## SUPPORTING INFORMATION

# Modifying the Luminescent Properties of a Cu(I) Diphosphine Complex Using Ligand-Centered Reactions in Single Crystals

Kyounghoon Lee,<sup>1</sup> Po-Ni Lai,<sup>2</sup> Riffat Parveen,<sup>3</sup> Courtney M. Donahue,<sup>1</sup> Mikayla M. Wymore,<sup>1</sup>

Blake A. Massman,<sup>1</sup> Bess Vlaisavljevich,<sup>3</sup> Thomas S. Teets,<sup>2</sup> Scott R. Daly<sup>\*,1</sup>

1) The University of Iowa, Department of Chemistry, E331 Chemistry Building, Iowa City, IA 52242

2) University of Houston, Department of Chemistry, 3585 Cullen Boulevard, Room 112, Houston, TX 77204

3) The University of South Dakota, Department of Chemistry, 414 E. Clark Street, Vermillion, SD 57069

### I. Experimental

**General Considerations.** Reactions were carried out under an atmosphere of N<sub>2</sub> or Ar using glovebox or standard Schlenk techniques unless stated otherwise. Glassware used for reactions performed under inert conditions was dried in an oven at 150 °C for at least 1.5 h and allowed to cool under vacuum before use. Solvents used under anhydrous conditions were dried and deoxygenated using a Pure Process Technologies Solvent Purification System. CuCl, HNPh<sub>2</sub>, and KN(SiMe<sub>3</sub>)<sub>2</sub> were purchased from commercial vendors and used without further purification. NEt<sub>3</sub> was distilled and stored over KOH. CDCl<sub>3</sub>, CD<sub>2</sub>Cl<sub>2</sub>, and THF-d<sub>8</sub> were distilled and stored over preactivated 3 Å molecular sieves. <sup>Ph</sup>TBDPhos was prepared as described previously.<sup>1</sup>

<sup>1</sup>H and <sup>31</sup>P{<sup>1</sup>H} NMR data were recorded on a Bruker AVANCE-300 or DPX-300 instrument operating at 300 MHz for <sup>1</sup>H and 121.4 MHz for <sup>31</sup>P. <sup>11</sup>B and <sup>13</sup>C{<sup>1</sup>H} NMR data were acquired

on a Bruker AVANCE-400 or DRX-400 instrument operating at 128.3 and 75.5 MHz, respectively. Chemical shifts are reported in  $\delta$  units referenced to residual solvent peaks (<sup>1</sup>H and <sup>13</sup>C), 85% H<sub>3</sub>PO<sub>4</sub> (<sup>31</sup>P;  $\delta$  0.0), or BF<sub>3</sub>·Et<sub>2</sub>O (<sup>11</sup>B;  $\delta$  0.0). Microanalysis data (CHN) were collected using an EAI CE-440 Elemental Analyzer at the University of Iowa. IR spectra were collected on a Thermo Scientific Nicolet iS5 using an attenuated total reflection (ATR) accessory in an N<sub>2</sub>-filled glovebox. HR-EI mass spectra were recorded on Waters GCT Premier instrument using TOF, and fragment ions (M: molecule, L: ligand) were assigned based on comparison to calculated natural abundance isotopic distributions.

(PhTBDPhos)CuCl (1). To a stirring solution of CuCl (0.045 g, 0.46 mmol) in CH<sub>2</sub>Cl<sub>2</sub> was added a solution of <sup>Ph</sup>TBDPhos (0.21 g, 0.42 mmol) in CH<sub>2</sub>Cl<sub>2</sub>. The reaction was stirred overnight, filtered, and concentrated under vacuum. Greenish-yellow blocks were obtained by layering the CH<sub>2</sub>Cl<sub>2</sub> solution with Et<sub>2</sub>O. The mother liquor was decanted, concentrated, and layered with additional Et<sub>2</sub>O to yield a second crop of crystals. Yield: 0.14 g (55%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 20 °C): δ 1.54 (quint, CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>, 4H), 2.87 (t, NCH<sub>2</sub>, 4H), 2.97 (m, NCH<sub>2</sub>, 4H), 7.34 (m, Ph, 12H), 7.48 (m, Ph, 8H). <sup>11</sup>B NMR (CDCl<sub>3</sub>, 20 °C):  $\delta$  24.8 (br s, FWHM = 460 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR  $(CDCl_3, 20 \ ^{\circ}C)$ :  $\delta 26.8$  (s,  $CH_2$ - $CH_2$ - $CH_2$ ), 46.7 (t,  $NCH_2$ ,  $J = 4 \ Hz$ ), 49.3 (s,  $NCH_2$ ), 128.6 (t, Ph, J = 5 Hz), 129.9 (s, Ph), 132.6 (t, Ph, J = 9 Hz), 133.9 (t, Ph, J = 16 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 20 °C): δ 40.9 (s). <sup>1</sup>H NMR (CD<sub>2</sub>Cl<sub>2</sub>, 25 °C): δ 1.55 (quint, CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>), 1.70 (quint, CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>), 2.78 (m, NCH<sub>2</sub>), 2.87 (t, NCH<sub>2</sub>), 2.94 – 3.02 (m, NCH<sub>2</sub>), 6.99 – 7.11 (m, Ph), 7.27 – 7.43 (m, Ph), 7.43 - 7.53 (m, Ph). <sup>11</sup>B NMR (CD<sub>2</sub>Cl<sub>2</sub>, 25 °C):  $\delta$  24.9 (br s, FWHM = 440 Hz). <sup>13</sup>C{<sup>1</sup>H} NMR (CD<sub>2</sub>Cl<sub>2</sub>, 25 °C):  $\delta$  27.1 (s, CH<sub>2</sub>-<u>C</u>H<sub>2</sub>-CH<sub>2</sub>), 27.2 (s, CH<sub>2</sub>-<u>C</u>H<sub>2</sub>-CH<sub>2</sub>), 47.1 (t, NCH<sub>2</sub>, J = 4Hz), 47.6 (s, NCH<sub>2</sub>), 49.6 (s, NCH<sub>2</sub>), 128.7 (t, Ph, J = 4 Hz), 128.8 (t, Ph, J = 4 Hz), 130.0 (s, Ph), 130.2 (s, Ph), 132.7 (t, Ph, J = 8 Hz), 132.8 (t, Ph, J = 9 Hz), 134.6 (t, Ph, J = 15 Hz), 134.8 (t, Ph,

J = 14 Hz). <sup>31</sup>P{<sup>1</sup>H} NMR (CD<sub>2</sub>Cl<sub>2</sub>, 25 °C):  $\delta$  39.9 (s), 56.8 (br s, FWHM = 440 Hz). Anal. calcd for C<sub>30</sub>H<sub>32</sub>BClCuN<sub>3</sub>P<sub>2</sub>: C, 59.4; H, 5.32; N, 6.93. Found: C, 59.3; H, 5.21; N, 6.83. MS(EI) [fragment ion, relative abundance]: *m/z* 108 [PPh, 33], 185 [PPh<sub>2</sub>, 13], 322 [L-PPh<sub>2</sub>, 7], 430 [L-Ph, 100], 507 [L, 6], 605 [M, 10]. IR (ATR, cm<sup>-1</sup>): 3068 vw, 3045 vw, 2946 vw, 2926 vw, 2845 brw, 1586 vw, 1571 vw,1500 w, 1479 w, 1466 vw, 1431 m, 1369 w, 1360 w, 1346 w, 1314 w, 1285 w, 1264 m, 1206 m, 1183 vw, 1157 w, 1096 m, 1070 vw, 1026 m, 997 vw, 964 vw, 881 w, 846 vw, 819 w, 758 w, 740 s, 691 s. UV-vis  $\lambda_{max}$ , nm ( $\epsilon$ , M<sup>-1</sup>cm<sup>-1</sup>): 301 (1.0 x 10<sup>4</sup>), 330 (9.4 x 10<sup>3</sup>) in CH<sub>2</sub>Cl<sub>2</sub>; 304 (1.0 x 10<sup>4</sup>), 367 (7.0 x 10<sup>3</sup>) in toluene.

(<sup>Ph</sup>TBDPhos-MeOH)CuCl (1-MeOH). To crystalline 1 (0.20 g, 0.33 mmol) was added NEt<sub>3</sub> (1 mL) followed by MeOH (10 mL). The greenish-yellow crystals changed to colorless over the course of a few hours. The mixture was left for two days, filtered, and evaporated to dryness under vacuum. Yield: 0.16 g (76%). Anal. Calcd for C<sub>31</sub>H<sub>36</sub>BClCuN<sub>3</sub>OP<sub>2</sub>: C, 58.3; H, 5.68; N, 6.58. Found: C, 58.3; H, 5.43; N, 6.27. IR (ATR, cm<sup>-1</sup>): 3105 m (NH), 3072 vw, 3049 w, 2942 vw, 2962 m, 2922 m, 2912 w, 2868 m, 2805 m, 1584 w, 1570 vw, 1499 vw, 1479 m, 1452 w, 1431 m, 1417 w, 1404 vw, 1387 vw, 1367 m, 1351 w, 1319 vw, 1294 m, 1259 w, 1238 m, 1188 m, 1154 vw, 1132 m, 1104 vw, 1078 s, 1063 s, 1034 vs, 1026 s, 997 m, 976 w, 959 m, 939 m, 909 s, 880 vw, 865 vs, 831 m, 805 w, 780 s, 740 vs, 692 vs, 640 vw, 618 w, 598 s, 574 w, 568 w, 563 m, 558 m.

(<sup>Ph</sup>TBDPhos)Cu(NPh<sub>2</sub>) (2). To a stirring mixture of 1 (0.10 g, 0.16 mmol) and HNPh<sub>2</sub> (0.028 g, 0.16 mmol) in toluene (10 mL) was added a solution of KN(SiMe<sub>3</sub>)<sub>2</sub> (0.033 g, 0.16 mmol) in toluene (5 mL) at -78 °C. The resulting yellow solution was allowed to slowly warm to room temperature, stirred for 3 h, filtered through Celite, and crystallized by vapor diffusion with pentane to yield yellow needles. Yield: 0.090 g (74%). Anal. Calcd for  $C_{42}H_{42}BCuN_4P_2$ : C, 68.3; H, 5.73; N, 7.58. Found: C, 68.4; H, 5.45; N, 7.49. <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 20 °C):  $\delta$  1.21 (quint, CH<sub>2</sub>-

C<u>H<sub>2</sub>-CH<sub>2</sub>, 4H</u>), 2.44 (t, NCH<sub>2</sub>, 4H), 2.79 (m, NCH<sub>2</sub>, 4H), 6.62 – 6.76 (m, Ph, 2H), 6.77 – 6.94 (m, Ph, 4H), 6.97 – 7.06 (m, Ph, 12H), 7.06 – 7.12 (m, Ph, 2H), 7.20 – 7.30 (m, Ph, 4H), 7.38 – 7.46 (m, Ph, 6H). <sup>11</sup>B NMR (C<sub>6</sub>D<sub>6</sub>, 20 °C):  $\delta$  25.0 (br s). <sup>31</sup>P{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 20 °C):  $\delta$  41.9 (s). IR (ATR, cm<sup>-1</sup>): 3061 w, 3046 w, 3012 w, 2958 vw, 2927 w, 2868 w, 2839 vw, 1587 w, 1572 m, 1501 w, 1479 m, 1471 m, 1435 m, 1430 m, 1384 m, 1366 m, 1353 m, 1317 m, 1294 s, 1266 s, 1222 vw, 1206 s, 1178 vw, 1164 s, 1116 vw, 1101 m, 1091 m, 1066 w, 1025 m, 991 m, 964 w, 943 m, 912 vw, 893 m, 864 w, 849 w, 823 w, 781 w, 740 s, 690 vs, 653 w, 632 m, 616 w, 588 m, 575 vw, 570 vw, 561 w. UV-vis (toluene)  $\lambda_{max}$ , nm ( $\epsilon$ , M<sup>-1</sup>cm<sup>-1</sup>): 287 (1.7 x 10<sup>4</sup>).

**Crystallographic studies.** Single crystals were obtained from  $Et_2O/CH_2Cl_2$  (1), pentane/toluene (2), or soaking crystalline 1 in MeOH/NEt<sub>3</sub> (1-MeOH). The crystals were mounted on a MiTeGen micromount using ParatoneN oil in air. The data collection, structural solution, and refinement were carried out as reported previously.<sup>2</sup> Briefly, the structures were solved with Direct Methods (SHELXT) and non-hydrogen atoms were confirmed with least-square method (SHELXL).<sup>3</sup> The positions of all hydrogen atoms were idealized and allowed to ride on the attached carbon or nitrogen atoms. The final refinement included anisotropic temperature factor on all non-hydrogen atoms. Structure solution and refinement were performed in  $Olex^{2,4}$  and publication figures were generated using  $Olex^2$  or Mercury. The details in data collection and refinement are available in Table S1.

**Photophysical Measurements.** UV-vis absorption spectra were recorded in deoxygenated CH<sub>2</sub>Cl<sub>2</sub> or toluene in screw-capped 1 cm quartz cuvettes using an Agilent Cary 8454 UV-vis spectrophotometer. To exclude air, all samples were prepared in a nitrogen-filled glovebox and sealed under nitrogen. Solid-state emission spectra were recorded using a Horiba FluoroMax-4 spectrofluorometer. The absolute quantum yields of the complexes were recorded using a

Spectralon-coated integrating sphere integrated with the FluoroMax-4 spectrofluorometer. Phosphorescence lifetimes were measured on a Horiba DeltaFlex Lifetime System, using pulsed diode excitation sources. Solid-state samples were prepared following the described procedure. 4 mg of Cu complex was ground into fine powder using a mortar and pestle in a nitrogen-filled glovebox. The powder was dropped on to the center of a clean quartz substrate. To ensure the sample was sealed tight, a minimum amount of grease was added on the edges of the slide, and the substrate was carefully covered with a second quartz slide to completely sandwich the compound.

**DFT Calculations.** DFT calculations were performed, using the Gaussian16 program.<sup>5</sup> Geometry optimizations were performed using the CAM-B3LYP<sup>6</sup> density functional and the def2-SVP basis set for C and H while the def2-TZVP and was used for Cu, Cl, N, B and P.<sup>7,8</sup> The nature of all stationary points was verified by harmonic vibrational analysis. The SMD<sup>9</sup> solvation model was used to perform geometry optimizations in both CH<sub>2</sub>Cl<sub>2</sub> and toluene. Calculations were performed at room temperature for both the gas phase and solution. Singlet ground state and triplet excited states were optimized using DFT. Energy minima were confirmed by harmonic vibrational analysis.

**TDDFT Calculations.** TDDFT calculations were used to investigate the photophysical differences in **1**, **1-MeOH**, and **2**. Calculations were performed with the same functional and basis set as described for the DFT optimizations. UV-vis transition energies were calculated for the first 10 states for singlet wavefunctions. Key transitions are assigned below in Table S3.



**Figure S1.** UV-vis absorption spectra for 1 in  $CH_2Cl_2$  (red; •) or in toluene (green; •) and 2 in toluene (blue;  $\blacktriangle$ ).

# II. XRD Data



**Figure S2.** Molecular structure of **2** with thermal ellipsoids at the 35% probability level. Phenyl groups on phosphorus are depicted as wire frames. Hydrogen atoms were omitted from the figure.

 Table S1. Crystallographic data for (<sup>Ph</sup>TBDPhos)CuCl (1), (<sup>Ph</sup>TBDPhos-MeOH)CuCl (1-MeOH),

 and (<sup>Ph</sup>TBDPhos)Cu(NPh<sub>2</sub>) (2).

	1	1-MeOH	2	
formula	$C_{30}H_{32}BClCuN_3P_2$	C <sub>31</sub> H <sub>36</sub> BClCuN <sub>3</sub> OP <sub>2</sub>	$C_{42}H_{42}BcuN_4P_2$	
FW (g mol <sup>-1</sup> )	606.32	638.37	739.08	
crystal system	Monoclinic	Monoclinic	Monoclinic	
space group	$P2_1/n$	$P2_1/c$	C2/c	
a (Å)	12.4036(12)	11.1940(11)	13.3593(15)	
b (Å)	19.0304(19)	21.080(2)	16.3964(17)	
c (Å)	12.5089(13)	13.3883(13)	17.537(2)	
α (deg)	90	90	90	
β (deg)	105.131(5)	107.235(5)	108.015(5)	
γ (deg)	90	90	90	
volume (Å <sup>3</sup> )	2850.3(5)	3017.4(5)	3653.1(7)	
Ζ	4	4	4	
$\rho_{calc} (g \text{ cm}^{-3})$	1.413	1.405	1.344	
$\mu$ (mm <sup>-1</sup> )	0.998	0.948	0.722	
F(000)	1256	1328	1544	
$\theta$ range (deg)	2.32/26.33	2.30/22.07	2.44/27.97	
R(int)	0.0403	0.1115	0.438	
data/restraints/para meters	5848/0/343	6202/1/327	4351/0/228	
GOF	0.983	1.013	1.059	
$R_1 [I > 2\sigma(I)]^a$	0.0309	0.0479	0.0346	
wR <sub>2</sub> (all data) <sup>b</sup>	0.1261	0.1060	0.0873	
Ext. Coeff	-	-	-	
Largest Peak/Hole (e·Å <sup>-3</sup> )	0.302/-0.398	0.531/-0.529	0.359/-0.497	
Temp (K)	190(2)	150(2)	150(2)	

<sup>a</sup> $\mathbf{R}_1 = \sum |F_o| - |F_c| | / |\sum |F_o|$  for reflections with  $F_o^2 > 2 \sigma(F_o^2)$ .

 ${}^{b}wR_{2} = \left[\sum w(F_{o}{}^{2} - F_{c}{}^{2})^{2} / \sum (F_{o}{}^{2})^{2}\right]^{1/2}$  for all reflections.

		1			1-MeOH			2	
	exp	calc (S)	calc (T)	exp	calc (S)	calc (T)	exp	calc (S)	calc (T)
Cu-P	2.1952(6)	2.24	2.24	2.183(1)	2.25	2.25	2.1903(5)	2.25	2.26
	2.1953(6)	2.24	2.27	2.193(1)	2.25	2.26		2.25	2.26
Cu-X	2.1681(6)	2.21	2.17	2.179(1)	2.22	2.25	1.899(2)	1.95	1.9
B-N	1.427(3)	1.43	1.42	1.628(5)	1.7	1.66	1.424(4)	1.43	1.44
B-N(P)	1.464(3)	1.47	1.45	1.529(5)	1.54	1.53	1.469(2)	1.47	1.48
	1.468(3)	1.47	1.47	1.544(5)	1.53	1.53		1.47	1.45
P-N	1.697(2)	1.7	1.73	1.662(3)	1.68	1.66	1.693(2)	1.7	1.68
	1.697(2)	1.7	1.67	1.666(3)	1.68	1.66		1.7	1.75
B-O	-	-	-	1.467(5)	1.44	1.44	-	-	-
P-M-P	101.52(2)	100.8	95.5	105.13(4)	102.8	86.7	102.03(3)	98.8	99.8
Σ NBN	360.0(2)	360	359.95	333.2(3)	331.87	330.295	360.0(2)	360	360.71

**Table S2.** Comparison of select bond distances and angles from XRD studies and optimized singlet(S) and triplet (T) DFT calculations in toluene.

## **III. DFT and TDDFT Data**

			TDDFT i	n toluene	TDDFT in DCM		
Complex	λ <sub>abs</sub> in toluene (ε/10 <sup>3</sup> M <sup>-1</sup> cm <sup>-1</sup> )	Energy (nm)	Oscillator Strength	Description	Energy (nm)	Oscillator Strength	Description
1	301 (10)	273	0.29	HOMO→LUMO+3	270	0.28	HOMO→LUMO+3
	333 (sh, 9.4)	302	0.23	HOMO→LUMO+1	297	0.23	HOMO→LUMO+1
2	287 (17)	285	0.40	HOMO→LUMO+9	272	0.15	HOMO-1→LUMO+1
		305	0.28	HOMO→LUMO+8	300	0.19	HOMO→LUMO+9
					310	0.38	HOMO→LUMO+8
1-MeOH	(not soluble)	299	0.19	HOMO→LUMO	295	0.22	HOMO→LUMO+1
		285	0.13	HOMO→LUMO+2	281	0.14	HOMO→LUMO+2

**Table S3.** Experimental and theoretical absorption data for 1, 2, and 1-MeOH at room temperature.  $\lambda_{abs}$  values are expressed in nm.

Table S4. Calculated excitation  $(E_{exc})$  and emission  $(E_P)$  energies from TDDFT.

	E (eV)	1	1-MeOH	2
GAS	E <sub>exc</sub>	3.60	3.63	3.43
	E <sub>P</sub>	2.18	2.07	2.20
DCM	E <sub>exc</sub>	3.85	3.84	3.63
	E <sub>P</sub>	2.17	2.30	2.02
TOLUENE	E <sub>exc</sub>	3.74	3.74	3.65
	E <sub>P</sub>	2.19	2.19	2.04



Figure S3. Kohn-Sham plots of select orbitals from the gas-phase DFT calculations of 1.



Figure S4. Kohn-Sham plots of select orbitals from the gas-phase DFT calculations of 1-MeOH.



Figure S5. Kohn-Sham plots of select orbitals from the gas-phase DFT calculations of 2.





Figure S6. Variable temperature <sup>1</sup>H NMR spectra of (<sup>Ph</sup>TBDPhos)CuCl (1) in CD<sub>2</sub>Cl<sub>2</sub>.



Figure S7. Variable temperature  ${}^{31}P{}^{1}H$  NMR spectra of ( ${}^{Ph}TBDPhos$ )CuCl (1) in CD<sub>2</sub>Cl<sub>2</sub>.



**Figure S8.** <sup>1</sup>H NMR spectrum of ( $^{Ph}TBDPhos$ )CuCl (1) in CDCl<sub>3</sub>. The \* symbol indicates resonances assigned to residual Et<sub>2</sub>O and CH<sub>2</sub>Cl<sub>2</sub>.



Figure S9. <sup>11</sup>B NMR spectrum of (<sup>Ph</sup>TBDPhos)CuCl (1) in CDCl<sub>3</sub>.



**Figure S10.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of ( $^{Ph}TBDPhos$ )CuCl (1) in CDCl<sub>3</sub>. The \* symbol indicates resonances assigned to residual CH<sub>2</sub>Cl<sub>2</sub>.



Figure S11. <sup>31</sup>P{<sup>1</sup>H} NMR spectrum of (<sup>Ph</sup>TBDPhos)CuCl (1) in CDCl<sub>3</sub>.



**Figure S12.** <sup>1</sup>H NMR spectrum of ( $^{Ph}TBDPhos$ )CuCl (1) in CD<sub>2</sub>Cl<sub>2</sub>. The \* symbol indicates resonances assigned to residual Et<sub>2</sub>O.



Figure S13. <sup>11</sup>B NMR spectrum of (<sup>Ph</sup>TBDPhos)CuCl (1) in CD<sub>2</sub>Cl<sub>2</sub>.



Figure S15. <sup>31</sup>P{<sup>1</sup>H} NMR spectrum of ( $^{Ph}TBDPhos$ )CuCl (1) in CD<sub>2</sub>Cl<sub>2</sub>.





Figure S17. <sup>11</sup>B NMR spectrum of (<sup>Ph</sup>TBDPhos)Cu(NPh<sub>2</sub>) (2) in C<sub>6</sub>D<sub>6</sub>.



### **V. Supporting Information References**

- (1) Lee, K.; Donahue, C. M.; Daly, S. R. Dalton Trans. 2017, 46, 9394-9406.
- (2) Lee, K.; Wei, H.; Blake, A. V.; Donahue, C. M.; Keith, J. M.; Daly, S. R. *Dalton Trans.* **2016**, *45*, 9774-9785.
- (3) Sheldrick, G. M. Acta Crystallogr. A 2008, 64, 112-122.
- (4) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. J. Appl. Crystallogr. 2009, 42, 339-341.
- (5) Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Hon-da, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.
- (6) Yanai, T.; Tew, D. P.; Handy, N. C. Chem. Phys. Lett. 2004, 393, 51-57.
- (7) Schäfer, A.; Horn, H.; Ahlrichs, R. J. Chem. Phys. 1992, 97, 2571-2577.
- (8) Schäfer, A.; Huber, C.; Ahlrichs, R. J. Chem. Phys. 1994, 100, 5829-5835.
- (9) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. J Phys. Chem. B 2009, 113, 6378-6396.