972369
C	4.27658632603924	2.39107494311889	5.97383679287360
C	9.33284532127369	10.34608691080952	5.36601461071126
C	5.54612396256271	10.46950402590114	5.79429651918962
H	4.73504649855799	1.48514094035480	6.35015209182230
C	1.57474965374428	8.58332980369932	4.67731493131860
H	3.34758571709464	2.55687185888313	6.52642587103158
N	4.71626529636557	4.77983096075846	5.84161939327108

C	5.15997449261304	3.58783741968967	6.09946239750029
H	1.06661240007451	9.52042558906379	4.49591939262836
Zn	6.35132471169209	6.29237089842072	5.79791585406657
C	5.86247711058723	9.16254672908675	6.16103896918437
H	5.57845713203289	11.27367810501054	6.51126212372552
N	8.73541920908264	6.85252081510856	6.11806116665816
N	9.26629389226693	8.07785160906618	6.14056569070407
C	6.56260286622987	3.48661518561202	6.52565022823312
H	9.60969570238330	10.65166423663466	6.36801450970147
C	3.00853388684928	7.21564078649435	6.05519372492366
N	7.28925235414323	4.61802586701455	6.49817996875176
H	6.56254244519783	1.38241959565896	6.99616690429908
C	2.36815342751952	8.42251035191906	5.80754023736474
C	7.13473648341785	2.29401861364021	6.95920550362050
H	10.06192505457656	8.24147384524135	6.74209552952708
C	8.56852647554665	4.64048506322470	6.90275379882928
C	9.27643354508570	5.92575470355216	6.84539123675025
H	3.59415163882368	7.08074722952813	6.95277869065099
C	8.45798047399781	2.29485046468133	7.36960140887841
C	6.25632179322461	8.77521417294262	7.52449223580558
H	2.46786308919192	9.23378691081857	6.51659784945135
H	11.32578114329452	6.55739783518969	6.97173979536239
C	9.18416954368590	3.47095444004730	7.34854913769451
H	8.92072176433275	1.37813527957350	7.70944402200645
N	6.27788401379360	7.50114793998300	7.76922137645107
H	6.41331050705169	10.80225507806396	8.24932682314585
C	10.53893430130704	6.15916991116770	7.61942360987692
H	10.21635515468551	3.47162575941536	7.65880038357190
C	6.66958694834028	9.79002199293044	8.54174998347048
H	10.91955221602645	5.25950832276003	8.08881293310861
H	7.75398809051782	9.76082250129282	8.69479157823031
H	4.48773868997070	5.69980437886240	8.53944647861879
H	10.37126718329571	6.88362358987817	8.42419634366167
N	6.77201257790431	7.04974580798207	8.92623625639821
H	6.19050790781620	9.59522323202179	9.50517459199726
C	5.21461257310811	5.17529643017426	9.14109797074317
H	7.12737668283708	7.72251813937747	9.59121164345105
H	3.96991121234100	3.46313304879309	9.44763370803625
C	6.44134345917331	5.76877825279412	9.42103691676587
C	4.92884090138778	3.91859699120865	9.65778170670379
C	7.36563514094998	5.11814345173821	10.23751832327338
C	5.84452401375036	3.26424116529028	10.47256986384930
H	8.31695260173571	5.58708058153841	10.45646823370549
H	5.60445334086135	2.29731924005504	10.89283273894596
C	7.06260317932369	3.87147013683485	10.76445527467691
H	7.77817342539751	3.37352554352947	11.40508315898289

### Zn-H (EtOH)

H	5.34868024558211	6.47675944420892	0.94202629689357
H	4.16579223960730	7.70424693817972	1.41552619374551
C	4.64183908988460	6.77879544145308	1.72076602407089
H	3.85681703576848	6.01875259593132	1.76454562085907
H	5.25569623071195	4.57865102809970	2.22331582238675
H	5.57119506200757	2.17572525957608	2.51899068863860

H	8.35007804507913	9.44287688206032	2.27786145789582
H	4.80106955494224	9.46332943950998	2.17862523209612
N	5.93007225454497	4.71722596840106	2.96399232633905
C	6.58250457405186	2.41832142620499	2.82070736987630
H	8.83384002711497	11.76879890411601	2.98921572317992
H	7.28093732918903	0.40489542976003	2.67061788611376
C	5.34534478816991	6.90043775852090	3.03309241762632
C	6.91694553004705	3.74225881184476	3.11737845428886
C	7.54714575694833	1.42699791041819	2.90897423173147
C	8.60464678999878	9.65454406415416	3.30850449090523
C	8.87868485936167	10.95927679695582	3.70591424935238
C	5.04588553606037	9.38631032606064	3.22594251608167
N	5.99937095461832	5.91306042286037	3.56008550171145
H	1.94342010527733	6.02848786615111	3.29212731507447
C	8.21376838882873	4.06341942622627	3.51624281618981
H	1.09229834356069	8.32648728170609	2.97578255751730
C	8.84344359813676	1.74019337196043	3.30833317470708
C	5.33826602201456	8.15109385574068	3.80177190408906
H	8.49053564394274	7.59096786107703	3.89606890435681
H	8.47544624002107	5.09108286717757	3.72330369316535
H	9.59525038829105	0.96476679545351	3.37686722107272
H	4.90713899701458	11.49199581122232	3.57900952716922
C	8.67146856370726	8.60658003618509	4.21708277562314
C	9.16625294924212	3.05758567319122	3.61570480255184
C	2.06266626991623	6.76776583884612	4.07421274260669
H	3.65714130840027	2.49140229228914	4.54609637253289
C	5.11406366682823	10.52289802594901	4.01207847433825
H	2.79441427369929	4.41808477452942	4.78907709034979
C	1.58477964465946	8.05818494796084	3.90156958485418
C	9.21614642285286	11.21497317044928	5.03188208448124
H	10.17231603532550	3.31253626737094	3.92348446239278
H	9.43116939144517	12.22543613613678	5.35610182962070
N	3.20492575903047	5.11555421963076	5.39608008940772
N	5.66343736512536	8.06911692445352	5.09948008134002
C	2.72464541090260	6.42457361793307	5.25326580520752
C	9.00294505091866	8.87115665438051	5.54570187264562
C	3.89811482638698	2.51169609809980	5.61465634406931
C	9.27256056989879	10.18068374835325	5.95285700696074
C	5.44361227439801	10.41914347691292	5.35442640195347
H	4.30709564456579	1.54192383882580	5.87473572801104
C	1.75594756579308	9.00943730099121	4.90190936948439
H	2.95780780296783	2.64447793456369	6.15648301724560
N	4.44756725603433	4.87015399683253	5.85412740465645
C	4.82695578220178	3.63256425777987	5.93497512085448
H	1.39634541239711	10.01973924135424	4.75865371557966
Zn	6.22272015784855	6.28904796177356	5.92333279128085
C	5.70510216709741	9.15828492203851	5.88400588770212
H	5.47729397365873	11.30131232749696	5.97235984503111
N	8.53420560505274	6.65702669242559	6.33291338785532
N	9.11170405515547	7.85377171498012	6.49397750215892
C	6.22020488381833	3.3992487776571	6.33634921644861
H	9.52769842635271	10.37809206781419	6.98679900975823
C	2.86568573695801	7.36172087502599	6.27389731285488
N	6.99991862725724	4.48382352090055	6.46297797816270
H	6.11697193326408	1.25091165029733	6.50070372246962
C	2.38546111332203	8.65181627282227	6.08941014994408
C	6.73062532502768	2.13069385621887	6.59962591290760

H	9.80852820923141	7.96554126033531	7.21821352076033
C	8.27195473264999	4.39044977268237	6.87544023581721
C	9.03212687928846	5.64239855947011	6.96800629549884
H	3.34447145517923	7.08138089372969	7.20191740648243
C	8.04626601099652	2.01435117741487	7.01851365184321
C	6.02473978297407	8.93647020892652	7.29986626024278
H	2.49749518688996	9.37959051808199	6.88266994556399
H	11.10761549044694	6.11322906134319	7.11749997922558
C	8.82637873092212	3.14694481661104	7.17149880950860
H	8.46276581922470	1.03920117304990	7.23116132467225
N	6.13872964172208	7.70128937573356	7.67998444674687
H	5.95813295658311	11.02369522611610	7.82709479951263
C	10.29855138374277	5.74082925614679	7.75313245658986
H	9.85341999631298	3.06042764691789	7.48721671247914
C	6.22892177481893	10.06437140963395	8.25255349390829
H	10.60186689911302	4.79050720853612	8.17852550785132
H	7.27486676453058	10.12816276013165	8.57179764313244
H	4.87153144924991	5.40463068581257	8.56750134745774
H	10.18511574303985	6.43841431886604	8.58768651885160
N	6.53305892167876	7.46561115343184	8.94360147299883
H	5.62637114902511	9.90169191752880	9.15032793623316
C	5.74974527035484	5.17060823437196	9.15200821493395
H	7.05902462631648	8.19382729892740	9.40863260760332
H	5.23050551407456	3.11083564924176	9.40163790343826
C	6.68671163476943	6.16326065708969	9.43220659470489
C	5.95395051809650	3.88269393539822	9.62991848434104
C	7.79003204436053	5.87718103080676	10.23839867918953
C	7.07261948339606	3.58199181150964	10.39912200591521
H	8.50312365737525	6.65888153312486	10.46804408594570
H	7.23533652669807	2.57356228655760	10.75604124774502
C	7.98003767364205	4.58896030407815	10.71565589407851
H	8.84896319100921	4.36720076078378	11.32191300625112

### Zn-OMe (vacuum)

H	-0.52675143113568	21.71122737913836	7.65635409734290
H	10.76777612233977	15.02841844437408	7.65587453524548
H	1.86674907861788	18.31126333719033	8.91225969747490
H	8.37296792529987	18.42740723639561	8.91130468922499
H	-1.78388619425559	20.45981773635381	7.81621213673600
H	12.02440719782980	16.28041655600833	7.81509448208593
O	-0.02072427892244	19.95101239616134	8.64685621020733
O	10.26127741063057	16.78859595497577	8.64620560797914
C	-0.96873845410131	20.96750798398341	8.32375104047444
C	11.20964632888396	15.77246044318974	8.32299081330968
C	2.11617790107798	19.29206448364468	9.29362298021626
C	8.12411026619388	17.44661168938699	9.29305366007468
C	1.15861577655646	20.30667240246985	9.19296372129859
C	9.08220543586955	16.43248399473499	9.19260773404000
H	4.10879970229985	18.76855296777472	9.83747615820090
H	6.13125903146135	17.96921056116396	9.83694428249332
C	3.36775061518769	19.55213722534236	9.81287710468268
C	6.87273894645469	17.18602989121550	9.81252010928592
C	1.47845984204560	21.59224313913358	9.63588873181933
C	8.76310964579089	15.14688672661210	9.63601258827665

H	0.76705223905475	22.40049016659063	9.55489347646035
H	9.47495389277737	14.33900199552281	9.55521990835619
H	-1.34834032122048	21.45845807241137	9.22339618118855
H	11.589754449324947	15.28184913077114	9.22260473829452
C	3.67590911178365	20.82741620555791	10.28604663416207
C	6.56533403545625	15.91075454373886	10.28617629168415
H	7.47905661581950	22.17749822738921	10.33990195891974
H	2.76262128264510	14.55923826544965	10.34066064989596
C	2.72835271679490	21.84026662696699	10.18737760650943
C	7.51341738673858	14.89837727061041	10.18774561956921
N	4.92923782722339	21.13788615375580	10.84842311478462
N	5.31224132248525	15.59987973243835	10.84886322106346
H	2.96433400427962	22.83664920356815	10.54144158954509
H	7.27802302197587	13.90200267994618	10.54221405803810
H	5.30379753526165	22.05637686528729	10.65634540417253
H	4.93801248640369	14.68120233008954	10.65701119216210
H	8.54132799843379	21.99414387756649	11.73681005358434
H	1.70022564682979	14.74295695701015	11.73743198744522
C	7.51723854797269	21.89010050448606	11.39568425569326
C	2.72430935855712	14.84709866250599	11.39631012665398
N	5.74617130235563	20.20532569991974	11.33103049721187
N	4.49495691292578	16.53233374411158	11.33106781866086
C	6.97710287512312	20.51242966089928	11.61269659442302
C	3.26409896002604	16.22499541997492	11.61277129273734
H	9.72393016227391	20.31018243053702	11.78014334530804
H	0.51718675004430	16.42696304456553	11.77920334628491
H	6.92002356948244	22.61488188934804	11.95826401146379
H	3.32167741516280	14.12271584282333	11.95924694472284
C	7.79392408186942	19.43694113162963	12.18146071720700
C	2.44695232019649	17.30051998824274	12.18101620617875
C	9.18757700712693	19.46694074139558	12.18448447025011
C	1.05329305693846	17.27036267609995	12.18355030550092
H	10.96138730636349	18.36836680558730	12.66793115730012
H	-0.72081177417330	18.36887078413919	12.66602721604614
C	9.87955513803114	18.36847762854826	12.66770633216768
N	7.14054034578418	18.36878099502900	12.66725108155222
C	0.36102055206894	18.36886825286756	12.66623783041688
N	3.10002630193845	18.36887817410280	12.66676129365056
Zn	5.12027964679150	18.36918414716784	12.66676424140063
C	9.18716821221239	17.27015475887471	13.15064676768282
C	1.05310910878241	19.46737991727325	13.14920441794606
C	7.79350735144757	17.30047322164649	13.15324704054019
C	2.44676415799808	19.43722368511830	13.15229749008062
H	6.91846214358563	14.12278268324766	13.37584619056226
H	3.32112645339289	22.61508745308159	13.37491869397936
H	9.72319093366118	16.42680091469929	13.55520192461364
H	0.51683845935940	20.31074641033062	13.55339647492287
C	6.97627757710907	16.22514093856713	13.72175853187104
C	3.26371793929237	20.51272056176516	13.72090831611738
N	5.74545126705894	16.53260209086606	14.00346020347332
N	4.49458001567460	20.20546892766249	14.00273783391617
C	7.51597623519526	14.84725990818126	13.93849594146994
C	2.72377808546877	21.89050807169228	13.93761329646023
H	8.54000101635929	14.74294012484619	13.59724744640894
H	1.69971783302600	21.99463499018491	13.59641974973308
H	5.30259056036970	14.68158951930015	14.67787337147973
H	4.93715648075213	22.05644425755357	14.67747874348255

H	2.96290325605599	13.90203123503687	14.79361817654453
H	7.27679575025307	22.83624309472208	14.79347282186096
N	4.92822288904595	15.60018088049717	14.48585876467839
N	5.31162877873458	21.13791923708445	14.48538802353877
C	2.72749435765201	14.89840646624947	15.14809350974979
C	7.51236022161856	21.83978147364208	15.14759911493029
H	7.47780416872590	14.55967888911879	14.99422848178715
H	2.76194767489022	22.17811126875441	14.99334091075623
C	3.67530585946895	15.91097960353134	15.04900908855302
C	6.56463464176202	20.82714759424512	15.04835296212661
H	-1.34847429925555	15.28077503528894	16.11649545961041
H	11.58836110436373	21.45741501956778	16.11469574425073
H	0.76644670772214	14.33863579169456	15.78177747011646
H	9.47340356089632	22.39957059154892	15.78127512565253
C	1.47807341854245	15.14667109405198	15.70055762112861
C	8.76186510878460	21.59147993897308	15.69985165283471
C	3.36786761644872	17.18623707358288	15.52269292039184
C	6.87225436268144	19.55177062786216	15.52161972132395
H	4.10918118925056	17.96955605406059	15.49780285908697
H	6.13101726667258	18.76837583679603	15.49654472234935
C	1.15895455732309	16.43221578024785	16.14409072761564
C	9.08117850755285	20.30582232687429	16.14291564026115
C	2.11677262169183	17.44654960504868	16.04300194220279
C	8.12345660353269	19.29141305228651	16.04163953084138
C	-0.96759224118104	15.77171672965174	17.01559754924710
C	11.20794739636612	20.96626785511315	17.01388712014892
O	-0.01987831253001	16.78808742460054	16.69117218618175
O	10.26013177904600	19.94991835826051	16.68971534373215
H	-1.78199585455647	16.27953748717768	17.52420482291420
H	12.02262468843349	20.45839127075530	17.52199665173665
H	1.86795335819262	18.42733319562750	16.42481078203220
H	8.37245225113122	18.31053173039385	16.42307982843383
H	-0.52477975804792	15.02798593574563	17.68243916523712
H	10.76543293700904	21.70984892911497	17.68109197226770

### Zn-OMe (EtOH)

H	-0.60629229463933	21.76108414768678	7.73225483140284
H	10.87210442221396	14.98331673719822	7.76430573897278
H	1.87697760864899	18.29035441609587	8.90162065199599
H	8.35511180769564	18.45356924243549	8.89819356187387
H	-1.83707235160251	20.48909385829565	7.91889232362864
H	12.08780116459746	16.26932904977201	7.95033292187813
O	-0.01113209039233	19.95313318206710	8.58563336124266
O	10.24919051244876	16.79594193355585	8.58875012520924
C	-0.98636577797382	20.97575329212699	8.39082906728066
C	11.23611673376326	15.78018683799248	8.41792275587236
C	2.12534768646537	19.27937746433070	9.26446202794798
C	8.10843899018973	17.46389064916936	9.26026658060243
C	1.17907781311124	20.29878388607557	9.15191423221498
C	9.05782320645056	16.44700815552560	9.15049093675443
H	4.10300521711239	18.74209300190428	9.84452099758439
H	6.12837293115370	17.99652470292273	9.83638988795638
C	3.37351515940356	19.53516504161274	9.80019072959646
C	6.86003588199341	17.20530452014409	9.79405851004178

C	1.49765588415292	21.58288889375566	9.59178489039108
C	8.74082506359673	15.16183064545440	9.58835895119450
H	0.78974835807734	22.39430252315838	9.50904264996808
H	9.45018516367608	14.35168241585633	9.50573584381837
H	-1.30078462172859	21.41413637327622	9.34149809642378
H	11.54269688777919	15.35637357455518	9.37779198789310
C	3.68493536608188	20.81193020795752	10.27128509333295
C	6.55136758380878	15.92834674782756	10.26639820002730
H	7.43856497612757	22.20064693496177	10.39460062546248
H	2.80671175601905	14.53406718794411	10.39928568962434
C	2.74252308725037	21.82946249589159	10.15556410735915
C	7.49575674077240	14.91257729281002	10.15053133770886
N	4.92020150391328	21.11960301929899	10.85084981772146
N	5.31740392734022	15.61934419514542	10.84829163811339
H	2.98059146493210	22.82380337374942	10.51197998006465
H	7.26005634137962	13.91725480343569	10.50577373375222
H	5.24033029596903	22.07689612239960	10.78718311371433
H	4.99599103301538	14.66294774699539	10.78240380993216
H	8.50639507441533	22.00839477004682	11.79060696422756
H	1.73392658554322	14.72498954577888	11.79100054805834
C	7.48318514179780	21.89962490128318	11.44599740863157
C	2.75844131424419	14.83466541150805	11.45070332493508
N	5.74304557472985	20.18682805563223	11.32437619497637
N	4.49538759163082	16.55038822390724	11.32661829610300
C	6.96248592662825	20.51422845418098	11.63078925299886
C	3.27736969631206	16.22073961796108	11.63675147347402
H	9.71518059300309	20.31842561482399	11.78992755995320
H	0.52412850299245	16.40739550803218	11.81815078869461
H	6.87159634719546	22.60817927589036	12.01317966454764
H	3.36828658145827	14.12573940794528	12.01953417859306
C	7.78736530972798	19.43923792439614	12.18801172969091
C	2.45256054814831	17.29386569632505	12.19811517003353
C	9.18060004952663	19.46940102547469	12.18552875000667
C	1.05938285097728	17.25929279773840	12.20642720856296
H	10.95307036576786	18.35665059578828	12.63978920901838
H	-0.71322188710556	18.36623833819160	12.67503225877060
C	9.87109688573445	18.36034844495693	12.64877847379277
N	7.13658739045593	18.36763611562840	12.66611851834888
C	0.36878840960070	18.36696343469892	12.67292356017301
N	3.10314756443765	18.36836145547094	12.67015441125465
Zn	5.11986872605650	18.36963386662804	12.66938958914002
C	9.18047696713178	17.25571761368417	13.12251588457117
C	1.05925070102014	19.47554622874389	13.13752101373182
C	7.78739047621492	17.29280167819485	13.13729445274994
C	2.45239069958817	19.44233134176255	13.14324065650500
H	6.87455641227236	14.12651013085902	13.31917020364843
H	3.36267902894019	22.60977457914092	13.31418230529890
H	9.71585992756816	16.40385559451530	13.51053198187391
H	0.52409443286218	20.32677661674857	13.52734502647175
C	6.96312391557589	16.22149951110972	13.70264252976781
C	3.27731391695576	20.51612525868020	13.70313447014321
N	5.74502586746870	16.55111869249149	14.01285185589010
N	4.49646340186658	20.18760874488782	14.00979853371113
C	7.48204137245739	14.83567755389824	13.89030389942244
C	2.75815266262667	21.90205304198816	13.89022855529928
H	8.50752121553455	14.72588892004009	13.55290758403482
H	1.73118040507681	22.01015102258415	13.55687427486014

H	5.24809369259247	14.66574628150306	14.56763528943000
H	4.99605636887265	22.07427248935638	14.55798739635575
H	2.98852402249193	13.91433840791333	14.83845948185274
H	7.26158048782144	22.82050622333830	14.82286147918739
N	4.92387620304882	15.62047176392743	14.49287759764624
N	5.31979276516912	21.11914002519512	14.48452478651982
C	2.74811659718820	14.90928761130710	15.19165999632317
C	7.49824076239111	21.82629393296329	15.18020576359538
H	7.43074632830514	14.53503477694017	14.94142609886903
H	2.81431532210522	22.20498927655743	14.94043902756201
C	3.68890033557565	15.92818015402296	15.07368317688198
C	6.55451183480760	20.80994195751409	15.06515639413236
H	-1.30264403869845	15.34445644163585	15.96365532501365
H	11.54050006260368	21.40042125724195	15.97664468209943
H	0.79593248824931	14.34309918283210	15.83878730804131
H	9.45222162856965	22.38873227614153	15.82560386902746
C	1.50239032389816	15.15549759486617	15.75356949745969
C	8.74316268659853	21.57830689722782	15.74310466600123
C	3.37615705196432	17.20505302208573	15.54336248084832
C	6.86445866943998	19.53296896085228	15.53639373072779
H	4.10514252691669	17.99864406026729	15.49949208047776
H	6.13385035023314	18.74091808585080	15.49272822270117
C	1.18132509259465	16.44037798470241	16.18949783920213
C	9.06066517472475	20.29362742291851	16.18223021835966
C	2.12707260747603	17.46039136669093	16.07737085291519
C	8.11287009192371	19.27545493945758	16.07077261913667
C	-0.99442443274982	15.76711499729103	16.92358784660658
C	11.23122242040146	20.96680641948393	16.93119391549375
O	-0.01068715041859	16.78580115445379	16.75194698300139
O	10.25121556740037	19.94670844888852	16.74671614248571
H	-1.84617016711529	16.25313612470173	17.39431130407021
H	12.08331405773286	20.47903591914732	17.39946874091242
H	1.87767197085572	18.44987005896596	16.43806464377739
H	8.36011600297672	18.28603925481811	16.43325049326508
H	-0.62637172734778	14.96978422633725	17.57429934719162
H	10.85810804215856	21.75611331760063	17.58890813230436

### Zn-OCF<sub>3</sub> (vacuum)

F	11.87610748968526	9.71899059073163	1.37545725192904
F	10.74801070681955	11.56899743902355	1.30450102940131
O	9.73852613495380	9.58106740314130	1.06741752931199
F	-1.31397229210496	9.10168139037920	-0.90252861660178
O	-0.06370852226649	7.42755553889898	-0.32521896081791
C	10.72396558340717	10.28733109548957	1.68226692916528
H	8.08733241483520	7.69012512921374	0.92126511578262
H	2.53241650223520	7.85251857923137	-0.59427738155835
C	8.41155703186588	9.73222206575396	1.43933458716303
C	7.63239396436060	8.59314023814447	1.30368851792588
C	-0.38926576673009	8.71209344018450	-0.05175568395494
C	0.94856702990587	6.82259578083584	0.41968706763005
C	2.27869117462425	7.12280232465517	0.16067209514572
H	8.43970929104607	11.82659382779158	1.94251600998359
C	7.84901700358900	10.92489974038925	1.88093194907371
C	6.29373630797505	8.62596139101538	1.65257645506347



H	5.68573264875162	7.74465808923336	1.53300751590795
H	-0.44759550011908	5.61992297121483	1.50733943710583
C	0.59654670050266	5.84669336450251	1.34118233656834
F	-0.86015608623627	8.85623429138812	1.20905225337159
C	3.26874885467189	6.43921858265296	0.84784136975849
H	4.30572118773383	6.63173309005068	0.61714998790536
F	10.58370849181150	10.27113797750395	3.03072058975757
F	0.67566478409379	9.54115278729494	-0.15002706027722
C	6.51463294554122	10.94226721405409	2.26622087557747
C	5.73533317767627	9.78915649419216	2.17765316534107
C	1.59419206072707	5.17046407216059	2.03062133620257
C	2.93094274087585	5.47101705672889	1.79007058686794
H	6.19301939642706	3.11334867503771	1.69016545825146
H	6.08226345647446	11.86059624761054	2.64391779838678
H	1.76555680300416	10.10857840110093	2.09270799295278
H	1.33546265403824	4.41652775439384	2.76194506248872
N	4.39368802653875	9.82084937442870	2.59881539902219
N	3.94352231437663	4.74956731217565	2.48863680001927
H	3.86556847228569	10.67477073837567	2.49568680543086
H	7.38042672604904	3.03738304792401	2.99354045251228
H	4.06282945472084	3.78242646557665	2.20916346177490
C	6.37915598092173	3.36932713566834	2.73782151023640
N	5.04965698601047	5.42864943582690	2.84372717527986
N	3.85094387151660	8.80227613592739	3.27468998358355
H	0.64270760037353	9.71713927890225	3.38228693999507
C	1.68441460742240	9.92191846013793	3.16641406869629
C	6.18276196285363	4.82934571036839	2.99553815682471
H	8.92793887752037	4.48959158773968	2.74681202293806
C	2.58915286316063	8.81031228850536	3.57986626079376
C	8.63023844306183	5.39275982739859	3.25698470335460
H	5.68334170316506	2.78298752782458	3.34505319621900
C	7.28565018406945	5.68885112795149	3.46676823327907
H	0.00198474354425	8.10388451278811	4.29796449902109
H	1.94834215272543	10.84364384999541	3.69484704482570
H	10.63610075262935	6.10071803250289	3.51604983789839
C	2.11225721324065	7.66365649157762	4.36996974716887
C	9.58617546993577	6.30434076711281	3.68034569705332
C	0.76790822469272	7.43309446603673	4.65096953703754
N	6.93516263191508	6.82536095164759	4.07909994701105
Zn	4.97550501348379	7.28046458735828	4.35511271539489
N	3.05155873899740	6.81068794212610	4.81664626085873
C	9.19970657425827	7.47641921401089	4.31401187734837
C	0.42014706306368	6.30618634281652	5.38186481806611
C	7.84203413883439	7.71620970314510	4.50836385235246
H	-0.61743130415435	6.11231814494888	5.61989362087598
H	7.85657505218031	10.96099794976510	5.02825952667889
H	9.94556997570524	8.17213974477310	4.65716580939830
C	2.73657613604661	5.71414220736617	5.51847462165999
H	4.34953945595558	2.80926880811135	5.73186122716766
C	1.40320406804532	5.43034026565620	5.81315888271988
C	7.30932452600120	8.90838863852863	5.19108713315774
H	1.14044067820933	4.56517512987451	6.40196280140196
C	3.84509118354158	4.87180317205078	5.99986816638011
C	8.17680965573637	10.06305669753143	5.56425171307027
H	9.21994480065219	9.90017224595847	5.32328964697536
N	6.03734324388892	8.88502003465477	5.44106283574913
N	4.98777327220634	5.46236823244837	6.13753944334502

C	3.63535019525006	3.41834659052391	6.29423628830127
H	5.95805934250512	3.77898653504610	6.72305536665357
H	2.64460696346259	3.08093625153517	6.00663045129415
H	5.97388115294834	10.72493030800545	6.29157136797107
N	6.06498706275615	4.76059682429383	6.50234350340391
N	5.42152660883534	9.92305534453668	6.02036950966774
H	8.51567555139345	3.84700752046264	6.27540378128746
H	8.11605022202765	10.26905461917956	6.63694797025842
H	3.49862535637552	11.74034649627468	6.09384077419599
H	3.77934355270779	3.19286691021111	7.35549855014936
C	7.22074946348715	5.40627478945796	6.99541602472983
C	8.45747984779346	4.78952381599106	6.80337172678862
C	4.14039807605925	9.75367771830163	6.59783697280783
C	3.22356308390615	10.80119759456472	6.55713372020344
F	10.68753251674591	9.21341087170453	7.50581342984719
F	-1.00530228934358	10.01862123279453	6.68078862208528
H	6.18910603436903	7.05899703796402	7.89529700101290
C	7.14707374337068	6.61151461402065	7.68864113975603
F	11.60446485694154	7.57775506710160	6.43491341835174
C	9.61251233365256	5.38741317536155	7.27973870118993
H	10.57809680213284	4.92035984155525	7.14645143719881
H	4.48505742976514	7.74746646539768	7.28192839567573
C	3.78021184193806	8.55942844380013	7.21776239424636
C	1.95238533369728	10.65569066320981	7.10068703838871
H	1.26294885132592	11.48520013008231	7.06999378878530
C	8.30498978613432	7.22381552305683	8.14730806798418
C	9.52746692081483	6.60906422514130	7.93027041198584
C	11.37063870314343	8.05631186678743	7.68030074332567
C	2.50879141105200	8.39697276897177	7.73485015274557
C	1.59235090626823	9.43688511154131	7.66839085336767
H	8.26273423803164	8.15144486547948	8.70023295024845
H	2.21539740400055	7.47125055043313	8.20856416641626
C	-0.73821932033201	9.91194290436246	8.00039788650525
O	10.69124845365380	7.17692578306127	8.45104036634658
F	12.52053393264171	8.32109632034835	8.26155264416754
O	0.36048821853541	9.13941028232753	8.22183305053184
F	-0.59927470674441	11.14967400100665	8.48701212549023
F	-1.76089878686090	9.32295230458815	8.59248117324817

CIE data

**ESI Table 1.** Changes in CIE L\*a\*b\* values recorded for 5 ppm of amine vapours.

		L*	a*	b*
Control filter		94.71	0.11	-0.69
Filter paper+MeOH		94.63	0.10	-0.49
Filter paper+DCM		94.67	0.08	-0.37
Original $2.3 \times 10^{-3}$	H	90.55	8.0	9.96
	OMe	76.35	14.64	14.54
	OCF3	89.29	7.58	12.71
TEA 5ppm	H	93.46	-0.80	5.75
	OCF3	94.36	0.02	1.04
	OMe	92.40	0.43	5.47
EtA 5ppm	H	93.37	-0.69	5.73
	OMe	93.59	-1.48	5.07
	OCF3	74.52	-0.65	1.65
Aniline 5ppm	H	93.68	-1.04	5.87
	OMe	87.52	5.22	9.36
	OCF3	93.90	0.26	1.98
NH <sub>3</sub> .H <sub>2</sub> O 5ppm	H	93.51	-0.87	6.02
	OMe	93.65	-0.83	4.29
	OCF3	94.36	-0.51	1.68

**ESI Table 2.** *dE* Values for 5 ppm 1H, 2-OMe and 3-OCF3 as a response function to amine vapor.

	EtA	TEA	Aniline	NH <sub>3</sub>
H-5	10.07	10.18	10.40	10.15
OMe-5	25.43	26.84	15.50	25.37
OCF3-5	20.20	10.64	13.78	14.59