

## Supporting Information

### Phenolate-Bonded Bis( $\mu$ -oxido)-bis-copper(III) Intermediates: Hydroxylation and Dehalogenation Reactivities

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## Experimental Details

### Materials and Methods

All the chemicals were purchased from commercial sources if not mentioned otherwise. THF and MeCN were of HPLC grade free of any stabilizer and further purified by a Pure-Solv 400 solvent purification system (Innovative Technology); anhydrous 2-methyltetrahydrofuran (MeTHF, Acros) was refluxed in the dark with Na/benzophenone for 6 h and distilled under an N<sub>2</sub> atmosphere. [Cu(MeCN)<sub>4</sub>](CF<sub>3</sub>SO<sub>3</sub>) was synthesized from Cu<sub>2</sub>O (Aldrich) and trifluoromethanesulfonate acid (Aldrich) by variation of the literature method.<sup>1</sup> Flash column chromatography was performed using SiliaFlash P60 flash silica gel (Silicycle, 230–400 mesh).

Preparation and manipulation of air-sensitive materials were carried out in a N<sub>2</sub> drybox (M. Braun, 1 ppm in O<sub>2</sub> and H<sub>2</sub>O). Low-temperature UV-Vis spectra were recorded on a Varian Cary 50 Bio spectrophotometer with a custom-designed quartz fiber-optic dip-probe (Hellma) of variable optical pathlength (0.10 or 1.0 cm) in custom-designed sample cells (ChemGlass). <sup>1</sup>H and <sup>19</sup>F NMR spectra were recorded on a Varian Inova 300 MHz or a Varian Mercury 400 MHz NMR spectrometer. High resolution mass spectra were acquired using API US QTOF (Waters) in positive electrospray mode. LC-MS was analyzed using a Waters 2795 HPLC system with a dual wavelength UV detector and a ZQ single quadrupole MS with an electrospray ionization source. A reverse phase Agilent Zorbax C8 column with 3.5  $\mu$ m Stablebond was used with a water/acetonitrile/0.1% formic acid as the mobile phase. The eluent was set at a flow rate of 0.3 mL min<sup>-1</sup> and monitored at 280 nm.

### Syntheses

***N,N'*-di-*tert*-butylpropane-1,3-diamine (DBPD)** DBPD was prepared from a previous literature report.<sup>2</sup> The unpurified product was obtained as light yellow powder, which was sublimed under vacuum to yield the pure ligand as colorless crystals. Yield: 45%. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  = 1.11 (s, 18H), 1.66 (quin, 2H, *J* = 6.8 Hz), 1.77 (br, 2H), 2.66 (t, 4H, *J* = 6.8 Hz).

**2-*tert*-butyl-4-bromophenol (3<sup>H</sup>)** 2-*tert*-butyl-4-bromophenol was synthesized according to a reported procedure.<sup>3</sup> 25 g (145 mmol) of p-bromophenol (Acros, 97%) and 6 g of DOWEX 50W-X8 resin were combined and the resulting suspension was saturated with isobutylene (TCI). After heating at 368 K for 6 h, the reaction mixture was purified by column chromatography (CH<sub>2</sub>Cl<sub>2</sub>/hexanes, 20:80). Evaporation of the solvent afforded a yellow oil, which was distilled over calcium chloride to give a clear yellow oil. Yield: 17 g (51%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ = 1.38 (s, 9H), 4.84 (s, 1H), 6.55 (d, 1H, *J* = 8.4 Hz), 7.17 (dd, 1H, *J* = 8.4 Hz, *J* = 2.4 Hz), 7.35 (d, 1H, *J* = 2.4 Hz).

**2-*tert*-butyl-4-cyanophenol (1<sup>H</sup>)** CuCN (0.60 g, 6.6 mmol) was dissolved in dimethylacetamide (DMA, 5 mL) under N<sub>2</sub>, and 2-*tert*-butyl-4-bromophenol (1.0 g, 4.4 mmol) in DMA (1 mL) was added with vigorous stirring. The reaction mixture was heated to reflux for 3 h under N<sub>2</sub> and cooled to RT. A 50% KBr aqueous solution (5 mL) was added and the resulting layers were separated. The aqueous phase was washed using Et<sub>2</sub>O (3 × 5 mL). The organic phases were combined, dried over MgSO<sub>4</sub>, and the solvent was removed, yielding a brown oil. The unpurified reaction mixture was purified by flash column chromatography using a solvent gradient starting from pure hexane to 1:1 hexane:Et<sub>2</sub>O. **1<sup>H</sup>** was isolated as a cotton-like white solid. Yield: 0.42 g (55%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ = 1.39 (s, 9H), 5.42 (s, 1H), 6.76 (dd, 1H, *J* = 8.4 Hz, *J* = 1.8 Hz), 7.38 (dd, 1H, *J* = 8.4 Hz, *J* = 1.8 Hz), 7.55 (d, 1H, *J* = 1.8 Hz). HRMS ES+ *m/z*: calculated: 176.1075; found: 176.1067.

### Syntheses of Phenolates

The phenolates **1 – 8** and **11** were synthesized by deprotonation of the corresponding phenol with NaH. To a THF solution (50 mL) of the phenol (*ca.* 1 g) was added 4 equiv of NaH (Aldrich, 95%) in a drybox. The reaction mixture was stirred until gas evolution ceased (2 h). The reaction mixture was filtered through celite and the solvent was removed under vacuum. White or light yellow powders were obtained and dried under vacuum for 12 h.

The phenolates **9**, **10** and **12 – 14** were synthesized by deprotonation of the corresponding phenol with equimolar amounts of triethylamine in THF. The prepared phenolate solutions (20 mM) were used directly for reactivity studies.

### Formation of <sup>s</sup>P<sup>DBPD</sup>

Under an inert atmosphere, equimolar amounts (0.100 mmol) of [Cu(MeCN)<sub>4</sub>](CF<sub>3</sub>SO<sub>3</sub>) and **DBPD** were mixed in THF (5 mL) to yield a clear colorless solution (20 mM Cu). The solution was used for oxygenation without further isolation of the Cu(I) complex, as this Cu(I) complex is not stable as a solid in the drybox. In a typical oxygenation reaction, a freshly prepared [(DBPD)Cu(I)(MeCN)](CF<sub>3</sub>SO<sub>3</sub>) THF solution (250 μL) was injected into MeTHF or THF (5 mL) saturated with O<sub>2</sub> (1 atm) with vigorous stirring at 183 K, yielding an <sup>s</sup>P<sup>DBPD</sup> solution (1 mM Cu).

### Alcohol Oxidation by <sup>s</sup>P<sup>DBPD</sup>

Excess O<sub>2</sub> in synthesizing the <sup>s</sup>P<sup>DBPD</sup> (1 mM in Cu, CF<sub>3</sub>SO<sub>3</sub><sup>-</sup>, 183 K, 5 mL THF) was removed by purging the reaction vessel with N<sub>2</sub> for 15 min. Two equivalents of substrate (benzyl alcohol or 1-octanol) were added to the <sup>s</sup>P<sup>DBPD</sup> solution, and the reaction mixture was kept at 193 K for 12 h. The reaction was quenched with aliquots of 30% NH<sub>3</sub> aqueous solution at 193 K and warmed to RT. Acetophenone was added to the solution as an internal GC standard. The mixture was dried over Na<sub>2</sub>SO<sub>4</sub> and passed through neutral activated alumina (Brockmann I, ~150 mesh, 58

Å). The column was washed with 2 mL methanol, and the combined eluent was analyzed by GC and GC-MS.

### Formation of $A^{DBPD}$

Excess  $O_2$  used in the synthesis of  $SP^{DBPD}$  (1 mM Cu,  $CF_3SO_3^-$ , 183 K, 5 mL MeTHF) was removed by purging the reaction vessel with  $N_2$  for 15 min. The solution was cooled to 153 K in a pentane/ $LN_2$  bath monitored with a thermocouple (Omega) inserted into the solution. The  $A^{DBPD}$  species was formed by injecting the desired phenolate in THF (20 mM, 375  $\mu$ L, 3.0 equivalents) to the  $SP^{DBPD}$  species with vigorous stirring, yielding a dark-colored species depending on the phenolate used.

### Titration of $SP^{DBPD}$ with Phenolate

In a pre-cooled MeTHF solution of  $SP^{DBPD}$  at 153 K, aliquots of phenolate **1** were added in 0.2 to 0.3 equivalent increments. The titrated solution was allowed to equilibrate for *ca.* 1 min until at least the difference of two consecutive UV-Vis scans was comparable to the spectral noise. Once the solution was insensitive to phenolate addition, two additional equivalents of phenolate were added to assure the complete formation of the  $A^{DBPD}$  species.

Each spectrum of the titration was corrected for dilution and deconvoluted into Gaussian-shape peaks using the GRAMS/32 program (Thermo Fisher Scientific). The concentration of  $SP^{DBPD}$  in each spectrum, calculated using an extinction coefficient of 30.8  $mM^{-1} cm^{-1}$  for the 365 nm band, was plotted versus the total concentration of **1** added. This plot was fit with proposed models by a nonlinear least-square regression using the Matlab program (The MathWorks, Natick, MA) and formation constants for each model.

### Thermal Decomposition Kinetics

$A^{DBPD}$  formed with 3 equivalents of phenolate **1** was allowed to decompose under  $N_2$  at various temperatures (153 – 193 K). The temperature of the solution was measured by immersing a thermocouple (Omega) directly into the solution. Data collection started only after the solution achieved the desired temperature (*ca.* 1 min). Multiwavelength (330 – 900 nm) component analyses of the spectral data by SPECFIT provided the decomposition rate constants.<sup>4</sup> The number of significant eigenvectors obtained for the multiwavelength analysis was two for all data sets, and a first-order kinetic ( $A \rightarrow B$ ) model provided a good fit for these data sets. The rate constants of decay at each temperature were used to obtain Eyring plot (Figure 8, left). Similar to the kinetics measurement described above, the decomposition rate constants of  $A^{DBPD}$  formed with 3 equivalents of phenolate **1–4** were obtained in MeTHF under  $N_2$  at 153 K and used in the Hammett analysis (Figure 8, right).

### Oxidation of Phenolate Substrates

The  $A^{DBPD}$  species formed with two equivalents of phenolate in MeTHF were allowed to thermally decay at 183 K. The distinct UV-Vis spectroscopic features bleached completely over a 5 – 120 min period depending on the phenolate added. The reaction mixture was quenched with an  $H_2SO_4$  aqueous solution (10%, 0.5 mL) at 183 K and allowed to warm to ambient temperatures. The MeTHF solvent was removed under vacuum, and  $CH_2Cl_2$  was used to extract the residue from aqueous phase. The organic phase was separated, dried over  $MgSO_4$ , and the solvent was removed under vacuum. The residue was dissolved in  $CDCl_3$  for  $^1H$ -NMR analysis or in MeOH for ESI-MS, LC-MS and GC-MS analyses. The yield of the phenolic product was

calculated from  $^1\text{H}$ -NMR by evaluating the area of signals internally or by comparing with an internal standard of 2-*t*-butyl-4-bromophenol, which was added after acidic quenching. The phenolic product recovery was greater than 90% for all the phenolates studied.

### X-ray Absorption Spectroscopy

Solution samples of the  $^s\text{P}^{\text{DBPD}}$  species and the  $^1\text{A}_2^{\text{DBPD}}$  species (4 mM Cu,  $\text{CF}_3\text{SO}_3^-$ , 3 equivalent of phenolate **1**, MeTHF) were loaded into Lucite XAS cells with 37 mM Kapton windows, frozen in liquid nitrogen ( $\text{LN}_2$ ) and stored under  $\text{LN}_2$  until use. Cu K-edge X-ray absorption data were collected on wiggler beam line 7-3 at the Stanford Synchrotron Radiation Laboratory under ring conditions of 3.0 GeV and 70–100 mA. A Si (220) monochromator was used for energy selection and detuned 50% to minimize higher harmonic components of the X-ray beam. During data collection, samples were maintained at 10–15 K using an Oxford Instruments CF1208 continuous flow liquid helium cryostat. Data were measured in fluorescence mode, monitoring the Cu  $K\alpha$  fluorescence signal with a 30-element Ge solid-state array detector. Internal energy calibration was performed by simultaneous measurement of the transmission signal through a Cu reference foil. The first inflection point of the copper reference data was aligned to 8980.3 eV. Data represent averages of 6–10 scans of each sample. Photoreduction was monitored and only scans with main edge shifts of less than 0.5 eV were included in the final data averages. Data reduction was performed according to established methods.<sup>5,6</sup>

The intensities and energies of the  $1s \rightarrow 3d$  pre-edge features were quantified using pseudo-Voigt line-shapes to model the rising edge background and absorption features of the Cu complexes according to established methods.<sup>5,6</sup> For each complex, a series of seven fits over varying energy ranges and with varying background features were performed and averaged using the program EDG\_FIT.<sup>7</sup> The reported area values ( $\text{FWHM} \times \text{Amplitude} \times 100$ ) are the average for each of the fits to a given complex.

Theoretical EXAFS signals were calculated using structural models based on appropriate model complexes as input parameters to FeFF (version 7) and fitted to the data using EXAFSPAK.<sup>7</sup> The structural parameters  $R$  ( $\text{\AA}$ ), the bond distance, and the bond variance,  $\sigma^2$  ( $\text{\AA}^2$ ), were varied for all shells in all fits. The  $\Delta E_0$  (eV) value representing the ionization threshold value was also varied for each fit, but was restrained to be a common value for all contributions within a given fit. Although EXAFS data were collected to  $k = 15 \text{ \AA}^{-1}$  for all samples, the EXAFS data were fit to  $k = 14 \text{ \AA}^{-1}$  for the  $^s\text{P}^{\text{DBPD}}$  sample in accordance with the noise level of the data.

### Computational

Density functional theory (DFT) calculations were performed using Gaussian 03 program (revision C.02)<sup>8</sup> and Gaussian 09 program (revision A.02, TD-DFT and NTO analysis)<sup>9</sup> on a Rocks Linux cluster. Restricted calculations were performed for species containing only Cu(III). The unrestricted wave function was used for the singlet ground state of the Cu(II) species with the broken-symmetry formalism. Both pure functional BLYP<sup>10,11</sup> and hybrid B3LYP<sup>12</sup> functionals were used. Basis Set 1 (BS1) calculations used the triple- $\zeta$  6-311+G(d) basis set on Cu, O and N atoms and the double- $\zeta$  6-31G(d) basis set on all other atoms.

Geometry optimization was performed with a B3LYP/6-31G(d) method in vacuum. All the ground state geometries were verified by frequency calculations to confirm the absence of imaginary frequencies and all the transition-state geometries were confirmed with only a single



imaginary frequency. Single point energies were calculated on the optimized structures using a PCM-BLYP/BS1 method. The Gaussian built-in parameterization of THF and UA0 radii were used to model the solvation. The singlet energy of the Cu diradical species was calculated from the corresponding broken-symmetry and triplet energies using a spin correction method.<sup>13</sup> Thermal corrections were calculated from the frequency analysis, from which the gas phase enthalpies and entropies (1 atm, 153 K) were obtained. Energy differences were calculated using the Wertz method.<sup>14</sup>

Time-dependent density functional theory<sup>15</sup> (TD-DFT) calculations were performed using a B3LYP/BS1 method in vacuum with Gaussian 09. The UV-Vis spectra were simulated using GaussView program (4.1.2, Gaussian, Inc.) with experimental FWHM values of 3600 cm<sup>-1</sup>. The natural transition orbital (NTO) method<sup>16</sup> was employed to analyze and visualize the TD-DFT calculated transitions with oscillator strengths larger than 0.06.

### DFT Calculated Geometries for DBPD Species

| <b>Table S1. <sup>SPDBPD</sup></b> |               |               |               |
|------------------------------------|---------------|---------------|---------------|
| Cu                                 | -1.4321740000 | 0.9656730000  | 0.5221000000  |
| Cu                                 | 1.4321740000  | -0.9656730000 | -0.5221000000 |
| O                                  | -0.4349720000 | -0.4800380000 | -0.3747800000 |
| O                                  | -3.2334820000 | 0.5201420000  | 0.0686000000  |
| O                                  | 0.4349720000  | 0.4800380000  | 0.3747800000  |
| O                                  | 3.2334820000  | -0.5201420000 | -0.0686000000 |
| N                                  | -6.0698850000 | -5.3437640000 | 1.8530220000  |
| N                                  | 6.0698850000  | 5.3437640000  | -1.8530220000 |
| N                                  | -2.0037540000 | 2.9405790000  | -0.6829200000 |
| N                                  | -1.7285740000 | 1.7331410000  | 2.4457930000  |
| N                                  | 1.7285740000  | -1.7331410000 | -2.4457930000 |
| N                                  | 2.0037540000  | -2.9405790000 | 0.6829200000  |
| C                                  | 0.9519950000  | -2.7143240000 | -4.6587570000 |
| C                                  | -0.1590940000 | -0.7248040000 | -3.6183250000 |
| C                                  | -0.4626790000 | -2.9835240000 | -2.5927490000 |
| C                                  | 0.5279100000  | -2.0682990000 | -3.3271200000 |
| C                                  | 1.9466740000  | -4.4324290000 | 2.7156530000  |
| C                                  | 0.3479960000  | -4.8062810000 | 0.8000430000  |
| C                                  | 0.1419830000  | -2.7686910000 | 2.2431230000  |
| C                                  | 1.1262400000  | -3.7509930000 | 1.5984000000  |
| C                                  | -0.9519950000 | 2.7143240000  | 4.6587570000  |
| C                                  | 0.4626790000  | 2.9835240000  | 2.5927490000  |
| C                                  | 0.1590940000  | 0.7248040000  | 3.6183250000  |
| C                                  | -0.5279100000 | 2.0682990000  | 3.3271200000  |
| C                                  | -1.9466740000 | 4.4324290000  | -2.7156530000 |
| C                                  | -0.1419830000 | 2.7686910000  | -2.2431230000 |
| C                                  | -0.3479960000 | 4.8062810000  | -0.8000430000 |
| C                                  | -1.1262400000 | 3.7509930000  | -1.5984000000 |
| C                                  | 6.6812540000  | 1.1520400000  | 2.2142350000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | 6.0192200000  | -0.9847750000 | 1.1250990000  |
| C | 4.4077020000  | 0.2400330000  | 2.6522170000  |
| C | 5.4986760000  | 0.4032410000  | 1.5663590000  |
| C | -6.6812540000 | -1.1520400000 | -2.2142350000 |
| C | -4.4077020000 | -0.2400330000 | -2.6522170000 |
| C | -6.0192200000 | 0.9847750000  | -1.1250990000 |
| C | -5.4986760000 | -0.4032410000 | -1.5663590000 |
| C | -5.5778740000 | -4.3338730000 | 1.5421730000  |
| C | 5.5778740000  | 4.3338730000  | -1.5421730000 |
| C | -3.0315270000 | 3.7141750000  | 0.0637150000  |
| C | -2.7347900000 | 3.9332630000  | 1.5516520000  |
| C | -2.8784090000 | 2.6908260000  | 2.4388240000  |
| C | -3.2952050000 | -1.4007740000 | 1.4681020000  |
| C | -3.8617320000 | -2.5995310000 | 1.8626960000  |
| C | -4.9695130000 | -3.0983380000 | 1.1638560000  |
| C | -5.4670730000 | -2.3621450000 | 0.0704140000  |
| C | -4.9169000000 | -1.1540590000 | -0.3508320000 |
| C | -3.7881500000 | -0.6404860000 | 0.3780650000  |
| C | 2.8784090000  | -2.6908260000 | -2.4388240000 |
| C | 2.7347900000  | -3.9332630000 | -1.5516520000 |
| C | 3.0315270000  | -3.7141750000 | -0.0637150000 |
| C | 3.8617320000  | 2.5995310000  | -1.8626960000 |
| C | 3.2952050000  | 1.4007740000  | -1.4681020000 |
| C | 3.7881500000  | 0.6404860000  | -0.3780650000 |
| C | 4.9169000000  | 1.1540590000  | 0.3508320000  |
| C | 5.4670730000  | 2.3621450000  | -0.0704140000 |
| C | 4.9695130000  | 3.0983380000  | -1.1638560000 |
| H | 1.3569630000  | -3.7228110000 | -4.5281360000 |
| H | 1.6970860000  | -2.1069970000 | -5.1874970000 |
| H | 0.0754780000  | -2.7993030000 | -5.3096420000 |
| H | -0.4614270000 | -0.2484120000 | -2.6830990000 |
| H | -1.0504020000 | -0.8836380000 | -4.2336200000 |
| H | 0.5073280000  | -0.0475740000 | -4.1696210000 |
| H | -1.3810990000 | -3.0709620000 | -3.1834980000 |
| H | -0.7294070000 | -2.5692100000 | -1.6172500000 |
| H | -0.0708280000 | -3.9945580000 | -2.4545680000 |
| H | 2.5124600000  | -3.6895740000 | 3.2918120000  |
| H | 2.6545470000  | -5.1739380000 | 2.3312440000  |
| H | 1.2783230000  | -4.9535480000 | 3.4102870000  |
| H | -0.2595100000 | -4.3399600000 | 0.0193130000  |
| H | -0.3257090000 | -5.3519850000 | 1.4688390000  |
| H | 1.0108600000  | -5.5437060000 | 0.3341420000  |
| H | -0.5492990000 | -3.3004680000 | 2.9064720000  |
| H | -0.4366170000 | -2.2430240000 | 1.4794990000  |
| H | 0.6763600000  | -2.0261100000 | 2.8464250000  |
| H | -1.6970860000 | 2.1069970000  | 5.1874970000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -1.3569630000 | 3.7228110000  | 4.5281360000  |
| H | -0.0754780000 | 2.7993030000  | 5.3096420000  |
| H | 0.7294070000  | 2.5692100000  | 1.6172500000  |
| H | 1.3810990000  | 3.0709620000  | 3.1834980000  |
| H | 0.0708280000  | 3.9945580000  | 2.4545680000  |
| H | 1.0504020000  | 0.8836380000  | 4.2336200000  |
| H | 0.4614270000  | 0.2484120000  | 2.6830990000  |
| H | -0.5073280000 | 0.0475740000  | 4.1696210000  |
| H | -2.6545470000 | 5.1739380000  | -2.3312440000 |
| H | -2.5124600000 | 3.6895740000  | -3.2918120000 |
| H | -1.2783230000 | 4.9535480000  | -3.4102870000 |
| H | 0.4366170000  | 2.2430240000  | -1.4794990000 |
| H | 0.5492990000  | 3.3004680000  | -2.9064720000 |
| H | -0.6763600000 | 2.0261100000  | -2.8464250000 |
| H | 0.3257090000  | 5.3519850000  | -1.4688390000 |
| H | 0.2595100000  | 4.3399600000  | -0.0193130000 |
| H | -1.0108600000 | 5.5437060000  | -0.3341420000 |
| H | -2.5199730000 | 2.2973360000  | -1.2835430000 |
| H | -2.1224770000 | 0.8955120000  | 2.8783260000  |
| H | 2.1224770000  | -0.8955120000 | -2.8783260000 |
| H | 2.5199730000  | -2.2973360000 | 1.2835430000  |
| H | 6.3912960000  | 2.1426080000  | 2.5830540000  |
| H | 7.5216600000  | 1.2761180000  | 1.5218200000  |
| H | 7.0459580000  | 0.5755650000  | 3.0721300000  |
| H | 5.2212310000  | -1.5695510000 | 0.6654500000  |
| H | 6.4106770000  | -1.5394440000 | 1.9875080000  |
| H | 6.8312400000  | -0.8793310000 | 0.3958410000  |
| H | 4.8008330000  | -0.3278700000 | 3.5053130000  |
| H | 3.5325260000  | -0.2787870000 | 2.2568150000  |
| H | 4.0838770000  | 1.2206740000  | 3.0213900000  |
| H | -7.5216600000 | -1.2761180000 | -1.5218200000 |
| H | -6.3912960000 | -2.1426080000 | -2.5830540000 |
| H | -7.0459580000 | -0.5755650000 | -3.0721300000 |
| H | -3.5325260000 | 0.2787870000  | -2.2568150000 |
| H | -4.8008330000 | 0.3278700000  | -3.5053130000 |
| H | -4.0838770000 | -1.2206740000 | -3.0213900000 |
| H | -6.4106770000 | 1.5394440000  | -1.9875080000 |
| H | -5.2212310000 | 1.5695510000  | -0.6654500000 |
| H | -6.8312400000 | 0.8793310000  | -0.3958410000 |
| H | 3.4545060000  | 3.1524930000  | -2.7041580000 |
| H | 6.3173140000  | 2.7758600000  | 0.4572890000  |
| H | 2.4204580000  | 1.0294110000  | -1.9929860000 |
| H | 1.7590200000  | -4.4069140000 | -1.6839500000 |
| H | 3.4747560000  | -4.6597790000 | -1.9153550000 |
| H | 3.9779850000  | -3.1720780000 | 0.0164340000  |
| H | 3.1956870000  | -4.6926610000 | 0.4029020000  |

|                                   |               |               |               |
|-----------------------------------|---------------|---------------|---------------|
| H                                 | 3.1052520000  | -3.0012200000 | -3.4641440000 |
| H                                 | 3.7343380000  | -2.1088410000 | -2.0839070000 |
| H                                 | -3.4545060000 | -3.1524930000 | 2.7041580000  |
| H                                 | -6.3173140000 | -2.7758600000 | -0.4572890000 |
| H                                 | -2.4204580000 | -1.0294110000 | 1.9929860000  |
| H                                 | -1.7590200000 | 4.4069140000  | 1.6839500000  |
| H                                 | -3.4747560000 | 4.6597790000  | 1.9153550000  |
| H                                 | -3.9779850000 | 3.1720780000  | -0.0164340000 |
| H                                 | -3.1956870000 | 4.6926610000  | -0.4029020000 |
| H                                 | -3.7343380000 | 2.1088410000  | 2.0839070000  |
| H                                 | -3.1052520000 | 3.0012200000  | 3.4641440000  |
| <b>Table S2. O<sup>DBPD</sup></b> |               |               |               |
| Cu                                | -0.9140810000 | -0.3901570000 | 0.9452590000  |
| Cu                                | 0.9199220000  | 0.3827850000  | -0.9087140000 |
| O                                 | 0.1506590000  | -1.1104860000 | -0.2864730000 |
| O                                 | -1.6738560000 | -1.9667100000 | 1.5398650000  |
| O                                 | -0.1432770000 | 1.1033080000  | 0.3231110000  |
| O                                 | 1.6452480000  | 1.9556860000  | -1.5554290000 |
| N                                 | -0.4921210000 | 8.1057490000  | 0.1997380000  |
| N                                 | 0.4695430000  | -8.1074390000 | -0.2400400000 |
| N                                 | -5.6720860000 | 1.0485840000  | -0.2661250000 |
| N                                 | -2.0757750000 | 0.4740650000  | 2.2999000000  |
| N                                 | 2.0763720000  | -0.4898790000 | -2.2647210000 |
| N                                 | 5.6937920000  | -1.0348660000 | 0.2726570000  |
| C                                 | -0.1221620000 | 7.0426700000  | -0.1002520000 |
| C                                 | 0.0988540000  | -7.0458790000 | 0.0644390000  |
| C                                 | 0.0265570000  | -0.8604290000 | -3.5630100000 |
| C                                 | 1.2736700000  | -2.8489770000 | -2.6596490000 |
| C                                 | 2.2510500000  | -1.4786230000 | -4.5458100000 |
| C                                 | 1.4148800000  | -1.4422320000 | -3.2520380000 |
| C                                 | 7.6404230000  | -2.6194070000 | 0.5759690000  |
| C                                 | 6.5783030000  | -1.4339590000 | 2.5385870000  |
| C                                 | 7.8595000000  | -0.1262460000 | 0.8295430000  |
| C                                 | 6.9278650000  | -1.3308440000 | 1.0434220000  |
| C                                 | -0.0314330000 | 0.8280990000  | 3.6100260000  |
| C                                 | -2.2580990000 | 1.4505670000  | 4.5861210000  |
| C                                 | -1.2649450000 | 2.8270430000  | 2.7123730000  |
| C                                 | -1.4158660000 | 1.4177090000  | 3.2963390000  |
| C                                 | -7.6183060000 | 2.6352590000  | -0.5610110000 |
| C                                 | -7.8307580000 | 0.1469260000  | -0.8623160000 |
| C                                 | -6.5338770000 | 1.4870380000  | -2.5336180000 |
| C                                 | -6.8985970000 | 1.3564150000  | -1.0441520000 |
| C                                 | 4.3515160000  | 4.7999190000  | 0.5690960000  |
| C                                 | 4.3548230000  | 3.3304750000  | -1.4399570000 |
| C                                 | 3.5815280000  | 2.4459040000  | 0.8089610000  |
| C                                 | 3.5830630000  | 3.6668260000  | -0.1407120000 |
| C                                 | -4.3525960000 | -4.7758300000 | -0.6599350000 |
| C                                 | -3.5704390000 | -2.4220140000 | -0.8589930000 |
| C                                 | -4.3844230000 | -3.3303120000 | 1.3662360000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -3.5922300000 | -3.6540090000 | 0.0761240000  |
| C | -4.6666660000 | 2.1059430000  | -0.1275890000 |
| C | -3.3132100000 | 1.5477820000  | 0.3347400000  |
| C | -3.3932360000 | 0.9039970000  | 1.7213770000  |
| C | 0.0424490000  | -3.5965940000 | 1.4464370000  |
| C | 0.5060100000  | -4.8561480000 | 1.1105020000  |
| C | -0.3499130000 | -5.7388830000 | 0.4337650000  |
| C | -1.6571400000 | -5.3272660000 | 0.1168020000  |
| C | -2.1491850000 | -4.0610050000 | 0.4381500000  |
| C | -1.2659160000 | -3.1712120000 | 1.1263530000  |
| C | 3.3988650000  | -0.9121420000 | -1.6924310000 |
| C | 3.3292390000  | -1.5395610000 | -0.2977530000 |
| C | 4.6857440000  | -2.0930730000 | 0.1610810000  |
| C | -0.5380220000 | 4.8403490000  | -1.1158640000 |
| C | -0.0748340000 | 3.5792110000  | -1.4465920000 |
| C | 1.2410860000  | 3.1631110000  | -1.1458980000 |
| C | 2.1323560000  | 4.0637870000  | -0.4826650000 |
| C | 1.6402180000  | 5.3311160000  | -0.1654470000 |
| C | 0.3258540000  | 5.7337370000  | -0.4637600000 |
| H | 0.0965780000  | 0.1759760000  | -3.9170770000 |
| H | -0.6078150000 | -0.8926640000 | -2.6736550000 |
| H | -0.4566030000 | -1.4477110000 | -4.3508320000 |
| H | 2.2466540000  | -3.3181210000 | -2.4790700000 |
| H | 0.7376210000  | -3.4826820000 | -3.3743590000 |
| H | 0.7091010000  | -2.8207970000 | -1.7252830000 |
| H | 1.7616650000  | -2.1255950000 | -5.2811320000 |
| H | 3.2579890000  | -1.8762890000 | -4.3820130000 |
| H | 2.3429400000  | -0.4797190000 | -4.9906630000 |
| H | 7.8964320000  | -2.5603800000 | -0.4897440000 |
| H | 7.0126730000  | -3.5051800000 | 0.7235920000  |
| H | 8.5710950000  | -2.7785990000 | 1.1332830000  |
| H | 6.0466130000  | -0.5348710000 | 2.8664210000  |
| H | 7.4906290000  | -1.5386790000 | 3.1363510000  |
| H | 5.9478190000  | -2.3029600000 | 2.7569820000  |
| H | 8.7855190000  | -0.2402710000 | 1.4032450000  |
| H | 7.3665880000  | 0.8001340000  | 1.1424210000  |
| H | 8.1362760000  | -0.0251450000 | -0.2284340000 |
| H | 0.6075960000  | 0.8640780000  | 2.7240050000  |
| H | -0.1071480000 | -0.2104990000 | 3.9565940000  |
| H | 0.4505540000  | 1.4076630000  | 4.4042440000  |
| H | -3.2625080000 | 1.8532680000  | 4.4192490000  |
| H | -1.7697790000 | 2.0914550000  | 5.3274480000  |
| H | -2.3563910000 | 0.4496530000  | 5.0250630000  |
| H | -0.7262610000 | 3.4532930000  | 3.4316640000  |
| H | -2.2347300000 | 3.3030840000  | 2.5327900000  |
| H | -0.6989470000 | 2.8006140000  | 1.7786930000  |
| H | -6.9904530000 | 3.5244880000  | -0.6857630000 |
| H | -7.8856680000 | 2.5564020000  | 0.5006240000  |
| H | -8.5431980000 | 2.8032710000  | -1.1253020000 |
| H | -7.3337910000 | -0.7729480000 | -1.1877870000 |

|                                                            |               |               |               |
|------------------------------------------------------------|---------------|---------------|---------------|
| H                                                          | -8.7511290000 | 0.2711070000  | -1.4429440000 |
| H                                                          | -8.1179490000 | 0.0254450000  | 0.1907150000  |
| H                                                          | -7.4402990000 | 1.5993870000  | -3.1389020000 |
| H                                                          | -5.9958730000 | 0.5954790000  | -2.8715990000 |
| H                                                          | -5.9041030000 | 2.3617580000  | -2.7302960000 |
| H                                                          | -5.9684540000 | 0.7545200000  | 0.6634450000  |
| H                                                          | -2.2693450000 | -0.3810690000 | 2.8264670000  |
| H                                                          | 2.2625280000  | 0.3626940000  | -2.7980190000 |
| H                                                          | 5.9813250000  | -0.7569830000 | -0.6646550000 |
| H                                                          | 3.8834500000  | 5.0841540000  | 1.5184450000  |
| H                                                          | 4.4380640000  | 5.6970180000  | -0.0547170000 |
| H                                                          | 5.3679590000  | 4.4582020000  | 0.7949110000  |
| H                                                          | 3.8765780000  | 2.5121090000  | -1.9810110000 |
| H                                                          | 5.3861500000  | 3.0412080000  | -1.2014710000 |
| H                                                          | 4.3942700000  | 4.2017810000  | -2.1044140000 |
| H                                                          | 4.6034620000  | 2.0892570000  | 0.9845360000  |
| H                                                          | 3.0079510000  | 1.6193430000  | 0.3901030000  |
| H                                                          | 3.1386000000  | 2.7098020000  | 1.7765550000  |
| H                                                          | -4.4552070000 | -5.6789640000 | -0.0473420000 |
| H                                                          | -3.8680830000 | -5.0526410000 | -1.6032350000 |
| H                                                          | -5.3629090000 | -4.4266160000 | -0.9012160000 |
| H                                                          | -3.0028490000 | -1.6013540000 | -0.4208550000 |
| H                                                          | -4.5884360000 | -2.0611740000 | -1.0484650000 |
| H                                                          | -3.1113880000 | -2.6763690000 | -1.8216440000 |
| H                                                          | -5.4099750000 | -3.0321200000 | 1.1141430000  |
| H                                                          | -3.9109270000 | -2.5217580000 | 1.9258940000  |
| H                                                          | -4.4398490000 | -4.2100680000 | 2.0183220000  |
| H                                                          | -1.5514340000 | 5.1437700000  | -1.3603200000 |
| H                                                          | 2.2790740000  | 6.0492240000  | 0.3330160000  |
| H                                                          | -0.7218770000 | 2.8696180000  | -1.9516540000 |
| H                                                          | 3.0006330000  | -0.7844490000 | 0.4247550000  |
| H                                                          | 2.5851090000  | -2.3398580000 | -0.2798950000 |
| H                                                          | 4.9879090000  | -2.9187960000 | -0.5100230000 |
| H                                                          | 4.5441540000  | -2.5395370000 | 1.1497610000  |
| H                                                          | 3.8880490000  | -1.6022440000 | -2.3900010000 |
| H                                                          | 4.0114400000  | -0.0070070000 | -1.6464160000 |
| H                                                          | 1.5136850000  | -5.1664460000 | 1.3696220000  |
| H                                                          | -2.2903790000 | -6.0373580000 | -0.4000020000 |
| H                                                          | 0.6838480000  | -2.8954080000 | 1.9701220000  |
| H                                                          | -2.9782800000 | 0.8015590000  | -0.3939470000 |
| H                                                          | -2.5700880000 | 2.3490580000  | 0.3311370000  |
| H                                                          | -4.9763580000 | 2.9203900000  | 0.5538210000  |
| H                                                          | -4.5167070000 | 2.5683920000  | -1.1075880000 |
| H                                                          | -4.0052400000 | -0.0005160000 | 1.6595230000  |
| H                                                          | -3.8878190000 | 1.5856860000  | 2.4235600000  |
| <b>Table S3. <sup>1</sup>SP<sub>I</sub><sup>DBPD</sup></b> |               |               |               |
| Cu                                                         | 2.1520560000  | -0.3952050000 | 0.1178920000  |
| Cu                                                         | -1.2781990000 | -1.1173840000 | -0.2425200000 |
| O                                                          | -2.2526070000 | 0.5307270000  | -0.3633930000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| O | 0.2788250000  | -0.3935440000 | 0.4558280000  |
| O | 0.6879950000  | -1.5984520000 | -0.2570850000 |
| N | 0.9466170000  | 6.2818400000  | -1.8913040000 |
| N | 2.4967720000  | 1.5566180000  | 0.3833540000  |
| N | 3.6746730000  | -1.2106270000 | -0.8697010000 |
| N | -2.3885550000 | -2.2459000000 | -1.5162800000 |
| N | -2.1507050000 | -2.4313070000 | 1.4799110000  |
| C | 0.3467190000  | 5.3117010000  | -1.6544620000 |
| C | -3.7220360000 | 4.4527800000  | 1.2051310000  |
| C | -3.1162050000 | 2.2081080000  | 2.0983650000  |
| C | -4.6045500000 | 2.4254080000  | 0.0601420000  |
| C | -3.3745750000 | 3.0055990000  | 0.7999400000  |
| C | -0.3453730000 | 4.0984480000  | -1.3518230000 |
| C | 0.0752380000  | 2.8848040000  | -1.9162170000 |
| C | -1.4499530000 | 4.0903160000  | -0.4779280000 |
| C | -0.5729780000 | 1.7128550000  | -1.5616660000 |
| C | -2.1368390000 | 2.9303800000  | -0.1175360000 |
| C | -1.6663670000 | 1.6795740000  | -0.6529350000 |
| C | 5.6030080000  | -2.8400040000 | -1.0163340000 |
| C | 3.3293020000  | -3.5624690000 | -0.2417400000 |
| C | 4.7202580000  | -2.0606600000 | 1.2192330000  |
| C | 3.8333310000  | 1.6461920000  | 2.5016490000  |
| C | 2.5704320000  | 3.6908450000  | 1.7108860000  |
| C | 1.3278200000  | 1.6803310000  | 2.5470620000  |
| C | -2.5640350000 | -0.8724400000 | -3.6095670000 |
| C | -0.5495870000 | -2.3207960000 | -3.1515620000 |
| C | -2.7337050000 | -3.3901410000 | -3.7232590000 |
| C | -1.5537930000 | -1.0473420000 | 3.4586100000  |
| C | -0.1180160000 | -2.9811360000 | 2.7150280000  |
| C | -2.3210440000 | -3.4236190000 | 3.8061730000  |
| C | 3.8259500000  | 1.1449000000  | -1.7338480000 |
| C | -4.2535510000 | -2.6255150000 | 0.1380600000  |
| C | 2.5737770000  | 2.1527730000  | 1.7866460000  |
| C | 4.5885230000  | -0.1316470000 | -1.3485500000 |
| C | -3.5980460000 | -2.0921850000 | 1.4148100000  |
| C | 3.5208910000  | 2.0901340000  | -0.5675160000 |
| C | 4.3523410000  | -2.4164780000 | -0.2266180000 |
| C | -2.0723390000 | -2.1956530000 | -3.0085040000 |
| C | -1.5562990000 | -2.4628750000 | 2.8704830000  |
| C | -3.8249540000 | -1.9880000000 | -1.1839970000 |
| H | -3.9501900000 | 5.0828020000  | 0.3381270000  |
| H | -2.9174610000 | 4.9298670000  | 1.7767160000  |
| H | -4.6116630000 | 4.4421680000  | 1.8439150000  |
| H | -2.8613480000 | 1.1709960000  | 1.8771960000  |
| H | -4.0088320000 | 2.2215150000  | 2.7359260000  |
| H | -2.2926750000 | 2.6525890000  | 2.6708270000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -5.4898820000 | 2.4774890000  | 0.7053500000  |
| H | -4.4405940000 | 1.3840330000  | -0.2228670000 |
| H | -4.8182030000 | 3.0000880000  | -0.8484540000 |
| H | 0.8869770000  | 2.8737560000  | -2.6391010000 |
| H | -1.7709950000 | 5.0445920000  | -0.0801350000 |
| H | -0.2550230000 | 0.7725070000  | -2.0015580000 |
| H | 5.9982190000  | -3.7715080000 | -0.5993270000 |
| H | 5.3678520000  | -3.0271290000 | -2.0709910000 |
| H | 6.4036070000  | -2.0960040000 | -0.9668350000 |
| H | 3.7433450000  | -4.4364120000 | 0.2699540000  |
| H | 2.3977650000  | -3.2790950000 | 0.2564430000  |
| H | 3.0904960000  | -3.8653690000 | -1.2692130000 |
| H | 3.8217060000  | -1.8332810000 | 1.8056110000  |
| H | 5.2221340000  | -2.9071030000 | 1.6977340000  |
| H | 5.3975780000  | -1.2024120000 | 1.2778900000  |
| H | 3.8513540000  | 2.0367110000  | 3.5238000000  |
| H | 3.8434960000  | 0.5524580000  | 2.5636810000  |
| H | 4.7595970000  | 1.9744590000  | 2.0193730000  |
| H | 1.6917750000  | 4.0607420000  | 1.1702150000  |
| H | 2.5375760000  | 4.1081210000  | 2.7221940000  |
| H | 3.4657080000  | 4.0890150000  | 1.2242300000  |
| H | 1.3116670000  | 0.5920420000  | 2.6593300000  |
| H | 1.3176930000  | 2.1229040000  | 3.5477650000  |
| H | 0.4065650000  | 1.9832810000  | 2.0370390000  |
| H | 1.5890710000  | 1.8667760000  | 0.0152290000  |
| H | 3.2063420000  | -1.5766970000 | -1.7032930000 |
| H | -2.2255780000 | -0.8009350000 | -4.6481250000 |
| H | -3.6560500000 | -0.8080150000 | -3.6181160000 |
| H | -2.1777300000 | -0.0102920000 | -3.0612690000 |
| H | -0.1825220000 | -3.2456440000 | -2.6888660000 |
| H | -0.2744630000 | -2.3452450000 | -4.2107480000 |
| H | -0.0331980000 | -1.4835440000 | -2.6761480000 |
| H | -2.3828390000 | -4.3453420000 | -3.3120160000 |
| H | -3.8257000000 | -3.3688490000 | -3.6614550000 |
| H | -2.4723960000 | -3.3751180000 | -4.7861250000 |
| H | -2.5687070000 | -0.6568550000 | 3.5829130000  |
| H | -1.0844390000 | -1.0578000000 | 4.4481580000  |
| H | -0.9950180000 | -0.3602940000 | 2.8180510000  |
| H | 0.3903880000  | -2.9799800000 | 3.6848550000  |
| H | -0.1102740000 | -4.0146320000 | 2.3431490000  |
| H | 0.4441420000  | -2.3624120000 | 2.0139130000  |
| H | -3.3192830000 | -3.0613000000 | 4.0687250000  |
| H | -2.4225430000 | -4.4203940000 | 3.3582390000  |
| H | -1.7684610000 | -3.5407890000 | 4.7442500000  |
| H | -2.0673050000 | -3.3966060000 | 1.1502570000  |
| H | -2.1962180000 | -3.2153560000 | -1.2511040000 |



|                                            |               |               |               |
|--------------------------------------------|---------------|---------------|---------------|
| H                                          | 4.4501290000  | 1.7046150000  | -2.4403110000 |
| H                                          | 2.9093550000  | 0.8951460000  | -2.2879900000 |
| H                                          | 5.2969200000  | 0.0931670000  | -0.5461600000 |
| H                                          | 4.4464870000  | 2.2690030000  | -0.0162500000 |
| H                                          | -4.1213570000 | -3.7185540000 | 0.0855880000  |
| H                                          | -5.3344330000 | -2.4661600000 | 0.2306270000  |
| H                                          | -3.7028010000 | -1.0043030000 | 1.4584820000  |
| H                                          | -4.1463420000 | -2.5104040000 | 2.2667630000  |
| H                                          | 5.1688620000  | -0.4900480000 | -2.2050700000 |
| H                                          | 3.1864040000  | 3.0561440000  | -0.9597310000 |
| H                                          | -4.4694960000 | -2.3823280000 | -1.9758800000 |
| H                                          | -3.9564300000 | -0.9050440000 | -1.1447350000 |
| <b>Table S4. <math>^1A_1^{DBPD}</math></b> |               |               |               |
| Cu                                         | -2.2392740000 | -0.8251340000 | -0.1659960000 |
| Cu                                         | 0.2631570000  | -0.3789470000 | 0.8591130000  |
| O                                          | 1.2927830000  | 1.1062880000  | 1.1387420000  |
| O                                          | -0.8484310000 | -1.7613950000 | 0.4691700000  |
| O                                          | -1.1118120000 | 0.5184180000  | 0.1338330000  |
| N                                          | -1.7274870000 | 7.1246760000  | 0.7816060000  |
| N                                          | -3.6347120000 | 0.5559580000  | -0.4184940000 |
| N                                          | -3.3090650000 | -2.4924050000 | 0.0002230000  |
| N                                          | 1.5466480000  | -1.6369630000 | 1.6372040000  |
| N                                          | 4.8580140000  | -1.1135410000 | -1.1659510000 |
| C                                          | -1.1806870000 | 6.0997160000  | 0.8563850000  |
| C                                          | 2.4581030000  | 4.0927040000  | -1.9935510000 |
| C                                          | 1.7780780000  | 1.7013930000  | -1.8881390000 |
| C                                          | 3.5264580000  | 2.6230940000  | -0.2907920000 |
| C                                          | 2.1977580000  | 2.9172160000  | -1.0292570000 |
| C                                          | -0.5328580000 | 4.8264460000  | 0.9389740000  |
| C                                          | -0.8848970000 | 3.9168490000  | 1.9478930000  |
| C                                          | 0.4535840000  | 4.4763350000  | -0.0012480000 |
| C                                          | 1.0965360000  | 3.2368360000  | -0.0000090000 |
| C                                          | 0.7097820000  | 2.3068030000  | 1.0172330000  |
| C                                          | -3.2929500000 | -4.9465410000 | -0.4128400000 |
| C                                          | -2.0717690000 | -3.3681010000 | -1.9513140000 |
| C                                          | -4.5822870000 | -3.4586460000 | -1.9810050000 |
| C                                          | -4.4835330000 | 0.2868730000  | -2.7738850000 |
| C                                          | -4.7589430000 | 2.4818290000  | -1.5516850000 |
| C                                          | -2.4854200000 | 1.7161880000  | -2.2871750000 |
| C                                          | 2.5917320000  | -0.5142970000 | 3.6321800000  |
| C                                          | 0.2191230000  | -1.3606270000 | 3.6984570000  |
| C                                          | 2.1136090000  | -2.9995000000 | 3.6484590000  |
| C                                          | 7.0664450000  | -2.0179860000 | -0.5412430000 |
| C                                          | 6.8109090000  | 0.2451740000  | -1.5826840000 |
| C                                          | 6.4653570000  | -1.8136660000 | -2.9866660000 |
| C                                          | -4.6806490000 | -0.8855430000 | 1.3782560000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | 2.6974610000  | -2.1224790000 | -0.5329860000 |
| C | -3.8537850000 | 1.2535090000  | -1.7663730000 |
| C | -4.5817560000 | -2.2833200000 | 0.7563870000  |
| C | 4.0572030000  | -2.3344680000 | -1.2171780000 |
| C | -4.8786110000 | 0.2336320000  | 0.3480430000  |
| C | -3.3324690000 | -3.5681600000 | -1.0979190000 |
| C | 1.6363440000  | -1.6181970000 | 3.1626030000  |
| C | 6.2835050000  | -1.1990170000 | -1.5823360000 |
| C | 2.8517170000  | -1.6410120000 | 0.9110000000  |
| C | -0.2629360000 | 2.6821700000  | 1.9748420000  |
| H | 2.7992870000  | 4.9906790000  | -1.4670230000 |
| H | 1.5717720000  | 4.3531690000  | -2.5833930000 |
| H | 3.2471260000  | 3.8095280000  | -2.6983670000 |
| H | 1.5615900000  | 0.8299910000  | -1.2688150000 |
| H | 2.5807370000  | 1.4422080000  | -2.5900810000 |
| H | 0.8821220000  | 1.9305050000  | -2.4765650000 |
| H | 4.3197120000  | 2.4098200000  | -1.0169580000 |
| H | 3.4351040000  | 1.7682390000  | 0.3809770000  |
| H | 3.8398760000  | 3.4919280000  | 0.2990170000  |
| H | -1.6251010000 | 4.1878150000  | 2.6941070000  |
| H | 0.7100020000  | 5.2151560000  | -0.7494250000 |
| H | -0.5116620000 | 1.9625220000  | 2.7488690000  |
| H | -3.3148910000 | -5.7387300000 | -1.1678430000 |
| H | -2.3751060000 | -5.0735270000 | 0.1736880000  |
| H | -4.1536840000 | -5.0994200000 | 0.2474110000  |
| H | -1.9693540000 | -4.1961460000 | -2.6595970000 |
| H | -2.1323100000 | -2.4420230000 | -2.5367760000 |
| H | -1.1725500000 | -3.3198000000 | -1.3320030000 |
| H | -4.7469980000 | -2.4387160000 | -2.3371040000 |
| H | -4.4417970000 | -4.0947280000 | -2.8601730000 |
| H | -5.4901920000 | -3.8077940000 | -1.4798900000 |
| H | -4.6442640000 | 0.8115750000  | -3.7204020000 |
| H | -3.8196850000 | -0.5596250000 | -2.9767530000 |
| H | -5.4571640000 | -0.0961830000 | -2.4516730000 |
| H | -4.3374250000 | 3.1622550000  | -0.8025010000 |
| H | -4.8408340000 | 3.0394760000  | -2.4895510000 |
| H | -5.7733310000 | 2.2090250000  | -1.2451330000 |
| H | -1.8109780000 | 0.8740840000  | -2.4661440000 |
| H | -2.6288790000 | 2.2470390000  | -3.2334470000 |
| H | -1.9874240000 | 2.3914360000  | -1.5857700000 |
| H | -3.1011030000 | 1.2355010000  | 0.1344270000  |
| H | -2.6138520000 | -2.8433560000 | 0.6672070000  |
| H | 2.5483070000  | -0.4476320000 | 4.7240290000  |
| H | 3.6294290000  | -0.7269740000 | 3.3582700000  |
| H | 2.3100880000  | 0.4523250000  | 3.2091320000  |
| H | -0.5053230000 | -2.0574230000 | 3.2626820000  |

|                                                        |               |               |               |
|--------------------------------------------------------|---------------|---------------|---------------|
| H                                                      | 0.2033730000  | -1.4871340000 | 4.7853690000  |
| H                                                      | -0.1083250000 | -0.3378180000 | 3.4832860000  |
| H                                                      | 1.4215830000  | -3.7940580000 | 3.3419520000  |
| H                                                      | 3.1124910000  | -3.2485650000 | 3.2786850000  |
| H                                                      | 2.1608910000  | -3.0062060000 | 4.7419650000  |
| H                                                      | 6.7645740000  | -3.0713260000 | -0.5286230000 |
| H                                                      | 8.1374820000  | -1.9936360000 | -0.7683750000 |
| H                                                      | 6.9164870000  | -1.6035450000 | 0.4612780000  |
| H                                                      | 7.8759320000  | 0.2715490000  | -1.8349930000 |
| H                                                      | 6.2814870000  | 0.8579670000  | -2.3244160000 |
| H                                                      | 6.6744670000  | 0.7056750000  | -0.5987030000 |
| H                                                      | 6.1232630000  | -2.8541210000 | -3.0236250000 |
| H                                                      | 5.9051510000  | -1.2446910000 | -3.7395380000 |
| H                                                      | 7.5204720000  | -1.8060270000 | -3.2823120000 |
| H                                                      | 4.4039170000  | -0.4055190000 | -1.7433360000 |
| H                                                      | 1.0571970000  | -2.5055000000 | 1.4004800000  |
| H                                                      | -5.5583770000 | -0.8836770000 | 2.0354230000  |
| H                                                      | -3.8223500000 | -0.6738940000 | 2.0310510000  |
| H                                                      | -5.4208150000 | -2.4165140000 | 0.0730160000  |
| H                                                      | -5.6556910000 | -0.0657470000 | -0.3588880000 |
| H                                                      | 2.1018690000  | -1.4006960000 | -1.1079820000 |
| H                                                      | 2.1437610000  | -3.0719440000 | -0.5597630000 |
| H                                                      | 4.5968810000  | -3.1249240000 | -0.6835220000 |
| H                                                      | 3.8768030000  | -2.7163780000 | -2.2373840000 |
| H                                                      | -4.6705040000 | -3.0462960000 | 1.5374320000  |
| H                                                      | -5.2279610000 | 1.1389550000  | 0.8537670000  |
| H                                                      | 3.5541020000  | -2.2983320000 | 1.4356360000  |
| H                                                      | 3.2629430000  | -0.6332480000 | 0.9366620000  |
| <b>Table S5. <sup>1</sup>SP<sub>2-trans</sub> DBPD</b> |               |               |               |
| Cu                                                     | -1.4321740000 | 0.9656730000  | 0.5221000000  |
| Cu                                                     | 1.4321740000  | -0.9656730000 | -0.5221000000 |
| O                                                      | -0.4349720000 | -0.4800380000 | -0.3747800000 |
| O                                                      | -3.2334820000 | 0.5201420000  | 0.0686000000  |
| O                                                      | 0.4349720000  | 0.4800380000  | 0.3747800000  |
| O                                                      | 3.2334820000  | -0.5201420000 | -0.0686000000 |
| N                                                      | -6.0698850000 | -5.3437640000 | 1.8530220000  |
| N                                                      | 6.0698850000  | 5.3437640000  | -1.8530220000 |
| N                                                      | -2.0037540000 | 2.9405790000  | -0.6829200000 |
| N                                                      | -1.7285740000 | 1.7331410000  | 2.4457930000  |
| N                                                      | 1.7285740000  | -1.7331410000 | -2.4457930000 |
| N                                                      | 2.0037540000  | -2.9405790000 | 0.6829200000  |
| C                                                      | 0.9519950000  | -2.7143240000 | -4.6587570000 |
| C                                                      | -0.1590940000 | -0.7248040000 | -3.6183250000 |
| C                                                      | -0.4626790000 | -2.9835240000 | -2.5927490000 |
| C                                                      | 0.5279100000  | -2.0682990000 | -3.3271200000 |
| C                                                      | 1.9466740000  | -4.4324290000 | 2.7156530000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | 0.3479960000  | -4.8062810000 | 0.8000430000  |
| C | 0.1419830000  | -2.7686910000 | 2.2431230000  |
| C | 1.1262400000  | -3.7509930000 | 1.5984000000  |
| C | -0.9519950000 | 2.7143240000  | 4.6587570000  |
| C | 0.4626790000  | 2.9835240000  | 2.5927490000  |
| C | 0.1590940000  | 0.7248040000  | 3.6183250000  |
| C | -0.5279100000 | 2.0682990000  | 3.3271200000  |
| C | -1.9466740000 | 4.4324290000  | -2.7156530000 |
| C | -0.1419830000 | 2.7686910000  | -2.2431230000 |
| C | -0.3479960000 | 4.8062810000  | -0.8000430000 |
| C | -1.1262400000 | 3.7509930000  | -1.5984000000 |
| C | 6.6812540000  | 1.1520400000  | 2.2142350000  |
| C | 6.0192200000  | -0.9847750000 | 1.1250990000  |
| C | 4.4077020000  | 0.2400330000  | 2.6522170000  |
| C | 5.4986760000  | 0.4032410000  | 1.5663590000  |
| C | -6.6812540000 | -1.1520400000 | -2.2142350000 |
| C | -4.4077020000 | -0.2400330000 | -2.6522170000 |
| C | -6.0192200000 | 0.9847750000  | -1.1250990000 |
| C | -5.4986760000 | -0.4032410000 | -1.5663590000 |
| C | -5.5778740000 | -4.3338730000 | 1.5421730000  |
| C | 5.5778740000  | 4.3338730000  | -1.5421730000 |
| C | -3.0315270000 | 3.7141750000  | 0.0637150000  |
| C | -2.7347900000 | 3.9332630000  | 1.5516520000  |
| C | -2.8784090000 | 2.6908260000  | 2.4388240000  |
| C | -3.2952050000 | -1.4007740000 | 1.4681020000  |
| C | -3.8617320000 | -2.5995310000 | 1.8626960000  |
| C | -4.9695130000 | -3.0983380000 | 1.1638560000  |
| C | -5.4670730000 | -2.3621450000 | 0.0704140000  |
| C | -4.9169000000 | -1.1540590000 | -0.3508320000 |
| C | -3.7881500000 | -0.6404860000 | 0.3780650000  |
| C | 2.8784090000  | -2.6908260000 | -2.4388240000 |
| C | 2.7347900000  | -3.9332630000 | -1.5516520000 |
| C | 3.0315270000  | -3.7141750000 | -0.0637150000 |
| C | 3.8617320000  | 2.5995310000  | -1.8626960000 |
| C | 3.2952050000  | 1.4007740000  | -1.4681020000 |
| C | 3.7881500000  | 0.6404860000  | -0.3780650000 |
| C | 4.9169000000  | 1.1540590000  | 0.3508320000  |
| C | 5.4670730000  | 2.3621450000  | -0.0704140000 |
| C | 4.9695130000  | 3.0983380000  | -1.1638560000 |
| H | 1.3569630000  | -3.7228110000 | -4.5281360000 |
| H | 1.6970860000  | -2.1069970000 | -5.1874970000 |
| H | 0.0754780000  | -2.7993030000 | -5.3096420000 |
| H | -0.4614270000 | -0.2484120000 | -2.6830990000 |
| H | -1.0504020000 | -0.8836380000 | -4.2336200000 |
| H | 0.5073280000  | -0.0475740000 | -4.1696210000 |
| H | -1.3810990000 | -3.0709620000 | -3.1834980000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -0.7294070000 | -2.5692100000 | -1.6172500000 |
| H | -0.0708280000 | -3.9945580000 | -2.4545680000 |
| H | 2.5124600000  | -3.6895740000 | 3.2918120000  |
| H | 2.6545470000  | -5.1739380000 | 2.3312440000  |
| H | 1.2783230000  | -4.9535480000 | 3.4102870000  |
| H | -0.2595100000 | -4.3399600000 | 0.0193130000  |
| H | -0.3257090000 | -5.3519850000 | 1.4688390000  |
| H | 1.0108600000  | -5.5437060000 | 0.3341420000  |
| H | -0.5492990000 | -3.3004680000 | 2.9064720000  |
| H | -0.4366170000 | -2.2430240000 | 1.4794990000  |
| H | 0.6763600000  | -2.0261100000 | 2.8464250000  |
| H | -1.6970860000 | 2.1069970000  | 5.1874970000  |
| H | -1.3569630000 | 3.7228110000  | 4.5281360000  |
| H | -0.0754780000 | 2.7993030000  | 5.3096420000  |
| H | 0.7294070000  | 2.5692100000  | 1.6172500000  |
| H | 1.3810990000  | 3.0709620000  | 3.1834980000  |
| H | 0.0708280000  | 3.9945580000  | 2.4545680000  |
| H | 1.0504020000  | 0.8836380000  | 4.2336200000  |
| H | 0.4614270000  | 0.2484120000  | 2.6830990000  |
| H | -0.5073280000 | 0.0475740000  | 4.1696210000  |
| H | -2.6545470000 | 5.1739380000  | -2.3312440000 |
| H | -2.5124600000 | 3.6895740000  | -3.2918120000 |
| H | -1.2783230000 | 4.9535480000  | -3.4102870000 |
| H | 0.4366170000  | 2.2430240000  | -1.4794990000 |
| H | 0.5492990000  | 3.3004680000  | -2.9064720000 |
| H | -0.6763600000 | 2.0261100000  | -2.8464250000 |
| H | 0.3257090000  | 5.3519850000  | -1.4688390000 |
| H | 0.2595100000  | 4.3399600000  | -0.0193130000 |
| H | -1.0108600000 | 5.5437060000  | -0.3341420000 |
| H | -2.5199730000 | 2.2973360000  | -1.2835430000 |
| H | -2.1224770000 | 0.8955120000  | 2.8783260000  |
| H | 2.1224770000  | -0.8955120000 | -2.8783260000 |
| H | 2.5199730000  | -2.2973360000 | 1.2835430000  |
| H | 6.3912960000  | 2.1426080000  | 2.5830540000  |
| H | 7.5216600000  | 1.2761180000  | 1.5218200000  |
| H | 7.0459580000  | 0.5755650000  | 3.0721300000  |
| H | 5.2212310000  | -1.5695510000 | 0.6654500000  |
| H | 6.4106770000  | -1.5394440000 | 1.9875080000  |
| H | 6.8312400000  | -0.8793310000 | 0.3958410000  |
| H | 4.8008330000  | -0.3278700000 | 3.5053130000  |
| H | 3.5325260000  | -0.2787870000 | 2.2568150000  |
| H | 4.0838770000  | 1.2206740000  | 3.0213900000  |
| H | -7.5216600000 | -1.2761180000 | -1.5218200000 |
| H | -6.3912960000 | -2.1426080000 | -2.5830540000 |
| H | -7.0459580000 | -0.5755650000 | -3.0721300000 |
| H | -3.5325260000 | 0.2787870000  | -2.2568150000 |

|                                                                    |               |               |               |
|--------------------------------------------------------------------|---------------|---------------|---------------|
| H                                                                  | -4.8008330000 | 0.3278700000  | -3.5053130000 |
| H                                                                  | -4.0838770000 | -1.2206740000 | -3.0213900000 |
| H                                                                  | -6.4106770000 | 1.5394440000  | -1.9875080000 |
| H                                                                  | -5.2212310000 | 1.5695510000  | -0.6654500000 |
| H                                                                  | -6.8312400000 | 0.8793310000  | -0.3958410000 |
| H                                                                  | 3.4545060000  | 3.1524930000  | -2.7041580000 |
| H                                                                  | 6.3173140000  | 2.7758600000  | 0.4572890000  |
| H                                                                  | 2.4204580000  | 1.0294110000  | -1.9929860000 |
| H                                                                  | 1.7590200000  | -4.4069140000 | -1.6839500000 |
| H                                                                  | 3.4747560000  | -4.6597790000 | -1.9153550000 |
| H                                                                  | 3.9779850000  | -3.1720780000 | 0.0164340000  |
| H                                                                  | 3.1956870000  | -4.6926610000 | 0.4029020000  |
| H                                                                  | 3.1052520000  | -3.0012200000 | -3.4641440000 |
| H                                                                  | 3.7343380000  | -2.1088410000 | -2.0839070000 |
| H                                                                  | -3.4545060000 | -3.1524930000 | 2.7041580000  |
| H                                                                  | -6.3173140000 | -2.7758600000 | -0.4572890000 |
| H                                                                  | -2.4204580000 | -1.0294110000 | 1.9929860000  |
| H                                                                  | -1.7590200000 | 4.4069140000  | 1.6839500000  |
| H                                                                  | -3.4747560000 | 4.6597790000  | 1.9153550000  |
| H                                                                  | -3.9779850000 | 3.1720780000  | -0.0164340000 |
| H                                                                  | -3.1956870000 | 4.6926610000  | -0.4029020000 |
| H                                                                  | -3.7343380000 | 2.1088410000  | 2.0839070000  |
| H                                                                  | -3.1052520000 | 3.0012200000  | 3.4641440000  |
| <b>Table S6.</b> <sup>1</sup> A <sub>2-trans</sub> <sup>DBPD</sup> |               |               |               |
| Cu                                                                 | -0.9140810000 | -0.3901570000 | 0.9452590000  |
| Cu                                                                 | 0.9199220000  | 0.3827850000  | -0.9087140000 |
| O                                                                  | 0.1506590000  | -1.1104860000 | -0.2864730000 |
| O                                                                  | -1.6738560000 | -1.9667100000 | 1.5398650000  |
| O                                                                  | -0.1432770000 | 1.1033080000  | 0.3231110000  |
| O                                                                  | 1.6452480000  | 1.9556860000  | -1.5554290000 |
| N                                                                  | -0.4921210000 | 8.1057490000  | 0.1997380000  |
| N                                                                  | 0.4695430000  | -8.1074390000 | -0.2400400000 |
| N                                                                  | -5.6720860000 | 1.0485840000  | -0.2661250000 |
| N                                                                  | -2.0757750000 | 0.4740650000  | 2.2999000000  |
| N                                                                  | 2.0763720000  | -0.4898790000 | -2.2647210000 |
| N                                                                  | 5.6937920000  | -1.0348660000 | 0.2726570000  |
| C                                                                  | -0.1221620000 | 7.0426700000  | -0.1002520000 |
| C                                                                  | 0.0988540000  | -7.0458790000 | 0.0644390000  |
| C                                                                  | 0.0265570000  | -0.8604290000 | -3.5630100000 |
| C                                                                  | 1.2736700000  | -2.8489770000 | -2.6596490000 |
| C                                                                  | 2.2510500000  | -1.4786230000 | -4.5458100000 |
| C                                                                  | 1.4148800000  | -1.4422320000 | -3.2520380000 |
| C                                                                  | 7.6404230000  | -2.6194070000 | 0.5759690000  |
| C                                                                  | 6.5783030000  | -1.4339590000 | 2.5385870000  |
| C                                                                  | 7.8595000000  | -0.1262460000 | 0.8295430000  |
| C                                                                  | 6.9278650000  | -1.3308440000 | 1.0434220000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -0.0314330000 | 0.8280990000  | 3.6100260000  |
| C | -2.2580990000 | 1.4505670000  | 4.5861210000  |
| C | -1.2649450000 | 2.8270430000  | 2.7123730000  |
| C | -1.4158660000 | 1.4177090000  | 3.2963390000  |
| C | -7.6183060000 | 2.6352590000  | -0.5610110000 |
| C | -7.8307580000 | 0.1469260000  | -0.8623160000 |
| C | -6.5338770000 | 1.4870380000  | -2.5336180000 |
| C | -6.8985970000 | 1.3564150000  | -1.0441520000 |
| C | 4.3515160000  | 4.7999190000  | 0.5690960000  |
| C | 4.3548230000  | 3.3304750000  | -1.4399570000 |
| C | 3.5815280000  | 2.4459040000  | 0.8089610000  |
| C | 3.5830630000  | 3.6668260000  | -0.1407120000 |
| C | -4.3525960000 | -4.7758300000 | -0.6599350000 |
| C | -3.5704390000 | -2.4220140000 | -0.8589930000 |
| C | -4.3844230000 | -3.3303120000 | 1.3662360000  |
| C | -3.5922300000 | -3.6540090000 | 0.0761240000  |
| C | -4.6666660000 | 2.1059430000  | -0.1275890000 |
| C | -3.3132100000 | 1.5477820000  | 0.3347400000  |
| C | -3.3932360000 | 0.9039970000  | 1.7213770000  |
| C | 0.0424490000  | -3.5965940000 | 1.4464370000  |
| C | 0.5060100000  | -4.8561480000 | 1.1105020000  |
| C | -0.3499130000 | -5.7388830000 | 0.4337650000  |
| C | -1.6571400000 | -5.3272660000 | 0.1168020000  |
| C | -2.1491850000 | -4.0610050000 | 0.4381500000  |
| C | -1.2659160000 | -3.1712120000 | 1.1263530000  |
| C | 3.3988650000  | -0.9121420000 | -1.6924310000 |
| C | 3.3292390000  | -1.5395610000 | -0.2977530000 |
| C | 4.6857440000  | -2.0930730000 | 0.1610810000  |
| C | -0.5380220000 | 4.8403490000  | -1.1158640000 |
| C | -0.0748340000 | 3.5792110000  | -1.4465920000 |
| C | 1.2410860000  | 3.1631110000  | -1.1458980000 |
| C | 2.1323560000  | 4.0637870000  | -0.4826650000 |
| C | 1.6402180000  | 5.3311160000  | -0.1654470000 |
| C | 0.3258540000  | 5.7337370000  | -0.4637600000 |
| H | 0.0965780000  | 0.1759760000  | -3.9170770000 |
| H | -0.6078150000 | -0.8926640000 | -2.6736550000 |
| H | -0.4566030000 | -1.4477110000 | -4.3508320000 |
| H | 2.2466540000  | -3.3181210000 | -2.4790700000 |
| H | 0.7376210000  | -3.4826820000 | -3.3743590000 |
| H | 0.7091010000  | -2.8207970000 | -1.7252830000 |
| H | 1.7616650000  | -2.1255950000 | -5.2811320000 |
| H | 3.2579890000  | -1.8762890000 | -4.3820130000 |
| H | 2.3429400000  | -0.4797190000 | -4.9906630000 |
| H | 7.8964320000  | -2.5603800000 | -0.4897440000 |
| H | 7.0126730000  | -3.5051800000 | 0.7235920000  |
| H | 8.5710950000  | -2.7785990000 | 1.1332830000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | 6.0466130000  | -0.5348710000 | 2.8664210000  |
| H | 7.4906290000  | -1.5386790000 | 3.1363510000  |
| H | 5.9478190000  | -2.3029600000 | 2.7569820000  |
| H | 8.7855190000  | -0.2402710000 | 1.4032450000  |
| H | 7.3665880000  | 0.8001340000  | 1.1424210000  |
| H | 8.1362760000  | -0.0251450000 | -0.2284340000 |
| H | 0.6075960000  | 0.8640780000  | 2.7240050000  |
| H | -0.1071480000 | -0.2104990000 | 3.9565940000  |
| H | 0.4505540000  | 1.4076630000  | 4.4042440000  |
| H | -3.2625080000 | 1.8532680000  | 4.4192490000  |
| H | -1.7697790000 | 2.0914550000  | 5.3274480000  |
| H | -2.3563910000 | 0.4496530000  | 5.0250630000  |
| H | -0.7262610000 | 3.4532930000  | 3.4316640000  |
| H | -2.2347300000 | 3.3030840000  | 2.5327900000  |
| H | -0.6989470000 | 2.8006140000  | 1.7786930000  |
| H | -6.9904530000 | 3.5244880000  | -0.6857630000 |
| H | -7.8856680000 | 2.5564020000  | 0.5006240000  |
| H | -8.5431980000 | 2.8032710000  | -1.1253020000 |
| H | -7.3337910000 | -0.7729480000 | -1.1877870000 |
| H | -8.7511290000 | 0.2711070000  | -1.4429440000 |
| H | -8.1179490000 | 0.0254450000  | 0.1907150000  |
| H | -7.4402990000 | 1.5993870000  | -3.1389020000 |
| H | -5.9958730000 | 0.5954790000  | -2.8715990000 |
| H | -5.9041030000 | 2.3617580000  | -2.7302960000 |
| H | -5.9684540000 | 0.7545200000  | 0.6634450000  |
| H | -2.2693450000 | -0.3810690000 | 2.8264670000  |
| H | 2.2625280000  | 0.3626940000  | -2.7980190000 |
| H | 5.9813250000  | -0.7569830000 | -0.6646550000 |
| H | 3.8834500000  | 5.0841540000  | 1.5184450000  |
| H | 4.4380640000  | 5.6970180000  | -0.0547170000 |
| H | 5.3679590000  | 4.4582020000  | 0.7949110000  |
| H | 3.8765780000  | 2.5121090000  | -1.9810110000 |
| H | 5.3861500000  | 3.0412080000  | -1.2014710000 |
| H | 4.3942700000  | 4.2017810000  | -2.1044140000 |
| H | 4.6034620000  | 2.0892570000  | 0.9845360000  |
| H | 3.0079510000  | 1.6193430000  | 0.3901030000  |
| H | 3.1386000000  | 2.7098020000  | 1.7765550000  |
| H | -4.4552070000 | -5.6789640000 | -0.0473420000 |
| H | -3.8680830000 | -5.0526410000 | -1.6032350000 |
| H | -5.3629090000 | -4.4266160000 | -0.9012160000 |
| H | -3.0028490000 | -1.6013540000 | -0.4208550000 |
| H | -4.5884360000 | -2.0611740000 | -1.0484650000 |
| H | -3.1113880000 | -2.6763690000 | -1.8216440000 |
| H | -5.4099750000 | -3.0321200000 | 1.1141430000  |
| H | -3.9109270000 | -2.5217580000 | 1.9258940000  |
| H | -4.4398490000 | -4.2100680000 | 2.0183220000  |



|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -1.5514340000 | 5.1437700000  | -1.3603200000 |
| H | 2.2790740000  | 6.0492240000  | 0.3330160000  |
| H | -0.7218770000 | 2.8696180000  | -1.9516540000 |
| H | 3.0006330000  | -0.7844490000 | 0.4247550000  |
| H | 2.5851090000  | -2.3398580000 | -0.2798950000 |
| H | 4.9879090000  | -2.9187960000 | -0.5100230000 |
| H | 4.5441540000  | -2.5395370000 | 1.1497610000  |
| H | 3.8880490000  | -1.6022440000 | -2.3900010000 |
| H | 4.0114400000  | -0.0070070000 | -1.6464160000 |
| H | 1.5136850000  | -5.1664460000 | 1.3696220000  |
| H | -2.2903790000 | -6.0373580000 | -0.4000020000 |
| H | 0.6838480000  | -2.8954080000 | 1.9701220000  |
| H | -2.9782800000 | 0.8015590000  | -0.3939470000 |
| H | -2.5700880000 | 2.3490580000  | 0.3311370000  |
| H | -4.9763580000 | 2.9203900000  | 0.5538210000  |
| H | -4.5167070000 | 2.5683920000  | -1.1075880000 |
| H | -4.0052400000 | -0.0005160000 | 1.6595230000  |
| H | -3.8878190000 | 1.5856860000  | 2.4235600000  |

#### DFT Calculated Geometries for DBPD Phenolate Hydroxylation Free Energy Surface

| Table S7. TS <sub>1</sub> |               |               |               |
|---------------------------|---------------|---------------|---------------|
| Cu                        | -2.2008630000 | -0.6549240000 | -0.1049340000 |
| Cu                        | 0.3657990000  | -0.3849700000 | 1.1106920000  |
| O                         | 1.3208530000  | 1.1474300000  | 1.7062610000  |
| O                         | -0.8065020000 | -1.6108250000 | 0.5340710000  |
| O                         | -1.0424590000 | 0.7212640000  | 0.6358700000  |
| N                         | -2.6267890000 | 6.1654540000  | -0.3659670000 |
| N                         | -3.5018550000 | 0.7090560000  | -0.7071010000 |
| N                         | -3.3678870000 | -2.3000230000 | 0.1895790000  |
| N                         | 1.6342450000  | -1.8072910000 | 1.5250200000  |
| N                         | 4.5241990000  | -1.0698630000 | -1.6871460000 |
| C                         | -1.9229360000 | 5.3327280000  | 0.0409290000  |
| C                         | 3.0775610000  | 4.7157930000  | -0.3887570000 |
| C                         | 3.1262990000  | 2.2286220000  | -0.6010780000 |
| C                         | 3.5071720000  | 3.3354360000  | 1.6453690000  |
| C                         | 2.7081220000  | 3.3984000000  | 0.3205580000  |
| C                         | -1.0834170000 | 4.2727290000  | 0.5155680000  |
| C                         | -1.6202080000 | 3.2541200000  | 1.2716670000  |
| C                         | 0.3181020000  | 4.2985860000  | 0.2229420000  |
| C                         | 1.2007510000  | 3.3095710000  | 0.6203310000  |
| C                         | 0.6447220000  | 2.2039370000  | 1.3516650000  |
| C                         | -3.7314000000 | -4.7600110000 | 0.0384360000  |
| C                         | -2.1713870000 | -3.5722960000 | -1.5426070000 |
| C                         | -4.6492320000 | -3.2628140000 | -1.7694790000 |
| C                         | -3.9323740000 | 0.2514430000  | -3.1501320000 |
| C                         | -4.2535310000 | 2.5693560000  | -2.2089270000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -1.9485430000 | 1.5807630000  | -2.4101260000 |
| C | 3.0775510000  | -1.0631720000 | 3.4452690000  |
| C | 0.6545230000  | -1.6619590000 | 3.7769840000  |
| C | 2.3183500000  | -3.4687740000 | 3.2560110000  |
| C | 6.6576160000  | -2.3106170000 | -1.6269160000 |
| C | 6.5594960000  | 0.1266440000  | -2.1976600000 |
| C | 5.7220510000  | -1.5725750000 | -3.8542160000 |
| C | -4.7937310000 | -0.4157870000 | 1.1210390000  |
| C | 2.3733460000  | -1.9519250000 | -0.8624340000 |
| C | -3.4270270000 | 1.2732710000  | -2.1261280000 |
| C | -4.6094270000 | -1.9288460000 | 0.9394470000  |
| C | 3.5671550000  | -2.1689790000 | -1.8041340000 |
| C | -4.8640970000 | 0.3808650000  | -0.1924980000 |
| C | -3.4983400000 | -3.4739310000 | -0.7764390000 |
| C | 1.9423780000  | -1.9968490000 | 3.0075560000  |
| C | 5.8450750000  | -1.2258290000 | -2.3550530000 |
| C | 2.8070590000  | -1.8444450000 | 0.6012180000  |
| C | -0.7874800000 | 2.1544080000  | 1.6522610000  |
| H | 2.8231180000  | 5.5943560000  | 0.2147700000  |
| H | 2.5915730000  | 4.8131640000  | -1.3665250000 |
| H | 4.1585710000  | 4.7395390000  | -0.5600710000 |
| H | 2.9399250000  | 1.2626130000  | -0.1292300000 |
| H | 4.1978900000  | 2.2935470000  | -0.8215870000 |
| H | 2.5816790000  | 2.2688350000  | -1.5526160000 |
| H | 4.5800320000  | 3.4104020000  | 1.4343140000  |
| H | 3.3295630000  | 2.4004320000  | 2.1808800000  |
| H | 3.2371620000  | 4.1686230000  | 2.3041520000  |
| H | -2.6559360000 | 3.2911050000  | 1.5973700000  |
| H | 0.6823030000  | 5.1528660000  | -0.3336590000 |
| H | -1.0405840000 | 1.6587000000  | 2.5860240000  |
| H | -3.8347490000 | -5.6191510000 | -0.6321590000 |
| H | -2.8879180000 | -4.9629810000 | 0.7096400000  |
| H | -4.6450170000 | -4.7014370000 | 0.6401090000  |
| H | -2.1550820000 | -4.4868380000 | -2.1440110000 |
| H | -2.0440110000 | -2.7226120000 | -2.2239050000 |
| H | -1.3177410000 | -3.5804690000 | -0.8595690000 |
| H | -4.5985820000 | -2.2773650000 | -2.2385800000 |
| H | -4.5721910000 | -4.0125950000 | -2.5628830000 |
| H | -5.6380200000 | -3.3849390000 | -1.3166000000 |
| H | -3.8058460000 | 0.6648440000  | -4.1554610000 |
| H | -3.3570180000 | -0.6788810000 | -3.1032250000 |
| H | -4.9952380000 | 0.0178950000  | -3.0335950000 |
| H | -3.9096940000 | 3.3168590000  | -1.4839980000 |
| H | -4.1471420000 | 3.0123250000  | -3.2039950000 |
| H | -5.3212520000 | 2.3915000000  | -2.0460370000 |
| H | -1.3454220000 | 0.6661080000  | -2.4243570000 |

|                                 |               |               |               |
|---------------------------------|---------------|---------------|---------------|
| H                               | -1.8582620000 | 2.0591470000  | -3.3902390000 |
| H                               | -1.5199980000 | 2.2513070000  | -1.6607330000 |
| H                               | -3.1485850000 | 1.4710060000  | -0.1241190000 |
| H                               | -2.6772610000 | -2.6209880000 | 0.8733400000  |
| H                               | 3.1928290000  | -1.1292900000 | 4.5319170000  |
| H                               | 4.0359270000  | -1.3431420000 | 2.9980150000  |
| H                               | 2.8569470000  | -0.0243320000 | 3.1872010000  |
| H                               | -0.2018650000 | -2.2202700000 | 3.3819980000  |
| H                               | 0.7698890000  | -1.9195530000 | 4.8343020000  |
| H                               | 0.4324950000  | -0.5910440000 | 3.7199530000  |
| H                               | 1.5028490000  | -4.1437890000 | 2.9676310000  |
| H                               | 3.2212400000  | -3.7648470000 | 2.7132560000  |
| H                               | 2.5145050000  | -3.6241710000 | 4.3216350000  |
| H                               | 6.2240080000  | -3.3089730000 | -1.7531780000 |
| H                               | 7.6769070000  | -2.3505420000 | -2.0252230000 |
| H                               | 6.7141160000  | -2.0916190000 | -0.5553540000 |
| H                               | 7.5645250000  | 0.0898900000  | -2.6303270000 |
| H                               | 6.0083790000  | 0.9258820000  | -2.7108930000 |
| H                               | 6.6459360000  | 0.3951300000  | -1.1395040000 |
| H                               | 5.2362080000  | -2.5425380000 | -4.0078710000 |
| H                               | 5.1369760000  | -0.8114340000 | -4.3860430000 |
| H                               | 6.7096960000  | -1.6220620000 | -4.3263370000 |
| H                               | 4.0877800000  | -0.2262480000 | -2.0598090000 |
| H                               | 1.0191870000  | -2.5840670000 | 1.2625320000  |
| H                               | -5.7394820000 | -0.2740850000 | 1.6577310000  |
| H                               | -4.0175820000 | 0.0029270000  | 1.7767050000  |
| H                               | -5.4742250000 | -2.3138650000 | 0.3976400000  |
| H                               | -5.3905920000 | -0.2037080000 | -0.9505180000 |
| H                               | 1.8278940000  | -1.0447680000 | -1.1596190000 |
| H                               | 1.6676140000  | -2.7840180000 | -0.9868050000 |
| H                               | 4.0716820000  | -3.1000380000 | -1.5223970000 |
| H                               | 3.1797840000  | -2.3232670000 | -2.8263130000 |
| H                               | -4.6060190000 | -2.4134750000 | 1.9222250000  |
| H                               | -5.4334370000 | 1.3029600000  | -0.0353590000 |
| H                               | 3.4368500000  | -2.7057770000 | 0.8548560000  |
| H                               | 3.4058320000  | -0.9472970000 | 0.7532280000  |
| <b>Table S8. TS<sub>2</sub></b> |               |               |               |
| Cu                              | 1.0078050000  | 0.0295010000  | 0.7400570000  |
| Cu                              | -1.0885010000 | -0.3261880000 | -1.1798710000 |
| O                               | -0.1458830000 | 0.9061070000  | -0.2869310000 |
| O                               | 1.7044560000  | 1.6417560000  | 1.4128370000  |
| O                               | 0.0909880000  | -1.4390420000 | -0.2076010000 |
| O                               | -1.7321070000 | -1.8703570000 | -2.0900070000 |
| N                               | 0.9098980000  | -6.9476570000 | 1.4107340000  |
| N                               | -0.8181680000 | 7.8372140000  | 0.5734140000  |
| N                               | 5.8709300000  | -0.7717860000 | -0.2942120000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| N | 2.2087050000  | -0.7588280000 | 2.1847370000  |
| N | -2.3475360000 | 0.7847880000  | -2.2305840000 |
| N | -5.7362660000 | 0.9287760000  | 0.6309500000  |
| C | 0.4564710000  | -6.0628240000 | 0.8046590000  |
| C | -0.3794330000 | 6.7673830000  | 0.7180970000  |
| C | -0.4072900000 | 1.3037880000  | -3.6409110000 |
| C | -1.3973830000 | 3.1108550000  | -2.2057690000 |
| C | -2.6563600000 | 2.2487220000  | -4.2304480000 |
| C | -1.7103890000 | 1.8852700000  | -3.0708020000 |
| C | -7.4120000000 | 2.5103140000  | 1.6704450000  |
| C | -6.4091240000 | 0.5952140000  | 2.9787070000  |
| C | -7.9682440000 | 0.1286370000  | 1.0763830000  |
| C | -6.8632520000 | 1.0689730000  | 1.5866410000  |
| C | 0.1316560000  | -1.3245940000 | 3.3381260000  |
| C | 2.3038070000  | -1.3375020000 | 4.6069930000  |
| C | 1.8117130000  | -3.1420170000 | 2.9230350000  |
| C | 1.6287260000  | -1.6615930000 | 3.2595760000  |
| C | 8.1732400000  | -1.8077060000 | -0.4425290000 |
| C | 7.7183000000  | 0.5921820000  | -1.0427730000 |
| C | 6.8407600000  | -1.2355130000 | -2.5118660000 |
| C | 7.1433210000  | -0.8340870000 | -1.0572360000 |
| C | -4.3193120000 | -5.2197360000 | -0.6086400000 |
| C | -3.8931540000 | -3.9638530000 | -2.7206650000 |
| C | -4.3050410000 | -2.7264420000 | -0.5499970000 |
| C | -3.6404300000 | -3.9655500000 | -1.1934080000 |
| C | 3.8302070000  | 4.6411510000  | -1.1100110000 |
| C | 3.0552730000  | 2.2816670000  | -1.2733480000 |
| C | 4.3015570000  | 3.1007940000  | 0.7854100000  |
| C | 3.2549960000  | 3.4646450000  | -0.2961680000 |
| C | 5.2026190000  | -2.0363270000 | 0.0187290000  |
| C | 3.7451140000  | -1.8204360000 | 0.4539080000  |
| C | 3.6168920000  | -1.0151530000 | 1.7465930000  |
| C | 0.0080160000  | 3.2384290000  | 1.8163810000  |
| C | -0.5254650000 | 4.5064530000  | 1.6811850000  |
| C | 0.1507800000  | 5.4511170000  | 0.8909280000  |
| C | 1.3582940000  | 5.0883670000  | 0.2660580000  |
| C | 1.9175270000  | 3.8154990000  | 0.3849860000  |
| C | 1.2137950000  | 2.8585430000  | 1.1838460000  |
| C | -3.5834530000 | 1.1691360000  | -1.4661860000 |
| C | -3.3574030000 | 1.3068680000  | 0.0399010000  |
| C | -4.5944410000 | 1.8375590000  | 0.7757490000  |
| C | 0.7206620000  | -3.9702200000 | -0.4157150000 |
| C | 0.1537580000  | -2.8366250000 | -1.1051870000 |
| C | -1.2901080000 | -2.8988100000 | -1.4183840000 |
| C | -2.1247070000 | -3.9441360000 | -0.9126470000 |
| C | -1.5047790000 | -4.9499560000 | -0.1877360000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -0.1008320000 | -4.9656810000 | 0.0693080000  |
| H | -0.5865640000 | 0.3646340000  | -4.1798360000 |
| H | 0.3115570000  | 1.1235120000  | -2.8369670000 |
| H | 0.0400180000  | 2.0112790000  | -4.3470450000 |
| H | -2.3042160000 | 3.5932130000  | -1.8256950000 |
| H | -0.8691960000 | 3.8522320000  | -2.8147600000 |
| H | -0.7607090000 | 2.8267740000  | -1.3644970000 |
| H | -2.1905420000 | 3.0139900000  | -4.8598420000 |
| H | -3.6116740000 | 2.6536220000  | -3.8805420000 |
| H | -2.8635440000 | 1.3774400000  | -4.8653220000 |
| H | -7.7379880000 | 2.8623090000  | 0.6833780000  |
| H | -6.6554420000 | 3.2089380000  | 2.0445470000  |
| H | -8.2742950000 | 2.5649090000  | 2.3454070000  |
| H | -5.9964750000 | -0.4171230000 | 2.9190300000  |
| H | -7.2571190000 | 0.5871670000  | 3.6727190000  |
| H | -5.6447430000 | 1.2509150000  | 3.4099280000  |
| H | -8.8274300000 | 0.1277750000  | 1.7557200000  |
| H | -7.5889020000 | -0.8949170000 | 0.9894200000  |
| H | -8.3287350000 | 0.4439410000  | 0.0879240000  |
| H | -0.3656200000 | -1.5694420000 | 2.3948410000  |
| H | -0.0230110000 | -0.2594570000 | 3.5508900000  |
| H | -0.3459050000 | -1.8971190000 | 4.1404520000  |
| H | 3.3800430000  | -1.5414640000 | 4.5891400000  |
| H | 1.8678340000  | -1.9516010000 | 5.4020690000  |
| H | 2.1581960000  | -0.2851210000 | 4.8808720000  |
| H | 1.3393730000  | -3.7512370000 | 3.7004210000  |
| H | 2.8671960000  | -3.4307070000 | 2.8812080000  |
| H | 1.3373510000  | -3.3881530000 | 1.9718570000  |
| H | 7.8101200000  | -2.8414410000 | -0.4542970000 |
| H | 8.3936610000  | -1.5384200000 | 0.5982580000  |
| H | 9.1168170000  | -1.7839420000 | -1.0002230000 |
| H | 6.9954860000  | 1.3015610000  | -1.4592400000 |
| H | 8.6407510000  | 0.6483290000  | -1.6306200000 |
| H | 7.9581600000  | 0.9108850000  | -0.0195640000 |
| H | 7.7530710000  | -1.1899530000 | -3.1172340000 |
| H | 6.0989700000  | -0.5571080000 | -2.9455190000 |
| H | 6.4537790000  | -2.2578210000 | -2.5869730000 |
| H | 6.0600600000  | -0.2749950000 | 0.5746900000  |
| H | 2.2400900000  | 0.1651220000  | 2.6235840000  |
| H | -2.6345750000 | 0.0715060000  | -2.9034640000 |
| H | -6.1209310000 | 1.0348320000  | -0.3068150000 |
| H | -4.2189610000 | -5.2732670000 | 0.4815120000  |
| H | -3.9163590000 | -6.1442580000 | -1.0379070000 |
| H | -5.3901870000 | -5.1899830000 | -0.8381210000 |
| H | -3.4666020000 | -3.0770970000 | -3.1937380000 |
| H | -4.9715080000 | -3.9813140000 | -2.9221430000 |

|                                                         |               |               |               |
|---------------------------------------------------------|---------------|---------------|---------------|
| H                                                       | -3.4498440000 | -4.8501770000 | -3.1896850000 |
| H                                                       | -5.3836730000 | -2.7251450000 | -0.7493460000 |
| H                                                       | -3.8844360000 | -1.8028730000 | -0.9493110000 |
| H                                                       | -4.1654340000 | -2.7233880000 | 0.5370180000  |
| H                                                       | 4.0514710000  | 5.5116210000  | -0.4816310000 |
| H                                                       | 3.1525830000  | 4.9588210000  | -1.9110050000 |
| H                                                       | 4.7694760000  | 4.3285040000  | -1.5806470000 |
| H                                                       | 2.5214360000  | 1.4593800000  | -0.7988720000 |
| H                                                       | 4.0235750000  | 1.9080260000  | -1.6278590000 |
| H                                                       | 2.4691960000  | 2.6001520000  | -2.1433820000 |
| H                                                       | 5.2507910000  | 2.8173450000  | 0.3136110000  |
| H                                                       | 3.9539860000  | 2.2702340000  | 1.4019480000  |
| H                                                       | 4.4918270000  | 3.9577510000  | 1.4427790000  |
| H                                                       | 1.7962620000  | -4.0460570000 | -0.3088120000 |
| H                                                       | -2.0842180000 | -5.7772710000 | 0.2014050000  |
| H                                                       | 0.7571990000  | -2.4667830000 | -1.9361210000 |
| H                                                       | -3.1052550000 | 0.3242220000  | 0.4571510000  |
| H                                                       | -2.5028810000 | 1.9631890000  | 0.2287100000  |
| H                                                       | -4.8074490000 | 2.8682440000  | 0.4367530000  |
| H                                                       | -4.3428740000 | 1.9111560000  | 1.8378820000  |
| H                                                       | -3.9858050000 | 2.1033300000  | -1.8722630000 |
| H                                                       | -4.3283040000 | 0.3888410000  | -1.6493620000 |
| H                                                       | -1.4525640000 | 4.7773090000  | 2.1775710000  |
| H                                                       | 1.8581040000  | 5.8441270000  | -0.3276500000 |
| H                                                       | -0.4985400000 | 2.4875000000  | 2.4149230000  |
| H                                                       | 3.2096020000  | -1.2993100000 | -0.3487310000 |
| H                                                       | 3.2746780000  | -2.7996080000 | 0.5824420000  |
| H                                                       | 5.7260920000  | -2.6331870000 | 0.7890040000  |
| H                                                       | 5.1904020000  | -2.6514270000 | -0.8863250000 |
| H                                                       | 4.0622030000  | -0.0286070000 | 1.5907920000  |
| H                                                       | 4.1793690000  | -1.5030290000 | 2.5531190000  |
| <b>Table S9. <math>\sigma(\text{C}-\text{O})</math></b> |               |               |               |
| Cu                                                      | 0.4472080000  | 1.5963050000  | 1.0675180000  |
| Cu                                                      | -0.4186780000 | -1.1568970000 | -0.6418970000 |
| O                                                       | -0.4968970000 | 0.5924520000  | -0.0541180000 |
| O                                                       | 0.0566400000  | 3.5125200000  | 1.3172320000  |
| O                                                       | 1.1084950000  | -1.7484340000 | 0.4054690000  |
| O                                                       | -0.2651880000 | -3.1651110000 | -1.4293260000 |
| N                                                       | 4.2190210000  | -6.4264800000 | 2.3325670000  |
| N                                                       | -6.0292320000 | 6.4932620000  | 0.9545580000  |
| N                                                       | 5.2440860000  | 2.9420580000  | -0.5340950000 |
| N                                                       | 1.9887750000  | 1.9422390000  | 2.4551850000  |
| N                                                       | -2.1458910000 | -1.0829790000 | -1.8975340000 |
| N                                                       | -5.1191340000 | -2.8415620000 | 1.0316200000  |
| C                                                       | 3.5108540000  | -5.8043230000 | 1.6365990000  |
| C                                                       | -4.9755850000 | 5.9764760000  | 1.0130280000  |

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -0.8959070000 | 0.4401710000  | -3.3985320000 |
| C | -2.8750350000 | 1.3357930000  | -2.0881680000 |
| C | -3.2360890000 | -0.2802550000 | -4.0303820000 |
| C | -2.3073980000 | 0.1159160000  | -2.8481330000 |
| C | -7.5880520000 | -2.5318900000 | 1.5998810000  |
| C | -5.8684680000 | -3.1014400000 | 3.3901690000  |
| C | -6.4501780000 | -4.7994930000 | 1.6134270000  |
| C | -6.2598960000 | -3.2883640000 | 1.9007580000  |
| C | 0.5398150000  | 0.8892280000  | 4.1598070000  |
| C | 2.8075110000  | 1.7646900000  | 4.8471520000  |
| C | 2.6262110000  | -0.3172920000 | 3.3817620000  |
| C | 2.0128080000  | 1.0639770000  | 3.7091380000  |
| C | 7.7925440000  | 2.8127400000  | -0.5099010000 |
| C | 6.5237640000  | 4.7502780000  | -1.5455900000 |
| C | 6.4603360000  | 2.4822100000  | -2.6551740000 |
| C | 6.5081700000  | 3.2211200000  | -1.2917020000 |
| C | 0.7250900000  | -7.4936330000 | -2.2806370000 |
| C | 0.3477050000  | -5.3706200000 | -3.5858100000 |
| C | -1.3070770000 | -6.0916850000 | -1.7737170000 |
| C | 0.2014340000  | -6.0342730000 | -2.1797820000 |
| C | -0.3402530000 | 7.7431790000  | -0.1038540000 |
| C | 0.7245430000  | 5.5959760000  | -0.8607410000 |
| C | 1.0054750000  | 6.4136040000  | 1.5453560000  |
| C | 0.0174580000  | 6.2970470000  | 0.3420970000  |
| C | 5.0153710000  | 1.5688490000  | -0.0377430000 |
| C | 3.5832990000  | 1.3896850000  | 0.5217630000  |
| C | 3.3179460000  | 2.2295040000  | 1.7912520000  |
| C | -2.3240340000 | 3.3966490000  | 1.5552100000  |
| C | -3.5814880000 | 3.9886690000  | 1.4987850000  |
| C | -3.6946950000 | 5.3396080000  | 1.0842440000  |
| C | -2.5186720000 | 6.0521680000  | 0.7267240000  |
| C | -1.2369610000 | 5.4816840000  | 0.7594200000  |
| C | -1.1317160000 | 4.1029270000  | 1.2024910000  |
| C | -3.3899960000 | -1.5394610000 | -1.1618370000 |
| C | -3.4513950000 | -1.1031900000 | 0.3173290000  |
| C | -4.8203280000 | -1.3920820000 | 0.9769770000  |
| C | 2.4732270000  | -3.7037930000 | 0.9376680000  |
| C | 1.6592000000  | -2.9249070000 | -0.0570010000 |
| C | 0.7043920000  | -3.7817890000 | -0.9114650000 |
| C | 0.9960510000  | -5.2088880000 | -1.1365300000 |
| C | 1.9308880000  | -5.7741640000 | -0.2925320000 |
| C | 2.6392220000  | -5.0537850000 | 0.7685070000  |
| H | -0.4446020000 | -0.4417940000 | -3.8901360000 |
| H | -0.2347610000 | 0.7775830000  | -2.5858920000 |
| H | -0.9629480000 | 1.2411290000  | -4.1537590000 |
| H | -3.9059380000 | 1.1614480000  | -1.7378310000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -2.9050640000 | 2.2044940000  | -2.7667580000 |
| H | -2.2337010000 | 1.5755530000  | -1.2282760000 |
| H | -3.3180470000 | 0.5618890000  | -4.7372670000 |
| H | -4.2574570000 | -0.5292240000 | -3.6994890000 |
| H | -2.8315240000 | -1.1454430000 | -4.5869310000 |
| H | -7.8806870000 | -2.6535730000 | 0.5415140000  |
| H | -7.4972120000 | -1.4525320000 | 1.8057410000  |
| H | -8.4130260000 | -2.9189690000 | 2.2226830000  |
| H | -4.9228270000 | -3.6235600000 | 3.6079870000  |
| H | -6.6552160000 | -3.5119080000 | 4.0454210000  |
| H | -5.7453340000 | -2.0387090000 | 3.6569730000  |
| H | -7.2517850000 | -5.2205450000 | 2.2427460000  |
| H | -5.5184940000 | -5.3528060000 | 1.8149970000  |
| H | -6.7326960000 | -4.9720000000 | 0.5583400000  |
| H | -0.0486070000 | 0.3588820000  | 3.3927000000  |
| H | 0.0590930000  | 1.8639440000  | 4.3526460000  |
| H | 0.4985680000  | 0.3014990000  | 5.0921140000  |
| H | 3.8686970000  | 1.9144820000  | 4.5907870000  |
| H | 2.7764980000  | 1.1491480000  | 5.7616310000  |
| H | 2.3681890000  | 2.7483170000  | 5.0902160000  |
| H | 2.5514680000  | -0.9691640000 | 4.2684800000  |
| H | 3.6956070000  | -0.2400660000 | 3.1221190000  |
| H | 2.0894650000  | -0.7948520000 | 2.5460890000  |
| H | 7.8265070000  | 1.7267450000  | -0.3212260000 |
| H | 7.8413410000  | 3.3301340000  | 0.4649960000  |
| H | 8.7017290000  | 3.0787120000  | -1.0765500000 |
| H | 5.6209230000  | 5.0604700000  | -2.0959320000 |
| H | 7.4113590000  | 5.0422070000  | -2.1312120000 |
| H | 6.5560110000  | 5.3110000000  | -0.5933360000 |
| H | 7.3290720000  | 2.7659730000  | -3.2729730000 |
| H | 5.5405410000  | 2.7447220000  | -3.2022500000 |
| H | 6.4914170000  | 1.3861250000  | -2.5361290000 |
| H | 5.1990420000  | 3.5999450000  | 0.2540810000  |
| H | 1.5991920000  | 2.8504920000  | 2.7482200000  |
| H | -1.8639080000 | -1.8670210000 | -2.5020560000 |
| H | -5.3055140000 | -3.1814810000 | 0.0794250000  |
| H | 0.5843190000  | -8.0533240000 | -1.3403880000 |
| H | 1.7935240000  | -7.5340800000 | -2.5536530000 |
| H | 0.1629340000  | -8.0268890000 | -3.0645480000 |
| H | -0.0393700000 | -4.3415070000 | -3.5913150000 |
| H | -0.2173240000 | -5.9538050000 | -4.3327650000 |
| H | 1.4041570000  | -5.3482680000 | -3.9041670000 |
| H | -1.8649550000 | -6.6958240000 | -2.5098840000 |
| H | -1.7554660000 | -5.0889440000 | -1.7373800000 |
| H | -1.4314790000 | -6.5629560000 | -0.7840610000 |
| H | -0.8106050000 | 8.3254310000  | 0.7068620000  |



|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -1.0177670000 | 7.7538310000  | -0.9744390000 |
| H | 0.5828070000  | 8.2714400000  | -0.3971260000 |
| H | 1.0189690000  | 4.5676040000  | -0.6087330000 |
| H | 1.6304770000  | 6.1587120000  | -1.1494660000 |
| H | 0.0548800000  | 5.5606740000  | -1.7376840000 |
| H | 1.8969770000  | 6.9956990000  | 1.2501600000  |
| H | 1.3323250000  | 5.4199250000  | 1.8838260000  |
| H | 0.5283500000  | 6.9311100000  | 2.3957910000  |
| H | 2.9765610000  | -3.1473270000 | 1.7312650000  |
| H | 2.1545350000  | -6.8388110000 | -0.3735380000 |
| H | 2.4524230000  | -2.7252110000 | -0.8585760000 |
| H | -2.6616360000 | -1.6268840000 | 0.8846610000  |
| H | -3.2379580000 | -0.0259740000 | 0.3928370000  |
| H | -5.6062560000 | -0.8005260000 | 0.4554260000  |
| H | -4.7805210000 | -1.0155150000 | 2.0112360000  |
| H | -4.2861670000 | -1.1766990000 | -1.6956980000 |
| H | -3.4008920000 | -2.6405730000 | -1.2184190000 |
| H | -4.4772340000 | 3.4244860000  | 1.7716370000  |
| H | -2.6416600000 | 7.0865410000  | 0.4054780000  |
| H | -2.2156750000 | 2.3508840000  | 1.8575660000  |
| H | 2.8552320000  | 1.6690950000  | -0.2596210000 |
| H | 3.4225530000  | 0.3221590000  | 0.7440110000  |
| H | 5.7496340000  | 1.2474770000  | 0.7370420000  |
| H | 5.1360320000  | 0.8788330000  | -0.8881980000 |
| H | 3.3025860000  | 3.2991970000  | 1.5273640000  |
| H | 4.1403630000  | 2.0830810000  | 2.5145190000  |

**Table S10. B**

|    |               |               |               |
|----|---------------|---------------|---------------|
| Cu | 0.5663230000  | 0.7587250000  | 0.3134310000  |
| Cu | -1.2297880000 | -0.9497140000 | -1.2703370000 |
| O  | -1.1533740000 | 0.8060350000  | -0.5679800000 |
| O  | 0.6333240000  | 2.5864550000  | 0.7840200000  |
| O  | 0.6787670000  | -0.7796580000 | -0.9283350000 |
| O  | -0.8827370000 | -2.7657830000 | -1.6083800000 |
| N  | 5.7835120000  | -3.7174770000 | -1.4713260000 |
| N  | -4.5570500000 | 6.7823450000  | -0.1999960000 |
| N  | 5.2353000000  | 2.8863360000  | 1.1344150000  |
| N  | 1.6418360000  | 0.4524490000  | 2.0588370000  |
| N  | -3.0857360000 | -1.2160330000 | -2.0421310000 |
| N  | -4.9839110000 | -2.3117150000 | 1.7777940000  |
| C  | 4.6270830000  | -3.5734970000 | -1.4920050000 |
| C  | -3.6527400000 | 6.0691020000  | -0.0236920000 |
| C  | -2.1383600000 | -0.1113160000 | -4.0075890000 |
| C  | -3.9590480000 | 1.0422660000  | -2.7237910000 |
| C  | -4.4837450000 | -1.0049620000 | -4.1060600000 |
| C  | -3.4380240000 | -0.3150490000 | -3.2105430000 |
| C  | -7.1595340000 | -2.3112190000 | 3.0642790000  |

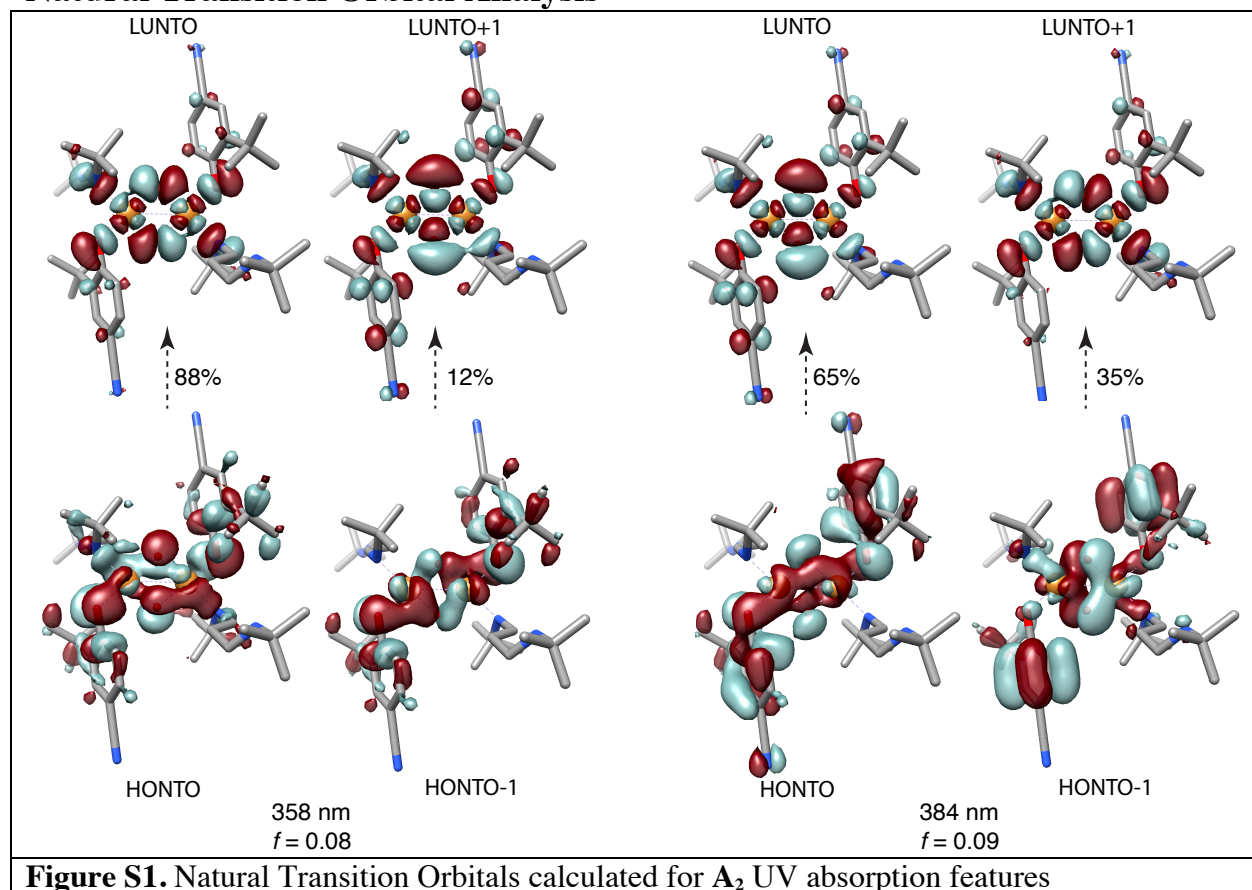
|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -4.9411400000 | -1.9267820000 | 4.2121580000  |
| C | -5.4714850000 | -4.1712050000 | 3.2369250000  |
| C | -5.6538660000 | -2.6546580000 | 3.0584980000  |
| C | 0.0970030000  | -1.3933140000 | 2.5229260000  |
| C | 1.5456560000  | -0.5028940000 | 4.3658850000  |
| C | 2.5650630000  | -1.8533250000 | 2.4975960000  |
| C | 1.4853620000  | -0.8282910000 | 2.8601660000  |
| C | 7.6506140000  | 3.1459000000  | 1.8305390000  |
| C | 6.1780160000  | 5.1053840000  | 1.2619100000  |
| C | 6.9099200000  | 3.5414710000  | -0.5525490000 |
| C | 6.4984670000  | 3.6391870000  | 0.9271830000  |
| C | 0.8395240000  | -6.7973280000 | -2.4878090000 |
| C | -0.7268160000 | -5.1648410000 | -3.5340750000 |
| C | -0.9468570000 | -5.7710130000 | -1.0843410000 |
| C | 0.0489340000  | -5.4979310000 | -2.2369990000 |
| C | 0.8286810000  | 5.8017210000  | -2.3187240000 |
| C | 1.2272670000  | 3.3507090000  | -2.1528620000 |
| C | 2.2051640000  | 4.9278580000  | -0.4342700000 |
| C | 0.9736300000  | 4.6321560000  | -1.3238290000 |
| C | 5.2903850000  | 1.4261210000  | 1.0491990000  |
| C | 3.8905560000  | 0.8107440000  | 0.9039040000  |
| C | 2.9884040000  | 1.1142310000  | 2.0989690000  |
| C | -1.5350460000 | 3.3393300000  | 1.3450740000  |
| C | -2.6166870000 | 4.1882460000  | 1.1756720000  |
| C | -2.5507550000 | 5.1839680000  | 0.1904330000  |
| C | -1.3837970000 | 5.3005730000  | -0.5900160000 |
| C | -0.2821140000 | 4.4573530000  | -0.4453640000 |
| C | -0.3641080000 | 3.4303170000  | 0.5508910000  |
| C | -4.1490280000 | -1.4865050000 | -1.0246630000 |
| C | -4.0673590000 | -0.6078400000 | 0.2260050000  |
| C | -5.1443650000 | -0.9492640000 | 1.2663950000  |
| C | 2.6688480000  | -2.1240660000 | -1.2000340000 |
| C | 1.2934010000  | -1.9663350000 | -1.1946370000 |
| C | 0.4251350000  | -3.0391760000 | -1.5609830000 |
| C | 0.9664330000  | -4.3165800000 | -1.8642570000 |
| C | 2.3577290000  | -4.4564900000 | -1.8211620000 |
| C | 3.2101550000  | -3.3863010000 | -1.5052680000 |
| H | -1.8522250000 | 1.3474530000  | -0.1758960000 |
| H | -1.6933390000 | -1.0691200000 | -4.3027810000 |
| H | -1.4026810000 | 0.4518480000  | -3.4236690000 |
| H | -2.3413440000 | 0.4559750000  | -4.9218690000 |
| H | -4.9063430000 | 0.9528200000  | -2.1825040000 |
| H | -4.1379850000 | 1.6900390000  | -3.5880700000 |
| H | -3.2243550000 | 1.5363680000  | -2.0820600000 |
| H | -4.7097190000 | -0.3753430000 | -4.9729510000 |
| H | -5.4270270000 | -1.1857770000 | -3.5801980000 |

|   |               |               |               |
|---|---------------|---------------|---------------|
| H | -4.1101630000 | -1.9656800000 | -4.4814990000 |
| H | -7.6816530000 | -2.8276360000 | 2.2486870000  |
| H | -7.3281290000 | -1.2351640000 | 2.9454210000  |
| H | -7.6290130000 | -2.6172290000 | 4.0065090000  |
| H | -3.8678250000 | -2.1419890000 | 4.1893590000  |
| H | -5.3433120000 | -2.2570740000 | 5.1763170000  |
| H | -5.0745420000 | -0.8402560000 | 4.1622760000  |
| H | -5.8983290000 | -4.5073740000 | 4.1878340000  |
| H | -4.4088960000 | -4.4345430000 | 3.2172490000  |
| H | -5.9747160000 | -4.7261610000 | 2.4340020000  |
| H | 0.0416450000  | -1.6927970000 | 1.4729860000  |
| H | -0.6936570000 | -0.6581760000 | 2.7237160000  |
| H | -0.1148210000 | -2.2757940000 | 3.1354680000  |
| H | 2.5099730000  | -0.0761390000 | 4.6600870000  |
| H | 1.3993360000  | -1.4151050000 | 4.9538080000  |
| H | 0.7571180000  | 0.2054650000  | 4.6507920000  |
| H | 2.3786880000  | -2.7809710000 | 3.0490850000  |
| H | 3.5673010000  | -1.5083860000 | 2.7707180000  |
| H | 2.5529120000  | -2.0902020000 | 1.4308590000  |
| H | 7.9162660000  | 2.1053020000  | 1.6141260000  |
| H | 7.3716320000  | 3.2111060000  | 2.8902340000  |
| H | 8.5517490000  | 3.7533850000  | 1.6856020000  |
| H | 5.3515020000  | 5.4686830000  | 0.6426760000  |
| H | 7.0510570000  | 5.7446910000  | 1.0917840000  |
| H | 5.8878290000  | 5.2146920000  | 2.3155460000  |
| H | 7.7761110000  | 4.1832730000  | -0.7487330000 |
| H | 6.0850140000  | 3.8612100000  | -1.1972840000 |
| H | 7.1915540000  | 2.5219120000  | -0.8376520000 |
| H | 4.8699520000  | 3.1502180000  | 2.0480800000  |
| H | 1.0304670000  | 1.1238360000  | 2.5285420000  |
| H | -2.8616720000 | -2.1213770000 | -2.4608920000 |
| H | -5.3184820000 | -2.9693120000 | 1.0752760000  |
| H | 1.4062330000  | -7.1109250000 | -1.6035660000 |
| H | 1.5380070000  | -6.7013860000 | -3.3269220000 |
| H | 0.1399230000  | -7.6044330000 | -2.7340830000 |
| H | -1.3173170000 | -4.2542450000 | -3.4131080000 |
| H | -1.4032040000 | -5.9887570000 | -3.7955520000 |
| H | -0.0350590000 | -5.0174000000 | -4.3718620000 |
| H | -1.6230650000 | -6.5924200000 | -1.3542300000 |
| H | -1.5441070000 | -4.8843930000 | -0.8619510000 |
| H | -0.4115380000 | -6.0630080000 | -0.1728600000 |
| H | 0.6849570000  | 6.7619570000  | -1.8099830000 |
| H | -0.0046890000 | 5.6530810000  | -3.0153890000 |
| H | 1.7441220000  | 5.8812580000  | -2.9152790000 |
| H | 1.3889300000  | 2.4878650000  | -1.5055910000 |
| H | 2.1179800000  | 3.4776670000  | -2.7804050000 |

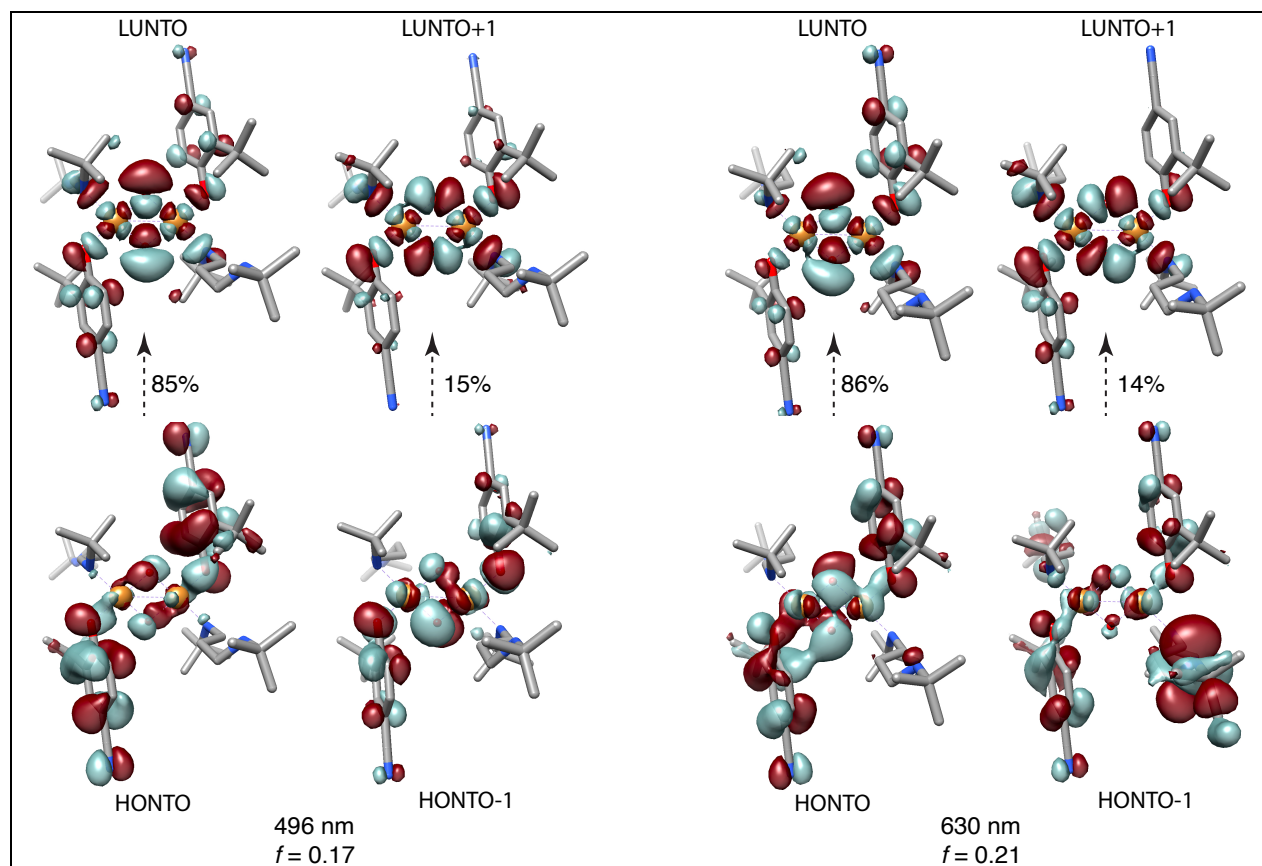
|                                                          |               |               |               |
|----------------------------------------------------------|---------------|---------------|---------------|
| H                                                        | 0.3770770000  | 3.1317470000  | -2.8093350000 |
| H                                                        | 3.0879350000  | 5.0967330000  | -1.0637040000 |
| H                                                        | 2.4274510000  | 4.0974410000  | 0.2369910000  |
| H                                                        | 2.0410040000  | 5.8309600000  | 0.1660520000  |
| H                                                        | 3.3144080000  | -1.2806540000 | -0.9862910000 |
| H                                                        | 2.8134810000  | -5.4126450000 | -2.0445060000 |
| H                                                        | -3.0809930000 | -0.7367610000 | 0.6856070000  |
| H                                                        | -4.1686160000 | 0.4486270000  | -0.0463230000 |
| H                                                        | -6.1434570000 | -0.7528680000 | 0.8350210000  |
| H                                                        | -5.0316680000 | -0.2514500000 | 2.1013720000  |
| H                                                        | -5.1433490000 | -1.4037430000 | -1.4817510000 |
| H                                                        | -4.0154950000 | -2.5298850000 | -0.7228550000 |
| H                                                        | -3.5006920000 | 4.0961430000  | 1.7998650000  |
| H                                                        | -1.3648520000 | 6.0861440000  | -1.3351220000 |
| H                                                        | -1.5539480000 | 2.5768720000  | 2.1210110000  |
| H                                                        | 3.4229790000  | 1.2066260000  | -0.0060990000 |
| H                                                        | 4.0043300000  | -0.2702620000 | 0.7810400000  |
| H                                                        | 5.8021040000  | 0.9524020000  | 1.9081260000  |
| H                                                        | 5.8680000000  | 1.1518290000  | 0.1616610000  |
| H                                                        | 2.7880080000  | 2.1875530000  | 2.1204360000  |
| H                                                        | 3.5011950000  | 0.8509470000  | 3.0330880000  |
| <b>Table S11.</b> 2- <i>tert</i> -butyl-4-cyanophenolate |               |               |               |
| O                                                        | -1.4354650000 | 2.1909840000  | -0.0004120000 |
| N                                                        | 4.2336040000  | -1.4593800000 | 0.0004850000  |
| C                                                        | 3.2484470000  | -0.8248300000 | 0.0003360000  |
| C                                                        | -1.6345220000 | -2.2502530000 | -0.0004440000 |
| C                                                        | -2.5727890000 | -0.3072730000 | -1.2601570000 |
| C                                                        | -2.5725060000 | -0.3079340000 | 1.2604910000  |
| C                                                        | -1.7710010000 | -0.7164610000 | -0.0000310000 |
| C                                                        | 2.0919030000  | 1.3582950000  | -0.0000190000 |
| C                                                        | 0.7846560000  | -0.6896390000 | 0.0001490000  |
| C                                                        | -0.4112710000 | 0.0057780000  | 0.0000000000  |
| C                                                        | 0.9240170000  | 2.0834230000  | -0.0002040000 |
| C                                                        | 2.0559960000  | -0.0568660000 | 0.0001550000  |
| C                                                        | -0.3915230000 | 1.4763570000  | -0.0002140000 |
| H                                                        | -1.1016680000 | -2.6143490000 | -0.8876550000 |
| H                                                        | -1.1013910000 | -2.6148020000 | 0.8864140000  |
| H                                                        | -2.6319600000 | -2.7099630000 | -0.0004070000 |
| H                                                        | -2.6760910000 | 0.7793680000  | -1.2884850000 |
| H                                                        | -2.0549350000 | -0.6380190000 | -2.1699740000 |
| H                                                        | -3.5718670000 | -0.7683610000 | -1.2519050000 |
| H                                                        | -2.0544960000 | -0.6392510000 | 2.1700100000  |
| H                                                        | -2.6756980000 | 0.7786990000  | 1.2894670000  |
| H                                                        | -3.5716230000 | -0.7689390000 | 1.2521750000  |
| H                                                        | 3.0564550000  | 1.8642300000  | -0.0000240000 |
| H                                                        | 0.7806680000  | -1.7758200000 | 0.0002810000  |

|   |              |              |               |
|---|--------------|--------------|---------------|
| H | 0.9426490000 | 3.1714100000 | -0.0003580000 |
|---|--------------|--------------|---------------|

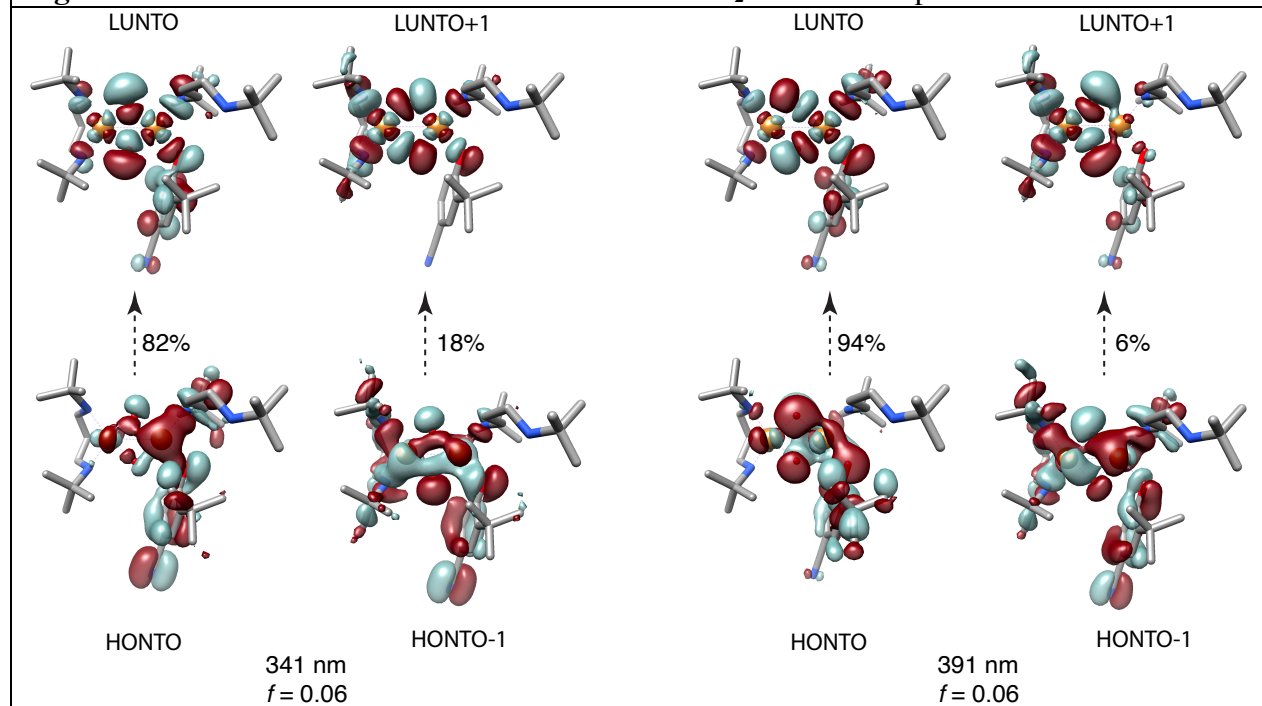
### Natural Transition Orbital Analysis



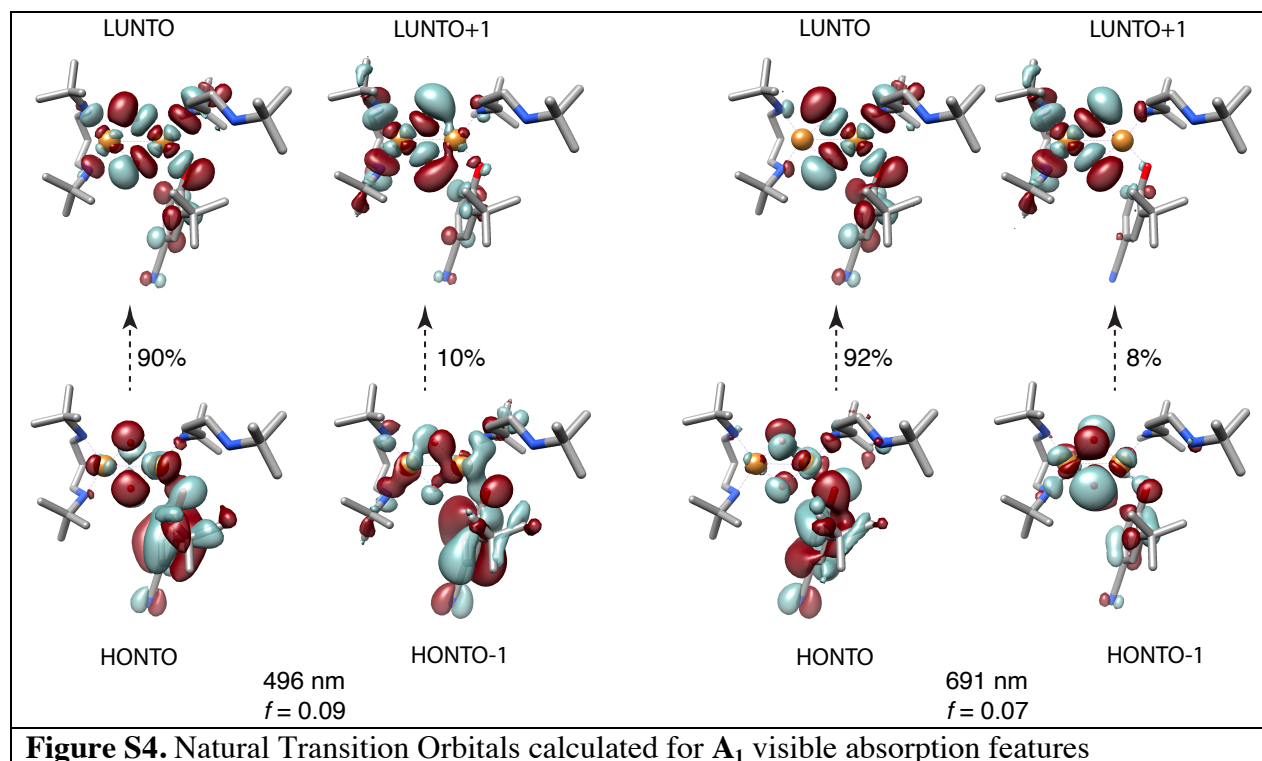
**Figure S1.** Natural Transition Orbitals calculated for  $A_2$  UV absorption features



**Figure S2.** Natural Transition Orbitals calculated for  $A_2$  visible absorption features



**Figure S3.** Natural Transition Orbitals calculated for  $A_1$  UV absorption features



**Figure S4.** Natural Transition Orbitals calculated for  $A_1$  visible absorption features

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