Electronic Supplementary Information for

Preparation and photophysical properties of fluorescent difluoroboronated β -diketones having phenanthrene studied by emission and transient absorption measurements

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1. Procedure for the compound preparations and analytical data

Synthesis of 1-acethylphenanthrene, β -diketones and difluoroboronated β -diketones. Acetylphenathrenes (AcPhe) are the key precursors to the desired boron complexes. 2-, 3-, and 9-Acetylphenathrenes (2-AcPhe, 3-AcPhe and 9-AcPhe, respectively) are commercially available whereas 1-acetylphenanthren (1-AcPhe) was synthesized by using photocyclization of a stilbene derivative. The synthesis procedures are illustrated in Scheme S1.



Scheme S1. Synthetic procedures to 1-acetylphenanthrene.

We performed acetal protection of the carbonyl group in *o*-acetylstilbene as it did not undergo photocyclization in the presence of iodine in aerated cyclohexane. The acetaled stilbene was subjected to photocyclization to form the phenanthrene derivative with the protected acetyl group. The deprotection of the acetal provided the desired 1-acetylphenanthrene.

General procedures for preparing the diketones. The used diketones were prepared by Claisen condensation between appropriate aromatic acetyl compounds and aromatic methyl ethers $(Ar^1CO_2Me, Scheme S2)$. Acetyl compounds of phenyl, 2-naphthyl, 2-anthryl and phenanthryl rings (3.0 mmol) and methyl ethers (methyl benzoate, methyl 2-furoate and methyl thiophene-2-carboxylate) (3.3 mmol) were refluxed for 4 h in THF (15 ml) in the presence of NaH. After cooling to room temperature, HCl was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. The product was purified by silica-gel chromatography using a mixture of hexane and ethyl acetate to give the desired compound.



Scheme S2. Preparation of BF₂DKs.

Analytical Data for the employed compounds

2-NpDKPh. Yield 85 %. ¹H NMR (CDCl₃, 400 MHz) $\delta_{\rm H}$ 7.00 (s, 1H), 7.49-7.61 (m, 5H), 7.88-8.04 (m, 6H), 8.54 (brs, 1H).The ¹H NMR spectral data were agreed with those reported in the literature.¹

2-AntDKPh. Yield 52 %. ¹H NMR (CDCl₃, 400 MHz) $\delta_{\rm H}$ 8.75 (s, 1H), 8.60 (s, 1H), 8.46 (s, 1H), 8.07-7.97 (m, 7H), 7.68-7.51 (m, 5H), 7.00 (s, 1H). The ¹H NMR spectral data were agreed with those reported in the literature.²

1-PheDKPh. Yield 48 %. mp 142–143 °C. ¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 16.80 (brs, 1H), 8.85 (d, 1H, J = 8.3 Hz), 8.71 (d, 1H, J = 8.3 Hz), 8.38 (d, 1H, J = 9.1 Hz), 7.99 (d, 2H, J = 7.6 Hz), 7.91 (d, 1H, J = 7.3 Hz), 7.88 (d, 1H, J = 7.3 Hz), 7.83 (d, 1H, J = 9.1 Hz), 7.72–7.66 (two triplets overlapped, 2H), 7.63 (t, 1H, J = 7.3 Hz), 7.56 (t, 1H, J = 7.6 Hz), 7.48 (t, 2H, J = 7.6 Hz), 6.72 (s, 1H); ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 191.0, 184.6, 136.0, 135.1, 132.8, 131.9, 131.0, 130.2, 129.2, 128.9, 128.7, 128.4, 127.4, 127.2, 127.1, 125.9, 125.8, 123.8, 123.0, 98.8; HRMS (FAB-TOF) *m*/*z* calcd. for C₂₃H₁₇O₂ 325.1229 [M+1], found 325.1249.

2-PheDKPh. Yield 76 %. mp 117–118 °C. ¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 17.02 (s, 1H), 8.77 (d, 1H, J = 8.7 Hz), 8.73 (d, 1H, J = 8.1 Hz), 8.55 (d, 1H, J = 1.5 Hz), 8.21 (dd, 1H, J = 8.7, 1.5 Hz), 8.06 (m, 2H), 7.93 (d, 1H, J = 7.7 Hz), 7.85 (d, 1H, J = 8.9 Hz), 7.82 (d, 1H, J = 8.9 Hz), 7.59 (m, 1H), 7.70 (ddd, 1H, J = 7.7, 7.1, 1.4 Hz), 7.68 (ddd, 1H, J = 7.7, 7.1, 1.0 Hz), 7.60 (m, 1H), 7.53 (m, 2H). ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 186.0, 185.5, 135.7, 138.4, 138.2, 133.0, 132.7, 131.8, 129.9, 128.9, 128.4, 128.1, 127.8, 127.40, 127.38 (overlapped), 127.2, 124.5, 123.4 (overlapped), 93.6. HRMS (FAB-TOF) *m*/*z* calcd. for C₂₃H₁₇O₂ 325.1229 [M+1], found 325.1227.

3-PheDKPh. Yield 60 %. mp 123–125 °C. ¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 17.1 (s, 1H), 8.83 (d, 2H J = 8.3 Hz), 8.13 (dd, 1H, J = 8.2, 1.5 Hz), 8.08–8.05 (m, 2H), 7.97 (d, 1H, J = 8.2 Hz), 7.93 (brd, 1H, J = 7.9 Hz), 7.85 (d, 2H, J = 8.7 Hz), 7.78 (d, 2H, J = 8.7 Hz), 7.74 (ddd, 1H, J = 8.3, 7.1, 1.3 Hz), 7.65 (ddd, 1H, J = 7.9, 7.1, 1.3 Hz), 7.61–7.56 (m, 1H), 7.57–7.51 (m, 2H), 7.07 (s, 1H). ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 186.0, 185.8, 135.8, 134.8, 133.4, 132.7, 132.4, 130.7, 130.2, 129.6, 129.1, 129.0, 128.9 (overlapped), 127.40, 127.35, 126.5, 124.5, 123.0, 122.7, 93.7. HRMS (FAB-TOF) m/z calcd. for C₂₃H₁₇O₂ 325.1229 [M+1], found 325.1247.

9-PheDKPh. Yield 82 %. mp 172–174 °C.¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 16.82(brs, 1H), 8.76 (d, 1H, J = 8.3 Hz), 8.71 (d, 1H, J = 8.3 Hz), 8.54 (d, 1H, J = 8.3 Hz), 8.10 (s, 1H), 8.02 (m, 2H), 7.97

(d, 1H, J = 7.8 Hz), 7.77–7.70 (m, 2H), 7.70–7.63 (m, 4H), 7.57 (t, 1H, J = 7.4 Hz), 7.51 (t, 2H, J = 7.4 Hz), 6.80(s, 2H); ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 191.0, 184.6, 135.1, 134.2, 132.7, 131.6, 130.9, 130.5, 129.7, 128.9, 128.8, 128.6, 128.5, 127.35(two lines overlapped), 127.26 (two lines overlapped), 126.9, 123.1, 1232.8, 98.4; HRMS (FAB-TOF) m/z calcd. for C₂₃H₁₇O₂ 325.1229 [M+1], found 325.1242.

3-PheDKF. Yield 50 %. mp 216–217 °C. ¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 16.40(brs, 1H), 9.31 (s, 1H), 8.79 (d, 1H, *J* = 8.3 Hz), 8.08 (dd, 1H, *J* = 8.3, 1.6 Hz), 7.92 (d, 1H, *J* = 8.4), 7.90 (d, 1H, *J* = 7.8 Hz), 7.82 (d, 1H, *J* = 7.8 Hz), 7.75–7.70 (m, 2H), 7.68–7.62 (m, 2H), 7.30 (d, 1H, *J* = 3.4 Hz), 6.95 (s, 1H), 6.95(s, 2H); ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 182.5.0, 177.7, 151.2, 146.3, 134.7, 132.4, 132.3, 130.6, 130.1, 129.5, 129.0, 128.9, 127.32, 127.28, 126.4, 124.3, 122.9, 122.4,116.0, 122.9, 93.2. HRMS (FAB-TOF) *m*/*z* calcd. for C₂₁H₁₄O₃ 314.0943 [M+1], found 314.0944.

3-PheDKT. Yield 56 %. mp 235–238 °C. ¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 16.54(brs, 1H), 9.27 (s, 1H), 8.02 (dd, 1H, J = 8.5, 1.2 Hz), 7.92–786 (m, 2H), 7.86 (dd, 1H, J = 3.7, 0.8 Hz), 7.81 (d, 1H, J = 8.7 Hz), 7.74–7.69 (m, 3H), 7.66–7.61 (m, 2H), 7.19 (dd, 1H, J = 4.9, 3.8 Hz), 6.84 (s, 1H); ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 183.1, 180.7, 142.5, 134.6, 132.8, 132.3, 132.1, 130.5, 130.1, 129.4, 129.0, 128.9, 128.4, 127.30, 127.27, 126.4, 124.1, 122.9, 122.2, 93.6. HRMS (FAB-TOF) *m/z* calcd. for C₂₁H₁₄O₂S 3304.0715 [M+1], found 330.0719.

General procedures for BF_2DKs . The prepared diketone compound was refluxed in benzene for 1 h in the presence of boron trifluoride diethyl etherate. The desired product was filtrated and washed with benzene.

Ph@Ph. Yield 86 %. ¹H NMR (CDCl₃, 400 MHz,) $\delta_{\rm H}$ 7.20 (s, 1H), 7.56 (t, 4H, *J* = 7.33), 7.70 (t, 2H, *J* = 7.33), 8.16 (d, 4H, *J* = 7.33). The ¹H NMR spectral data were agreed with those reported in the literature.³

2-Np@Ph. Yield 85 %. ¹H NMR (CDCl₃, 400 MHz,) $\delta_{\rm H}$ 7.00 (s, 1H), 7.49–7.61 (m, 5H), 7.88–8.04 (m, 6H), 8.54 (brs, 1H). The ¹H NMR data were agreed with those reported in the literature.¹

2-Ant@Ph. Yield 48 %. ¹H NMR (DMSO- d_6 , 400 MHz) δ_H 8.92 (s, 1H), 8.70 (s, 1H), 8.41 (dd, 2H, J=1.37, 8.70), 8.29–8.11 (m, 5H), 7.85–7.81 (m, 1H), 7.70–7.59 (m, 4H), 7.32 (s, 1H). The ¹H NMR data were agreed with those reported in the literature.²

1-Phe@Ph. Yield 47 %. mp 210–211 °C. H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 8.97 (d, 1H, J = 8.4 Hz), 8.70 (d, 1H, J = 8.2 Hz), 8.38 (d, 1H, J = 9.3 Hz), 8.17 (m, 2H), 8.04 (dd, 1H, J = 7.3, 1.0 Hz), 7.95 (dd, 1H, J = 7.8, 1.0 Hz), 7.91 (d, 1H, J = 9.3 Hz), 7.77–7.68 (m, 4H), 7.57 (m, 2H), 7.11 (s, 1H). ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 187.8, 183.3, 135.7, 132.0, 131.8, 131.4, 130.0, 129.9, 129.8, 129.4, 129.34, 129.29, 128.9, 128.6, 127.7, 127.5, 125.7, 123.04, 122.95, 99.0. HRMS (FAB-TOF) m/z calcd. for C₂₃H₁₅BF₂O₂ 372.1133 [M⁺], found 372.1149.

2-Phe@Ph. Yield 27%. mp 261–263 °C. ¹H NMR (600 MHz, CDCl₃) $\delta_{\rm H}$ 8.97 (d, 1H, J = 8.4 Hz), 8.70 (d, 1H, J = 8.2 Hz), 8.38 (d, 1H, J = 9.3 Hz), 8.17 (m, 2H), 8.04 (dd, 1H, J = 7.3, 1.0 Hz), 7.95 (dd, 1H, J = 7.8, 1.0 Hz), 7.91 (d, 1H, J = 9.3 Hz), 7.77–7.68 (m, 4H), 7.57 (m, 2H), 7.11 (s, 1H). ¹³C NMR (150 MHz, CDCl₃) $\delta_{\rm C}$ 187.8, 183.3, 135.7, 132.0, 131.8, 131.4, 130.0, 129.9, 129.8, 129.4, 129.34, 129.29, 128.9, 128.6, 127.7, 127.5, 125.7, 123.04, 122.95, 99.0. HRMS (FAB-TOF) *m/z* calcd. for C₂₃H₁₅BF₂O₂ 372.1133 [M⁺], found 372.1135.

3-Phe@Ph. Yield 60 %. mp 258–260 °C. ¹H NMR (600 MHz, DMSO- d_6) $\delta_{\rm H}$ 9.80 (d, 1H, J = 1.2 Hz), 9.21 (d, 1H, J = 8.3 Hz), 8.51–8.48 (m, 3H). 8.30 (s, 1H), 8.25 (d, 1H, J = 8.5 Hz), 8.12 (d, 1H, J = 8.5 Hz), 8.10 (d, 1H, J = 8.7 Hz), 8.00 (d, 1H, J = 7.7 Hz), 7.90–7.84 (two triplets overlapped, 2H), 7.78 (t, 1H, J = 7.7 Hz), 7.34, t, 2H, J = 7.7 Hz). ¹³C NMR (150 MHz, DMSO- d_6) $\delta_{\rm C}$ 182.5, 182.3, 136.3, 135.9, 131.9, 131.5, 131.4, 130.0, 129.8, 129.6, 129.50, 129.47, 129.27, 129.0, 127.9, 126.3, 125.9, 125.5, 123.7, 95.0. HRMS (FAB-TOF) *m*/*z* calcd. for C₂₃H₁₅BF₂O₂ 372.1133 [M⁺], found 372.1170.

9-Phe@Ph. Yield 92 %. mp 172–174 °C. ¹H NMR (600 MHz, DMSO- d_6) $\delta_{\rm H}$ 9.08 (d, 1H, J = 8.0 Hz), 8.96 (d, 1H, J = 8.3 Hz), 8.79 (s, 1H), 8.05 (dd, 1H, J = 7.8, 1.5 Hz), 8.41 (d, 2H, J = 7.8 Hz), 8.23 (d, 1H, J = 7.8 Hz), 7.93–7.79 (m, 6H), 7.72 (t, 2H, J = 7.8 Hz). ¹³C NMR (150 MHz, DMSO- d_6) $\delta_{\rm C}$ 187.0, 182.9, 136.2, 134.0, 132.0, 131.2, 130.6, 130.5, 130.3, 129.6, 129.5 (two lines

overlapped), 129.0, 128.0, 127.93, 127.91, 127.3, 125.6, 123.9, 123.3, 99.0. HRMS (FAB-TOF) m/z calcd. for C₂₃H₁₅BF₂O₂ 372.1133 [M⁺], found 372.1133.

3-Phe@F. Yield 92 %. mp 216–217 °C. ¹H NMR (600 MHz, DMSO- d_6) $\delta_{\rm H}$ 9.69 (bs, 1H), 9.15 (d, 1H, J = 8.4 Hz), 8.44 (m, 1H), 8.41 (dd, 1H, J = 8.3, 1.3 Hz), 8.28 (d, 1H, J = 3.6 Hz), 8.24 (d, 1H, J = 8.5 Hz), 8.10 (two doublets, 2H), 8.00 (two doublets, 2H), 7.85 (ddd, J = 8.4, 7.2, 1.1 Hz), 7.77 (t, 1H, J = 7.6 Hz), 7.06 (dd, 1H, 3.6, 1.5 Hz). ¹³C NMR (150 MHz, DMSO- d_6) $\delta_{\rm C}$ 180.7, 170.8, 152.5, 147.3, 136.0, 131.9, 131.2, 129.9, 129.8, 129.6, 129.3, 129.0, 127.90, 127.88, 126.3, 125.24, 125.18, 124.9, 123.6, 115.1, 93.9. HRMS (FAB-TOF) *m*/*z* calcd. for C₂₁H₁₃BF₂O₃ 362.0926 [M⁺], found 362.0917.

3-Phe@T. Yield 72 %. mp 235–238 °C. ¹H NMR (600 MHz, DMSO- d_6) $\delta_{\rm H}$ 9.71 (bs, 1H), 9.16 (d, 1H, J = 8.3 Hz), 8.86 (d, 1H, J = 4.1 Hz), 8.46 (dd, 1H, J = 4.8, 1.2 Hz), 8.44 (dd, 1H, J = 8.5, 1.2 Hz), 8.25 (d, 1H, J = 8.5 Hz), 8.19 (s, 1H), 8.11 (two doublets, 2H), 8.00 (d, J = 7.8 Hz), 7.86 (t, 1H, J = 7.6 Hz), 7.77 (t, 1H, 7.3 Hz), 7.56 (dd, 1H, J = 4.8, 4.1 Hz). ¹³C NMR (150 MHz, DMSO- d_6) $\delta_{\rm C}$ 180.7, 170.8, 152.5, 147.3, 136.0, 131.9, 131.1, 129.9, 129.8, 129.6, 129.3, 129.0, 127.89, 127.88, 126.3, 125.24, 125.18, 124.9, 123.6, 115.1, 93.9. HRMS (FAB-TOF) *m*/*z* calcd. for C₂₁H₁₃BF₂O₂S 378.0697 [M⁺], found 378.0695.

Detailed procedures

1.1. Preparation of 1-Phe@Ph

1.1.1 Synthesis of compound 1.



To 60 ml chloroform solution of benzyltriphenylphosphonium bromide (2.5 g, 5.77 mmol) and 2acetylbenzaldehyde (780 mg, 5.25 mmol), 30 ml of aqueous KOH (50 %) was dropwise added. After the solution was stirred for 30 min at room temperature, 100 ml chloroform was added. The organic layer was separated, washed with brine, and evaporated under reduced pressure. The product was purified by silica gel chromatography using hexane/ethyl acetate (9:1, v/v) providing compound **1** (913 mg, 76 %).

1.1.2 Synthesis of compound 2.



To 200 ml benzene (Bz), compound **1** (1.3 g, 5.85 mmol), 30 ml ethylene glycol and *p*-toluenesulfonic acid (0.77 g, 4.0 mmol) were added, the solution was refluxed for 48 h. After cooling to room temperature, the solution was washed with water and brine. The product was separated by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) providing compound **2** (1.42 g, 91%).

1.1.3 Synthesis of compound 3.



A cyclohexane (CH) solution (1000 ml) of compound **2** (600 mg, 2.26 mmol) and 50 mg I₂ was photolyzed using with a home-made microflow photoreactor.⁴ The photolyzed solution was washed with aqueous Na₂S₂O₃ and brine. After usual work-up, crude compound **3** was obtained (500 mg, 83 %). ¹H NMR (CDCl₃, 400 MHz) $\delta_{\rm H}$, 8.75-8.71 (m, 3H), 8.01 (d, 1H, J = 7.33), 7.95-7.92 (m, 1H), 7.85 (d, 1H, J = 9.39), 7.69-7.63 (m, 3H), 4.14-4.13 (m,2H), 3.85-3.83 (m, 2H), 2.04 (s, 3H).

1.1.4 Synthesis of 1-AcPhe



Compound **3** (1.0 g, 3.78 mmol) and chloral hydrate (3.8 g, 22.7 mmol) was added in a mixture of 6 ml hexane and 0.5 ml CH_2Cl_2 . The solution was stirred at room temperature under N₂ atmosphere for 2 h. After adding CH_2Cl_2 (100 ml), the solution was washed with water and brine. After evaporating the solvent, the residue was chromatographed on silica-gel using hexane/ethyl acetate (3:1, v/v) to give 1-AcPhe (600 mg, 72 %).

1.1.5 Synthesis of compound 1-PheDKPh



To 25 ml of dry THF, 1-AcPhe (550 mg, 2.5 mmol) and NaH (60 % in oil, 720 mg, 18 mmol) were added, and the mixture was stirred for 5 min at room temperature. Methyl benzoate (0.40 ml, 3.0 mmol) was added to the solution, which was refluxed for 5 h. After cooling to room temperature, aqueous NH₄Cl (20 %, 30 ml) was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. The product was purified by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) to give 1-PheDKPh (390 mg, 48 %).



1-PheDKPh (240 mg, 0.74 mmol) and a Et_2O solution of boron trifluoride diethyl etherate (46 %, 0.30 ml, 1.1 mmol) were added to 7 ml of benzene, and the solution was refluxed for 1 h. The precipitated 1-Phe@Ph was collected by filtration and washed with benzene (130 mg, 47 %).

1.2 Preparation of 2-Phe@Ph

1.2.1 Synthesis of 2-PheDKPh



To 20 ml of dry THF, 2-acetylphenanthrene (507 mg, 2.3 mmol) and NaH (60 % in oil, 720 mg, 18 mmol) were added, and the mixture was stirred for 5 min at room temperature. Methyl benzoate (0.34 ml, 2.5 mmol) was added to the solution, which was refluxed for 3 h. After cooling to room temperature, aqueous NH₄Cl (20 %, 30 ml) was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. After removal of the solvent, the product was purified by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) to give 2-PheDKPh (576 mg, 76 %).

1.2.2 Synthesis of 2-Phe@Ph



2-PheDKPh (324 mg, 1.0 mmol) and boron trifluoride diethyl etherate (46 %, 0.41 ml, 1.5 mmol) were added to 7 ml of benzene, and the solution was refluxed for 1 h. The precipitated 2-Phe@Ph was collected by filtration and washed with benzene (100 mg, 27 %).

1.3 Preprarion of 3-Phe@Ph

1.3.1 Synthesis of 3-PheDKPh



To 20 ml of dry THF, 3-acetylphenanthrene (507 mg, 2.3 mmol) and NaH 700 mg (60 % in oil, 720 mg, 18 mmol) were added, and the mixture was stirred for 5 min at room temperature. Methyl benzoate 0.34 ml (2.5 mmol) was added to the mixture, which was then refluxed for 3 h. After cooling to room temperature, aqueous NH₄Cl (20 %, 30 ml) was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. After removal of the solvent, the product was purified by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) to give 3-PheDKPh (444 mg, 60 %).

1.3.2 Synthesis of 3-Phe@Ph



3-PheDKPh (324 mg, 1.0 mmol) and boron trifluoride diethyl etherate (46 %, 0.41 ml, 1.5 mmol) were added to 10 ml benzene, and the solution was refluxed for 1 h. The precipitated product was filtrated and washed with benzene to give 3-Phe@Ph (100 mg, 48 %).

1.4 Preparation of 9-Phe@Ph

1.4.1 Synthesis of 9-PheDKPh



To 25 ml of dry THF, 9-acetylphenanthrene (500 mg, 2.3 mmol) and NaH 700 mg (60 % in oil, 720 mg, 18 mmol) were added, and the solution was stirred for 5 min at room temperature. Methyl benzoate (0.34 ml, 2.7 mmol) was added to the solution, which was refluxed for 24 h. After cooling to room temperature, aqueous NH₄Cl (20 %, 30 ml) was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. After removal of the solvent, the product was purified by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) to give 9-PheDKPh (600 mg, 82 %).

1.4.2 Synthesis of 9-Phe@Ph



9-PheDKPh (300 mg, 0.92 mmol) and boron trifluoride diethyl etherate (46 %, 0.41 ml, 1.5 mmol) were added to 10 ml of benzene, and the solution was refluxed for 1 h. The precipitated product was filtrated and washed with benzene to give 9-Phe@Ph (305 mg, 92 %).

1.5 Preparation of 3-Phe@F

1.5.1 Synthesis of 3-PheDKF



To 25 ml of dry THF, 3-acetylphenanthrene (500 mg,2.3 mmol) and NaH (60 % in oil, 720 mg, 18 mmol) were added, and the mixture was stirred for 5 min at room temperature. Methyl 2-furoate (0.40 ml, 3.9 mmol) was added to the solution, which was refluxed for 5 h. After cooling to room temperature, aqueous NH₄Cl (20 %, 30 ml) was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. After removal of the solvent, the product was purified by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) to give 3-PheDKF (358 mg, 50 %).

1.5.2 Synthesis of 3-Phe@F



3-PheDKF (300 mg, 0.95 mmol) and boron trifluoride diethyl etherate (46 %, 0.41 ml, 1.5 mmol) were added to 6 ml benzene, then the solution was refluxed for 1 h. The precipitated product was filtrated and washed with benzene to give 3-Phe@F (320 mg, 92 %).

1.6. Preparation of 3-Phe@T

1.6.1 Synthesis of compound 3-PheDKT



To 25 ml of dry THF, 3-acetylphenanthrene (500 mg, 2.3 mmol) and NaH 700 mg (60 % in oil, 720 mg, 18 mmol) were added, and the mixture was stirred for 15 min at room temperature. Methyl 2-thiophenecarboxylate (0.35 ml, 3.0 mmol) was added to the mixture, which was refluxed for 3 h. After cooling to room temperature, aqueous NH₄Cl (20 %, 30 ml) was added. The product was extracted with ethyl acetate, and the solution was washed with aqueous NH₄Cl and brine. After removal of the solvent, the product was purified by silica-gel chromatography using hexane/ethyl acetate (3:1, v/v) to give 3-PheDKT (426 mg, 56 %).

1.6.2 Synthesis of 3-Phe@T



3-PheDKF (376 mg, 1.14 mmol) and boron trifluoride diethyl etherate (46 %, 0.41 ml, 1.5 mmol) were added to 6 ml of benzene, then the solution was refluxed for 1 h. The precipitated product was filtrated and washed with benzene to give 3-Phe@T (309 mg, 72 %).

2. Absorption and fluorescence spectra in ACN

Figure S1 shows absorption and fluorescence spectra of the used compounds in acetonitrile (ACN). All the compounds show stokes shifts. The fluorescence spectrum of Ph@Ph has vibrational structures while others show structureless emission bands.



Figure S1. Absorption (black) and fluorescence (blue) spectra in ACN for Ph@Ph (a), 2-Np@Ph (b), 2-Ant@Ph (c), 1-Phe@Ph (d), 2-Phe@Ph (e), 3-Phe@Ph (f), 9-Phe@Ph (g), 3-Phe@F (h) and 3-Phe@T (i). The fluorescence spectra are not corrected.

3. Transient absorption spectra in ACN

Figure S2 shows transient absorption spectra obtained upon 355 and 400 nm laser pulsing in the ACN solution of the DF_2DKs .



Figure S2. Transient absorption spectra obtained at 200 ns upon laser pulsing in the Ar-purged ACN solution of Ph@Ph (a), 2-Np@Ph (b), 2-Ant@Ph (c), 1-Phe@Ph (d), 2-Phe@Ph (e), 3-Phe@Ph (f), 9-Phe@Ph (g), 3-Phe@F (h) and 3-Phe@T (i) at 295 K. A 355 nm Laser pulse was used for Ph@Ph whereas 400 nm laser pulses were employed for exciting the other BF₂DK.

4. Results of DFT and TD-DFT calculations (atom coordinates and sum of electronic and zeropoint energies)

The calculation was carried out at the DFT level, using the Gaussian 09 software package.⁵ The geometries of the difluoroboronated β -diketones were fully optimized by using the 6-31G(d) base set at the B3LYP method considering a dielectric constant of CF in the CPCM model. Atom coordinates for the optimized geometries of the difluoroboronated β -diketones in vaccum and chloroform are as follows.

	X	Y	Z
С	-5. 57662	1.21084	-1.40909
С	-6. 73661	0. 47573	-1.26593
С	-6. 71366	-0. 75171	-0. 56427
С	-5. 53449	-1. 22196	-0. 01991
C	-4. 32699	-0. 48511	-0. 15314
С	-4. 35565	0. 74193	-0. 85552
С	-3. 06719	-0.95796	0. 41035
C	-1.88902	-0. 18477	0. 23964
C	-1. 96551	1.06988	-0. 47857
С	-3. 13789	1.51012	-0. 99829
С	-2. 99650	-2. 17620	1.13200
С	-1.80000	-2. 62557	1.66016
С	-0. 62364	-1.87531	1. 47668
С	-0.66145	-0. 67501	0. 77461
С	0.61450	0.06335	0. 60682
С	1. 78877	-0. 55963	0. 17022
С	2. 98315	0. 15899	0. 04047
С	4. 26597	-0. 42467	-0. 40381
С	4. 32040	-1.71538	-0. 95828
С	5. 54387	-2. 24548	-1.36984
С	6. 71722	-1. 49423	-1. 23221
С	6. 66802	-0. 20834	-0.68466
С	5. 44727	0. 32874	-0. 27274
0	0. 57060	1.32204	0.90214
0	3. 04780	1. 42459	0. 31920
В	1.81713	2. 18454	0.77909
F	2. 09017	2. 64773	2.00309
F	1. 55370	3. 09115	-0. 17066
H	-5, 58506	2. 15843	-1. 94728
Н	-7. 67525	0.83171	-1. 68822
Н	-7. 63625	-1. 32098	-0, 45796
Н	-5. 52350	-2, 16919	0. 52085
Н	-1. 05533	1.67167	-0. 57346
Н	-3, 19226	2.46006	-1. 53341
H	-3. 90772	-2. 76422	1. 27189
•	0.00772		

Table S1. Atom coordinates for the optimized geometry of 1-Phe@Ph in vacuum.

Н	-1. 75780	-3.55899	2. 22067	
Н	0. 31446	-2. 24084	1.89964	
Н	1. 76507	-1.61731	-0. 08349	
Н	3. 40713	-2. 30230	-1.07265	
Н	5. 58579	-3. 24538	-1.80041	
Н	7. 67146	-1.91295	-1.55427	
Н	7. 58152	0. 37747	-0. 58024	
Н	5. 39652	1. 33785	0. 15211	
~				

Sum of electronic and zero-point energies = -1260.62705140 Hartree

Table S2.	Atom	coordinates	for tl	he op	ptimized	geometry	y of	1-Phe	@Ph i	n chlorof	orm.
						1.7	/				

1 a	ole 32. Atom coordinates for the	optimized	
	Х	Y	Z
С	-5. 70865	1.33807	-1. 02252
С	-6.86930	0. 60226	-0. 87128
С	-6. 79983	-0. 70195	-0. 34009
С	-5. 58077	-1.24797	0. 02801
С	-4. 37356	-0. 51871	-0. 11305
С	-4. 45212	0.79966	-0. 65061
С	-3.06799	-1.05604	0. 26204
С	-1.89766	-0. 24331	0. 11796
С	-2. 03261	1.07265	-0. 44569
С	-3. 25034	1.56263	-0. 81295
С	-2. 92417	-2.37336	0. 75825
С	-1. 68559	-2. 89518	1. 08784
С	-0. 53438	-2. 10968	0. 94313
С	-0. 62399	-0.79596	0. 48445
С	0. 62977	-0. 01669	0. 42706
С	1. 83014	-0. 57549	-0. 02091
С	3. 01775	0. 15966	0. 07635
С	4. 34533	-0. 36924	-0. 27583
С	4. 55116	-1.73801	-0. 53920
С	5. 81932	-2. 20623	-0. 87624
С	6. 89827	-1.31835	-0. 95624
С	6. 70483	0. 04230	-0. 69328
С	5. 43936	0. 51524	-0. 35283
0	0. 58128	1.21626	0. 85735
0	2. 99757	1.39320	0. 50869
В	1. 73205	2. 15822	0. 70518
F	1.84245	2.91290	1.85911
F	1. 50871	2.95307	-0. 41836
Н	-5. 74442	2.34589	-1. 42958
Н	-7. 82864	1.02425	-1. 15816
Н	-7.70796	-1.28586	-0. 21639
Н	-5.57130	-2. 25329	0. 43404
Н	-1. 15252	1.68690	-0.58217
Н	-3. 32436	2.55974	-1. 24052
Н	-3. 79693	-3.00389	0. 88256
H	-1.60464	-3. 90938	1. 46/45
H	0. 42983	-2.51563	1. 23233
H	1.83014	-1.57528	-0. 42/24
Н	3. 73171	-2. 44508	-0. 46827

Н	5.96709	-3. 26418	-1.07280			
Н	7. 88574	-1.68647	-1. 22095			
Н	7. 53980	0.73428	-0. 75542			
Н	5. 28517	1. 56945	-0. 15196			
Sum of electronic and zero-point energies = -1260.65477731 Hartree						

1 6

Table S3. Atom coordinates for the optimized geometry of 2-Phe@Ph in vacuum.

I dole bet I from	ecolumnates for the	opumizea	Seemen je	
	Х	Y	Z	
С	-7. 42023	-1. 25577	0.04064	
C	-6. 50732	-2. 32882	0. 00734	
С	-5. 14439	-2.08699	-0. 01217	
С	-4. 62916	-0. 76754	0.00067	
С	-5. 55926	0.31634	0. 03485	
С	-3. 20426	-0. 47257	-0. 01898	
C	-2. 77412	0.88920	-0. 00380	
С	-3. 74658	1.94669	0. 03178	
C	-5. 07897	1.67026	0.04990	
С	-2. 20470	-1. 47724	-0. 05563	
С	-0.86103	-1.16460	-0. 07041	
С	-0. 43097	0. 18670	-0. 05132	
С	-1.39680	1. 18933	-0. 02260	
С	0. 99371	0. 56217	-0. 05789	
С	2.03850	-0. 35517	0. 11706	
С	3. 36228	0. 07296	-0. 03834	
С	4. 52482	-0. 83807	-0. 01218	
C	5. 81486	-0. 29140	0. 11856	
C	6. 93188	-1. 12367	0. 15742	
C	6. 77897	-2. 51011	0.05913	
C	5. 50143	-3.06262	-0. 08037	
C	4. 38163	-2. 23409	-0. 11504	
0	1. 24322	1.82256	-0. 25979	
0	3. 63985	1. 32753	-0. 23444	
В	2. 61179	2. 41511	-0. 03405	
F	2. 68856	2.84725	1. 27702	
F	2. 82492	3. 39921	-0.96098	
Н	-7.64322	0.87970	0. 07997	
Н	-8. 48930	-1. 45025	0. 05577	
Н	-6. 87318	-3. 35211	-0. 00312	
Н	-4. 46771	-2. 93447	-0. 03737	
Н	-3. 39237	2.97436	0. 04335	
Н	-5.80838	2. 47639	0. 07623	
Н	-2. 48794	-2. 52373	-0. 07820	
Н	-0. 13819	-1.97234	-0. 11539	
Н	-1.07961	2. 22708	-0. 00832	
Н	1.82466	-1. 38949	0. 33557	
Н	5. 92467	0. 78474	0.19490	
Н	7. 92240	-0.69036	0. 26540	
Н	7.65109	-3. 15814	0. 08741	
Н	5. 37858	-4. 13865	-0. 16809	
Н	3. 40016	-2.67875	-0. 24480	

Sum of electronic and zero-point energies = -1260.66104196 Hartree

	Х	Y	Z	
С	2. 77487	0.89354	-0.00366	
С	1. 39808	1.19534	-0.01791	
С	3. 20166	-0. 47010	-0.01062	
С	2. 20072	-1. 47475	-0.03384	
С	0.85742	-1.16132	-0.04495	
С	0. 42991	0. 19235	-0. 03512	
С	-0. 99208	0. 56153	-0.04182	
С	-2. 03617	-0. 35728	0. 11427	
С	-3. 36085	0.06673	-0. 02947	
С	-4. 51940	-0.84236	-0.01060	
С	-4. 36811	-2. 23797	-0. 12902	
С	-5. 48449	-3. 07138	-0. 10274	
С	-6. 76527	-2. 52651	0.04413	
С	-6. 92617	-1. 14135	0. 15875	
С	-5.81339	-0. 30318	0. 12783	
0	-1. 24865	1.83172	-0. 22548	
0	-3. 64015	1. 33225	-0. 20644	
В	-2.61337	2. 40185	-0.03655	
F	-2.82462	3. 37702	-0.99588	
F	-2. 71167	2.91631	1.25631	
Н	2. 48060	-2. 52197	-0.04814	
Н	0. 13619	-1.97023	-0.07724	
Н	-1.82056	-1. 39514	0. 31058	
Н	-3. 38592	-2. 67843	-0. 26325	
Н	-5. 35608	-4. 14540	-0. 20188	
Н	-7. 63383	-3. 17904	0.06626	
Н	-7.91855	-0.71484	0. 27366	
Н	-5. 93437	0.77046	0. 21937	
Н	1.08794	2. 23502	-0.00848	
С	3.74969	1.95036	0.01857	
С	4. 62606	-0.76784	0.00375	
С	5. 55893	0.31480	0. 02418	
С	5. 08211	1.67081	0. 03132	
Н	5.81362	2. 47501	0.04724	
Н	3. 39838	2.97900	0. 02411	
С	5. 13679	-2. 08984	-0.00147	
С	6. 94782	0. 03933	0.03794	
С	7. 41602	-1.26249	0. 03213	
Н	8. 48450	-1.45980	0. 04281	
C	6. 49999	-2. 33425	0.01238	
Н	6.86340	-3. 35826	0.00800	
Н	7.64531	0.87352	0. 05331	
Н	4. 45831	-2. 93580	-0. 01626	

Table S4. Atom coordinates for the optimized geometry of 2-Phe@Ph in chloroform.

Sum of electronic and zero-point energies = -1260.63914126 Hartree

		Х	Y	Z	
	С	-6. 63909	0. 12096	-0.34686	
	С	-6. 64021	1. 47538	-0. 61529	
	С	-5. 42038	2. 18999	-0.65654	
	С	-4. 22280	1. 54014	-0. 43107	
	С	-4. 19474	0. 14695	-0. 15517	
	С	-5. 41733	-0. 56433	-0. 11207	
	С	-2. 94759	-0. 56850	0. 08333	
	С	-2. 98156	-1.95828	0.35710	
	С	-4. 25124	-2. 64996	0. 39621	
	С	-5. 41202	-1.98374	0. 17157	
	С	-1.69320	0.08764	0.05031	
	С	-0. 51214	-0. 61351	0.27050	
	С	-0. 55550	-2.00475	0. 54944	
	С	-1.76767	-2. 65974	0.59215	
	С	0.77799	0.10420	0.21940	
	С	2.02162	-0.51486	0. 04580	
	С	3. 19977	0.23751	-0.00513	
	С	4. 54925	-0. 34269	-0. 17987	
	С	5. 66887	0.37347	0.27940	
	С	6,94920	-0. 16254	0. 12724	
	С	7, 11821	-1, 40562	-0, 49056	
	С	6.00628	-2. 11545	-0.95935	
	C	4, 72291	-1. 58862	-0, 80587	
	0	0.66705	1, 39161	0, 33758	
	0	3, 19626	1. 52887	0, 11241	
	В	1, 89435	2, 28395	0, 30846	
	F	1. 75129	3, 09008	-0, 74995	
	F	1. 97168	2, 87057	1, 50880	
	Н	-7, 57486	-0, 43583	-0, 31210	
	H	-7. 57465	2.00497	-0. 79628	
	H	-5, 43594	3. 25944	-0.86760	
	Н	-3, 28442	2. 09826	-0. 46199	
	Н	-4, 24428	-3, 71837	0, 61135	
	Н	-6. 37297	-2, 49996	0, 19949	
	Н	-1. 64944	1, 16720	-0. 14995	
	Н	0.37324	-2. 54538	0. 73772	
	Н	-1 80828	-3 72713	0 80959	
	Н	2 07234	-1 59671	-0 04868	
	H	5 52575	1 35178	0 75063	
	 Н	7 81572	0 30217	0 48711	
	H	8 11879	-1 82244	-0 61045	
	 Н	6 14205	-3 07001		
	Н	0.1429J 2 850/1	-2 120/7	-1 10151	
_	11	0.00941	2.1094/	1. 10101	

 Table S5. Atom coordinates for the optimized geometry of 3-Phe@Ph in vacuum.

Sum of electronic and zero-point energies = -1260.62679147 Hartree

	Х	Y	Z	
С	-6.65582	0. 13055	0. 08332	
С	-6.68768	1.51313	0. 11170	
С	-5.47855	2. 23742	0.09771	
С	-4. 26189	1. 57471	0.05608	
С	-4. 19706	0. 16115	0. 02703	
С	-5. 42455	-0. 56833	0.04075	
С	-2.93917	-0. 57960	-0.01671	
С	-2.96887	-2.00827	-0. 04355	
С	-4. 22591	-2.69603	-0. 02936	
С	-5.40065	-2.00408	0.01127	
С	-1.68300	0.05729	-0. 03235	
С	-0. 48669	-0. 66310	-0.06783	
С	-0.53239	-2. 08189	-0. 09720	
С	-1.74806	-2. 72877	-0. 08649	
С	0. 78543	0.07170	-0. 07231	
С	2.03520	-0. 53337	0. 10635	
С	3. 20056	0. 22652	-0. 03213	
С	4. 56025	-0. 33793	0.01456	
С	5.66190	0. 53352	0. 12165	
С	6.95879	0. 02679	0. 17553	
С	7.17604	-1.35418	0. 11738	
С	6. 08880	-2. 22809	0.00355	
С	4. 78979	-1.72653	-0. 04688	
0	0. 69697	1.36220	-0. 27405	
0	3. 13409	1.51800	-0. 23027	
В	1.85842	2. 27854	-0. 09188	
F	1.81338	3. 25377	-1.07367	
F	1.80123	2.82990	1. 18836	
Н	-7. 58090	-0. 44112	0.09343	
Н	-7.63776	2. 03928	0.14460	
Н	-5. 49714	3. 32367	0.11946	
Н	-3.35166	2.16442	0.04587	
Н	-4. 22502	-3. 78283	-0. 05084	
Н	-6. 34922	-2. 53573	0. 02242	
Н	-1.61840	1. 13719	-0.00906	
Н	0. 37866	-2.66755	-0. 14781	
Н	-1. 78367	-3. 81475	-0.11619	
Н	2. 10032	-1.58811	0.31998	
Н	5. 49007	1.60297	0.16952	
Н	7.79998	0, 70830	0, 26451	
Н	8. 18779	-1.74839	0.15786	
Н	6. 25346	-3, 30034	-0. 05095	
Н	3.96247	-2. 41994	-0. 15361	

 Table S6. Atom coordinates for the optimized geometry of 3-Phe@Ph in chloroform.

Sum of electronic and zero-point energies = -1260.65976304 Hartree

Table S7. Ato	m coordinates for the	e optimized	geometry o	f 9-Phe@Ph in vacuum.
	Х	Y	Z	
С	-2. 97146	3. 11548	0.71705	
С	-4. 25649	3. 62172	0. 69983	
С	-2. 71729	1.76495	0.37135	
С	-3. 79269	0.90624	0.0022	
С	-5. 09786	1. 45464	-0.00199	
С	-5. 32586	2. 77828	0.33717	
С	-1. 38616	1.24944	0. 40272	
С	-1.09642	-0.05873	0. 10781	
С	-2. 15830	-0.96880	-0. 29486	
С	-3. 50172	-0. 47866	-0.35345	
С	0. 31148	-0. 49406	0.24679	
С	1. 37628	0. 30182	-0. 19377	
С	2. 69106	-0.08455	0.09771	
С	3. 87764	0.73947	-0. 20759	
С	3. 76770	2.07512	-0.63739	
С	4. 90972	2. 82121	-0. 92059	
С	6. 17693	2.24576	-0. 77914	
С	6. 29682	0. 92054	-0.34937	
С	5. 15726	0. 17155	-0.06309	
0	0. 52068	-1.63331	0.8343	
0	2. 93280	-1.21924	0. 68407	
В	1. 88137	-2. 29021	0. 83831	
F	2.06682	-2. 92106	2.03667	
F	1. 94973	-3. 12912	-0. 26093	
С	-4. 52083	-1.36621	-0.77546	
С	-4. 24238	-2.67202	-1.13639	
С	-2. 91886	-3. 14423	-1.0948	
С	-1.89795	-2. 30756	-0. 68239	
Н	-2, 13371	3, 74910	1.00001	
Н	-4, 44375	4. 65831	0,96621	
Н	-5, 94786	0.83766	-0. 27064	
Н	-6. 34080	3. 16699	0. 32509	
Н	-0, 59103	1.91886	0.72059	
Н	1, 16942	1.21103	-0. 73762	
Н	2, 79424	2.54349	-0. 73962	
Н	4, 81190	3.85265	-1. 24784	
Н	7.06647	2.82935	-1.00146	
Н	7, 27911	0.46965	-0. 23853	
Н	5. 24170	-0. 85727	0. 26879	
Н	-5 54759	-1. 02222	-0. 82912	
Н	-5 04755	-3, 32782	-1, 45714	
H	-2 69247	-4 16656	-1 38484	
Н	-0 88551	-2 68877	-0 64812	
Sum of electro	onic and zero-point er	hergies = -12	260.631914	.57 Hartree
	1	0		

 Table S7. Atom coordinates for the optimized geometry of 9-Phe@Ph in vacuum.

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			Х	Y	Z	
C -4.28227 -2.66788 1.09259 C -3.51127 -0.47326 0.33849 C -2.16818 -0.96816 0.31018 C -1.92468 -2.30812 0.70490 C -2.95888 -0.01069 C -2.95888 -0.31225 C -3.7835 0.91683 -0.32219 C -2.69968 1.77484 -0.34225 C -1.37087 1.25392 -0.35219 C -1.37087 1.25392 -0.0649 C 0.31116 -0.49655 -0.20418 C 1.38169 0.30296 0.06649 C 1.38169 0.30296 0.08458 C 3.8106 0.30216 0.86253 C 3.77128 2.08177 0.57377 C 6.18077 2.24437 0.75377 C 6.18077 2.24437 0.75377 C 6.30044 0.90475 0.36764 C 5.16068 0.15231 0.9197 O 0.51778 -1.65430	_	С	-4. 54546	-1.35896	0. 72882	
C -3.51127 -0.47326 0.33849 C -2.16818 -0.96816 0.31018 C -1.92468 -2.30812 0.70490 C -2.5588 -3.14374 1.08827 C -3.78835 0.91683 -0.01069 C -2.69968 1.77484 -0.34225 C -1.37087 1.25392 -0.35219 C -1.09283 -0.06050 -0.06649 C 0.31116 -0.49655 -0.20418 C 1.38169 0.30296 0.20786 C 2.69328 -0.08879 -0.08458 C 3.8106 0.73071 0.20537 C 3.77128 2.08117 0.59164 C 4.91437 2.83020 0.86253 C 6.18077 2.24437 0.75377 C 6.30044 0.90475 0.36764 C 5.16068 0.15231 0.9197 O 0.51778 -1.65430 -0.77401 O 2.92738 -2.06776 F 1.978		С	-4. 28227	-2.66788	1.09259	
C -2. 16818 -0. 96816 0. 31018 C -1. 92468 -2. 03012 0. 70490 C -2. 95888 -3. 14374 1. 08827 C -3. 78835 0. 91683 -0. 01069 C -2. 69968 1. 77484 -0. 34225 C -1. 37087 1. 25392 -0. 35219 C -1. 37087 1. 25392 -0. 06449 C 0. 31116 -0. 49655 -0. 20418 C 1. 38169 0. 30296 0. 20786 C 2. 69328 -0. 08879 -0. 08458 C 3. 87108 0. 73071 0. 20537 C 3. 77128 2. 08117 0. 59164 C 4. 91437 2. 83020 0. 86253 C 6. 30044 0. 90475 0. 36764 C 5. 16068 0. 15231 0. 09197 O 0. 51778 -1. 65430 -0. 77401 O 2. 92738 -1. 24012 -0. 65831 B 1. 87334 -2. 28197 -0. 83013 F 2. 03460 2. 878		С	-3. 51127	-0. 47326	0. 33849	
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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		С	-1.37087	1. 25392	-0.35219	
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C4.914372.830200.86253C6.180772.244370.75377C6.300440.904750.36764C5.160680.152310.09197O0.51778 -1.65430 -0.77401 O2.92738 -1.24012 -0.65831 B1.87334 -2.28197 -0.83013 F2.03460 -2.87808 -2.06776 F1.97895 -3.20417 0.21017 H -0.91211 -2.69014 0.70431 H -2.74384 -4.16629 1.38604 H 0.56850 1.92399 -0.64735 H1.18420 1.22324 0.73585 H2.80008 2.55820 0.66697 H4.81793 3.87192 1.15456 H 7.28177 0.44677 0.28302 H 5.24940 -0.88680 -0.20454 H -5.57183 -1.01150 0.75688 H -5.09821 -3.32143 1.38894 C -5.09150 1.46995 -0.03269 C -2.93716 3.13202 -0.67677 C -4.22089 3.64341 -0.68510 H -5.09150 1.46925 -0.93269 C -2.93716 3.13202 -0.67677 C -2.08961 3.19362 -0.36939 H -2.08961 3.76488 -0.92833 H -5.95166 0.85550 0.20708		С	3. 77128	2. 08117	0. 59164	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		С	4.91437	2.83020	0.86253	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		С	6. 18077	2. 24437	0.75377	
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$		С	5.16068	0. 15231	0.09197	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0	0. 51778	-1.65430	-0. 77401	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		0	2.92738	-1. 24012	-0. 65831	
F2.03460 -2.87808 -2.06776 F1.97895 -3.20417 0.21017 H -0.91211 -2.69014 0.70431 H -2.74384 -4.16629 1.38604 H -0.56850 1.92399 -0.64735 H 1.18420 1.22324 0.73585 H 2.80008 2.55820 0.66697 H 4.81793 3.87192 1.15456 H 7.07030 2.83070 0.96743 H 7.28177 0.44677 0.28302 H 5.24940 -0.88680 -0.20454 H -5.57183 -1.01150 0.75688 H -5.09821 -3.32143 1.38894 C -5.09150 1.46995 -0.03269 C -2.93716 3.13202 -0.67677 C -4.22089 3.64341 -0.68510 H -4.39713 4.68425 -0.94142 C -5.30344 2.79993 -0.36108 H -6.31628 3.19362 -0.28833 H -2.08961 3.76488 -0.92883		В	1.87334	-2. 28197	-0. 83013	
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H1. 184201. 223240. 73585H2. 800082. 558200. 66697H4. 817933. 871921. 15456H7. 070302. 830700. 96743H7. 281770. 446770. 28302H5. 24940-0. 88680-0. 20454H-5. 57183-1. 011500. 75688H-5. 09821-3. 321431. 38894C-5. 091501. 46995-0. 03269C-2. 937163. 13202-0. 67677C-4. 220893. 64341-0. 68510H-6. 316283. 19362-0. 36039H-2. 089613. 76488-0. 92883H-5. 951660. 855500. 20708		Н	-0.56850	1.92399	-0.64735	
H2.800082.558200.66697H4.817933.871921.15456H7.070302.830700.96743H7.281770.446770.28302H5.24940 -0.88680 -0.20454 H -5.57183 -1.01150 0.75688H -5.09821 -3.32143 1.38894C -5.09150 1.46995 -0.03269 C -2.93716 3.13202 -0.67677 C -4.39713 4.68425 -0.94142 C -5.30344 2.79993 -0.36108 H -6.31628 3.19362 -0.36939 H -2.08961 3.76488 -0.92883 H -5.95166 0.85550 0.20708		Н	1. 18420	1. 22324	0. 73585	
H4. 81793 3. 87192 1. 15456 H7. 07030 2. 83070 0. 96743 H7. 28177 0. 44677 0. 28302 H5. 24940 $-0. 88680$ $-0. 20454$ H $-5. 57183$ $-1. 01150$ 0. 75688 H $-5. 09821$ $-3. 32143$ 1. 38894 C $-5. 09150$ 1. 46995 $-0. 03269$ C $-2. 93716$ 3. 13202 $-0. 67677$ C $-4. 39713$ 4. 68425 $-0. 94142$ C $-5. 30344$ 2. 79993 $-0. 36108$ H $-6. 31628$ 3. 19362 $-0. 36939$ H $-2. 08961$ 3. 76488 $-0. 92883$ H $-5. 95166$ $0. 85550$ $0. 20708$		Н	2.80008	2. 55820	0. 66697	
H 7.07030 2.83070 0.96743 H 7.28177 0.44677 0.28302 H 5.24940 -0.88680 -0.20454 H -5.57183 -1.01150 0.75688 H -5.09821 -3.32143 1.38894 C -5.09150 1.46995 -0.03269 C -2.93716 3.13202 -0.67677 C -4.22089 3.64341 -0.68510 H -4.39713 4.68425 -0.94142 C -5.30344 2.79993 -0.36108 H -6.31628 3.19362 -0.36939 H -2.08961 3.76488 -0.92883 H -5.95166 0.85550 0.20708		Н	4.81793	3.87192	1.15456	
H 7.28177 0.44677 0.28302 H 5.24940 -0.88680 -0.20454 H -5.57183 -1.01150 0.75688 H -5.09821 -3.32143 1.38894 C -5.09150 1.46995 -0.03269 C -2.93716 3.13202 -0.67677 C -4.22089 3.64341 -0.68510 H -4.39713 4.68425 -0.94142 C -5.30344 2.79993 -0.36108 H -6.31628 3.19362 -0.36939 H -2.08961 3.76488 -0.92883 H -5.95166 0.85550 0.20708		Н	7.07030	2.83070	0.96743	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		Н	7. 28177	0. 44677	0. 28302	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		Н	5. 24940	-0. 88680	-0. 20454	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		Н	-5. 57183	-1.01150	0. 75688	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		Н	-5. 09821	-3. 32143	1. 38894	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		С	-5. 09150	1. 46995	-0. 03269	
C -4. 22089 3. 64341 -0. 68510 H -4. 39713 4. 68425 -0. 94142 C -5. 30344 2. 79993 -0. 36108 H -6. 31628 3. 19362 -0. 36939 H -2. 08961 3. 76488 -0. 92883 H -5. 95166 0. 85550 0. 20708		С	-2.93716	3. 13202	-0.67677	
H -4. 39713 4. 68425 -0. 94142 C -5. 30344 2. 79993 -0. 36108 H -6. 31628 3. 19362 -0. 36939 H -2. 08961 3. 76488 -0. 92883 H -5. 95166 0. 85550 0. 20708		С	-4. 22089	3. 64341	-0.68510	
C -5. 30344 2. 79993 -0. 36108 H -6. 31628 3. 19362 -0. 36939 H -2. 08961 3. 76488 -0. 92883 H -5. 95166 0. 85550 0. 20708		Н	-4. 39713	4. 68425	-0.94142	
H-6. 316283. 19362-0. 36939H-2. 089613. 76488-0. 92883H-5. 951660. 855500. 20708		С	-5. 30344	2. 79993	-0.36108	
H -2. 08961 3. 76488 -0. 92883 H -5. 95166 0. 85550 0. 20708		Н	-6.31628	3. 19362	-0. 36939	
Н –5. 95166 0. 85550 0. 20708		Н	-2. 08961	3.76488	-0. 92883	
		Н	-5.95166	0.85550	0. 20708	

 Table S8. Atom coordinates for the optimized geometry of 9-Phe@Ph in chloroform.

Sum of electronic and zero-point energies = -1260.65053126 Hartree

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Table S9.	Atom coordinates for the	optimized	geometry of	3-Phe@F in vacuum.
$ \begin{array}{c} C & 6. 3921 & 0. 19581 & 0.03267 \\ C & 6. 40721 & 1.57814 & 0.04602 \\ C & 5. 18846 & 2.28487 & 0.03692 \\ C & 3. 98174 & 1.60505 & 0.01486 \\ C & 3. 93609 & 0. 19095 & 0.00133 \\ C & 5. 17347 & -0.52079 & 0.1021 \\ C & 2. 68823 & -0.56609 & -0.02172 \\ C & 2. 68323 & -0.56609 & -0.02561 \\ C & 2. 73651 & -1.99371 & -0.03443 \\ C & 4. 00301 & -2.66367 & -0.02561 \\ C & 5. 16821 & -1.95634 & -0.00386 \\ C & 1. 42347 & 0.05441 & -0.03074 \\ C & 0. 23732 & -0.68016 & -0.04824 \\ C & 0. 30118 & -2.09718 & -0.06406 \\ C & 1. 52483 & -2.72904 & -0.05790 \\ C & -1.04457 & 0.04471 & -0.04524 \\ C & -2.28882 & -0.57934 & 0.11175 \\ C & -3.44860 & 0.18760 & -0.03391 \\ 0 & -0.96954 & 1.33257 & -0.22365 \\ 0 & -3.41686 & 1.47539 & -0.22465 \\ B & -2.14322 & 2.25599 & -0.00167 \\ F & -2.11697 & 2.68118 & 1.31371 \\ F & -2.08259 & 3.27137 & 0.91821 \\ H & 7.35028 & 2.11775 & 0.06332 \\ H & 5.19158 & 3.37152 & 0.04712 \\ H & 3.06241 & 2.18054 & 0.00802 \\ H & 4.01664 & -3.75092 & -0.3615 \\ H & 6.12427 & -2.47506 & 0.00328 \\ H & 1.33390 & 1.1333 & -0.01914 \\ H & -0.60464 & -2.69295 & -0.09637 \\ H & 1.519158 & 3.37152 & 0.04712 \\ H & 3.3966 & -0.89062 & -0.03815 \\ C & -4.77282 & -0.39034 & -0.01858 \\ C & -4.77282 & -0.39034 & -0.01858 \\ C & -4.77282 & -0.39034 & -0.01858 \\ C & -6.02088 & 0.17841 & -0.11129 \\ C & -6.21863 & -2.03451 & 0.0491 \\ H & -8.03656 & -0.89062 & -0.03185 \\ H & -6.22068 & 1.23498 & -0.21947 \\ C & -6.21863 & -2.03451 & 0.0491 \\ H & -8.03656 & -0.82385 & -0.06849 \\ H & -6.22068 & 1.23498 & -0.21947 \\ C & -6.21863 & -2.03451 & 0.10491 \\ H & -8.03656 & -0.82385 & -0.06849 \\ H & -6.22068 & 1.23498 & -0.21947 \\ C & -6.21863 & -2.03451 & 0.10491 \\ H & -8.03656 & -0.82385 & -0.06849 \\ H & -6.47682 & -3.07850 & 0.20383 \\ \hline \end{array}$		Х	Y	Z	
$ \begin{array}{c} {\rm C} & {\rm 6}, 40721 & {\rm 1}, 57814 & {\rm 0}, 4662 \\ {\rm C} & {\rm 5}, 18846 & {\rm 2}, 28487 & {\rm 0}, 03692 \\ {\rm C} & {\rm 3}, 9374 & {\rm 1}, 60505 & {\rm 0}, 01486 \\ {\rm C} & {\rm 3}, 93609 & {\rm 0}, 19095 & {\rm 0}, 00133 \\ {\rm C} & {\rm 5}, 17347 & {\rm -0}, 52079 & {\rm 0}, 01021 \\ {\rm C} & {\rm 2}, 68823 & {\rm 0}, 56609 & {\rm -0}, 02172 \\ {\rm C} & {\rm 2}, 73651 & {\rm -1}, 99371 & {\rm -0}, 03443 \\ {\rm C} & {\rm 4}, 00301 & {\rm -2}, 66367 & {\rm -0}, 02561 \\ {\rm C} & {\rm 5}, 16821 & {\rm -1}, 95634 & {\rm -0}, 00386 \\ {\rm C} & {\rm 1}, 42347 & {\rm 0}, 05441 & {\rm -0}, 03074 \\ {\rm C} & {\rm 0}, 23732 & {\rm -0}, 68016 & {\rm -0}, 04824 \\ {\rm C} & {\rm 0}, 03118 & {\rm -2}, 09718 & {\rm -0}, 06406 \\ {\rm C} & {\rm 1}, 52483 & {\rm -2}, 72904 & {\rm -0}, 05790 \\ {\rm C} & {\rm -1}, 04457 & {\rm 0}, 04471 & {\rm -0}, 04524 \\ {\rm C} & {\rm -2}, 28882 & {\rm -0}, 57934 & {\rm 0}, 11175 \\ {\rm C} & {\rm -3}, 44860 & {\rm 0}, 18760 & {\rm -0}, 03391 \\ {\rm 0} & {\rm -0}, 096954 & {\rm 1}, 33257 & {\rm -0}, 22365 \\ {\rm 0} & {\rm -3}, 41686 & {\rm 1}, 47539 & {\rm -0}, 22465 \\ {\rm 8} & {\rm -2}, 14322 & {\rm 2}, 25599 & {\rm -0}, 00167 \\ {\rm F} & {\rm -2}, 11697 & {\rm 2}, 68118 & {\rm 1}, 31371 \\ {\rm F} & {\rm -2}, 08259 & {\rm 3}, 27137 & {\rm -0}, 91821 \\ {\rm H} & {\rm 7}, 35028 & {\rm 3}, 1775 & {\rm 0}, 06332 \\ {\rm H} & {\rm 5}, 19158 & {\rm 3}, 37152 & {\rm 0}, 04712 \\ {\rm H} & {\rm 3}, 06241 & {\rm 2}, 18054 & {\rm 0}, 00802 \\ {\rm H} & {\rm 4}, 01664 & {\rm -3}, 35092 & {\rm -0}, 03615 \\ {\rm H} & {\rm 6}, 12427 & {\rm 2}, 45706 & {\rm 0}, 00328 \\ {\rm H} & {\rm 1}, 33390 & {\rm 1}, 1333 & {\rm -0}, 01914 \\ {\rm H} & {\rm -0}, 60464 & {\rm -2}, 69295 & {\rm -0}, 09637 \\ {\rm H} & {\rm -1}, 237448 & {\rm -1}, 64135 & {\rm 0}, 28393 \\ {\rm C} & {\rm -4}, 77282 & {\rm -0}, 39034 & {\rm -0}, 01858 \\ {\rm C} & {\rm -6}, 20088 & {\rm 0}, 17841 & {\rm -0}, 11129 \\ {\rm C} & {\rm -6}, 22068 & {\rm 1}, 23498 & {\rm -0}, 21947 \\ {\rm C} & {\rm -6}, 21663 & {\rm -2}, 03455 & {\rm -0}, 06649 \\ {\rm H} & {\rm -6}, 22068 & {\rm -1}, 75290 & {\rm 0}, 11426 \\ {\rm H} & {\rm -6}, 47628 & {\rm -1}, 75290 & {\rm 0}, 11426 \\ {\rm H} & {\rm -6}, 47826 & {\rm -1}, 75290 & {\rm 0}, 11426 \\ {\rm H} & {\rm -6}, 478264 & {\rm -1}, 75290 & {\rm 0}, 11426 \\ {\rm H} & {\rm -6}, 47662 $	С	6. 39421	0. 19581	0. 03267	
C5. 188462. 284870. 03692C3. 981741. 605050. 01486C3. 936090. 190950. 00133C5. 17347 $-0. 52079$ 0. 01021C2. 68823 $-0. 56609$ $-0. 02172$ C2. 73651 $-1. 99371$ $-0. 03443$ C4. 00301 $-2. 66367$ $-0. 02561$ C5. 16821 $-1. 95634$ $-0. 03074$ C0. 23732 $-0. 68016$ $-0. 04824$ C0. 30118 $-2. 09718$ $-0. 6406$ C1. 52483 $-2. 72904$ $-0. 5790$ C $-2. 2882$ -57934 $0. 11175$ C $-3. 44860$ $0. 18760$ $-0. 23911$ O -99554 $1. 33257$ $-0. 22865$ O $-3. 41686$ $1. 47539$ $-0. 22465$ B $-2. 14322$ $2. 25599$ $-0. 00167$ F $-2. 11697$ $2. 68118$ $1. 31371$ F $-2. 08259$ $3. 27137$ $-0. 91821$ H $7. 32761$ $-0. 36277$ $0. 03920$ H $7. 32761$ $-0. 36277$ $0. 0322$ H $5. 19158$ $3. 37152$ $0. 04712$ H $3. 00930$ $1. 13333$ $-0. 01941$ H $-0. 66241$ $2. 89295$ $-0. 03615$ H $-0. 20864$ $-1. 61333$ $-0. 01580$ H $-1. 62088$ $0. 17841$ $-0. 01580$ C $-6. 98062$ $-0. 03185$ H $-2. 37468$ $-1. 614135$ $0. 28393$ <td< td=""><td>С</td><td>6. 40721</td><td>1. 57814</td><td>0.04602</td><td></td></td<>	С	6. 40721	1. 57814	0.04602	
$ \begin{array}{c} C & 3.98174 & 1.60505 & 0.01486 \\ C & 3.93609 & 0.19095 & 0.00133 \\ C & 5.17347 & -0.52079 & 0.01021 \\ C & 2.68823 & -0.56609 & -0.02172 \\ C & 2.73651 & -1.9371 & -0.03433 \\ C & 4.00301 & -2.66367 & -0.02561 \\ C & 5.16821 & -1.95634 & -0.00386 \\ C & 1.42347 & 0.05441 & -0.03074 \\ C & 0.23732 & -0.68016 & -0.04824 \\ C & 0.30118 & -2.09718 & -0.06406 \\ C & 1.52483 & -2.72904 & -0.05790 \\ C & -1.04457 & 0.04471 & -0.04524 \\ C & -2.28882 & -0.57934 & 0.11775 \\ C & -3.44860 & 0.18760 & -0.03391 \\ 0 & -0.96954 & 1.33257 & -0.22365 \\ 0 & -3.41686 & 1.47539 & -0.22465 \\ 8 & -2.11697 & 2.68118 & 1.31371 \\ F & -2.08259 & 3.27137 & -0.91821 \\ H & 7.32761 & -0.36277 & 0.03920 \\ H & 7.35028 & 2.11775 & 0.06332 \\ H & 5.19158 & 3.37152 & 0.04712 \\ H & 3.06241 & 2.18054 & 0.00802 \\ H & 4.01664 & -2.69295 & -0.09637 \\ H & 1.33390 & 1.13333 & -0.01914 \\ H & -0.60464 & -2.69295 & -0.09637 \\ H & 1.519158 & 3.37152 & 0.04712 \\ H & 3.06241 & 2.18054 & 0.00802 \\ H & -2.37468 & -1.64135 & 0.28393 \\ C & -4.77282 & -0.39034 & -0.01885 \\ C & -6.02088 & 0.17841 & -0.11129 \\ C & -6.21863 & -2.03355 & -0.09637 \\ H & -2.37468 & -1.64135 & 0.28393 \\ C & -4.77282 & -0.39034 & -0.01858 \\ C & -6.02088 & 0.17841 & -0.011829 \\ C & -6.21863 & -2.03355 & -0.09637 \\ H & -6.37662 & -0.37500 \\ H & -6.27668 & -2.69295 & -0.09637 \\ H & -6.27688 & -1.75290 & -0.03315 \\ -6.20288 & -0.37540 \\ -7.5728 & -0.39034 & -0.01858 \\ C & -6.02088 & 0.17841 & -0.01129 \\ C & -6.21863 & -2.03451 & 0.01941 \\ H & -6.63666 & -0.83085 & -0.06849 \\ H & -6.7682 & -3.07850 & 0.20383 \\ 0 & -4.89246 & -1.75290 & 0.11426 \\ \end{array}$	С	5. 18846	2. 28487	0. 03692	
C3.936090.190950.00133C5.17347-0.520790.01021C2.6823-0.56609-0.02172C2.73651-1.99371-0.03443C4.00301-2.66367-0.02561C5.16821-1.95634-0.00386C1.423470.05441-0.03074C0.23732-0.68016-0.04824C0.30118-2.09718-0.06406C1.52483-2.72904-0.05790C-1.044570.04471-0.04524C-2.28882-0.579340.11175C-3.448600.18760-0.033910-0.969541.3257-0.223650-3.416861.47539-0.22465B-2.143222.25599-0.00167F-2.116972.681181.31371F-2.082593.27137-0.91821H7.350282.117750.06332H5.191583.371520.04712H3.062412.180540.00802H4.01664-3.75092-0.03615H6.12427-2.475060.00328H1.57434-3.81518-0.07540H-2.37468-1.641350.28393C-4.77282-0.39034-0.11858C-6.020880.17841-0.11129C-6.21863-2.034510.10491H-6.220681.23498-0.21947C-6.95806-0.89052<	С	3. 98174	1.60505	0.01486	
C5. 17347-0. 520790. 01021C2. 68823-0. 56609-0. 02172C2. 73651-1. 99371-0. 03443C4. 00301-2. 66367-0. 02561C5. 16821-1. 95634-0. 00386C1. 423470. 05441-0. 03074C0. 23732-0. 68016-0. 04824C0. 30118-2. 09718-0. 06406C1. 52483-2. 72904-0. 05790C-1. 044570. 04471-0. 04524C-2. 28882-0. 579340. 11175C-3. 448600. 18760-0. 3391O-0. 969541. 33257-0. 22365O-3. 416861. 47539-0. 22465B-2. 143222. 25599-0. 00167F-2. 16972. 681181. 31371F-2. 082593. 27137-0. 91821H7. 350282. 117750. 06332H3. 062412. 180540. 00320H3. 302412. 180540. 00328H4. 01664-3. 75092-0. 03615H6. 12427-2. 475060. 00328H1. 57434-3. 81518-0. 07540H-0. 60464-2. 69295-0. 09637H1. 57434-3. 81518-0. 07540H-6. 27688-0. 19441H-6. 206880. 17841C-6. 27688-0. 23345C-6. 27686-0. 82365C-6. 95806 </td <td>С</td> <td>3.93609</td> <td>0. 19095</td> <td>0. 00133</td> <td></td>	С	3.93609	0. 19095	0. 00133	
C2.68823-0.56609-0.02172C2.73651-1.99371-0.03443C4.00301-2.66367-0.02561C5.16821-1.95634-0.00366C1.423470.05441-0.03074C0.23732-0.68016-0.04824C0.30118-2.09718-0.06406C1.52483-2.72904-0.05790C-1.044570.04471-0.04524C-2.28882-0.57934-0.11175C-3.448600.18760-0.033910-0.969541.33257-0.223650-3.416861.47539-0.22465B-2.116972.681181.31371F-2.116972.681181.31371F-2.082593.27137-0.91821H7.350282.117750.06332H5.191583.371520.04712H3.062412.180540.00802H4.01664-3.75092-0.01914H-0.60464-2.69255-0.09637H1.57434-3.81518-0.07540H-2.37468-1.641350.28393C-4.7282-0.39034-0.11129C-6.95806-0.89062-0.03185H-6.220681.23489-0.21947C-6.95806-0.89062-0.03185H-6.220681.23489-0.21947C-6.95806-0.82365-0.06849H-6.47682-0.30	С	5. 17347	-0. 52079	0. 01021	
C2.73651 -1.99371 -0.02443 C4.00301 -2.66367 -0.02561 C5.16821 -1.95634 -0.03074 C0.23732 -0.68016 -0.04824 C0.30118 -2.09718 -0.06406 C1.242470.04471 -0.04524 C0.3018 -2.72904 -0.05790 C -1.04457 0.04471 -0.04524 C -2.28882 -0.57934 0.11175 C -3.44860 0.18760 -0.03391 0 -0.96954 1.33257 -0.22365 0 -3.41686 1.47539 -0.22465 B -2.14322 2.25599 -0.00167 F -2.11697 2.68118 1.31371 F -2.08259 3.27137 -0.91821 H 7.35028 2.11775 0.06332 H 5.19158 3.37152 0.04712 H 3.06241 2.18054 0.00802 H 4.01664 -3.75092 -0.03615 H 6.12427 -2.47506 0.00328 H 1.33390 1.13333 -0.01914 H -0.60464 -2.69255 -0.09637 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.11858 C -6.20686 1.23488 -0.1947 C -6.95806 -0.89062 -0.03185 H -6.20686 1	С	2. 68823	-0.56609	-0. 02172	
C4.00301 -2.66367 -0.02561 C5.16821 -1.95634 -0.00366 C1.423470.05441 -0.03074 C0.23732 -0.66016 -0.04824 C0.30118 -2.09718 -0.06406 C1.52483 -2.72904 -0.05790 C -1.04457 0.04471 -0.04524 C -2.28882 -0.57934 0.11175 C -2.28882 -0.57934 0.11175 C -3.44860 0.18760 -0.03391 0 -0.96954 1.3257 -0.22365 0 -3.41686 1.47539 -0.21465 B -2.14322 2.25599 -0.00167 F -2.11697 2.68118 1.31371 F -2.08259 3.27137 -0.91821 H 7.35028 2.11775 0.06332 H 5.19158 3.37152 0.04712 H 3.06241 2.18054 0.00802 H 4.01664 -3.75092 -0.03615 H 6.12427 -2.47506 0.00328 H 1.33390 1.13333 -0.01914 H -0.60464 -2.69295 -0.09637 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28333 C -4.77282 -0.39034 -0.11129 C -6.620268 0.17841 -0.11129 C -6.95806 -0.89062 -0.03185 H -6.22068 <t< td=""><td>С</td><td>2. 73651</td><td>-1.99371</td><td>-0. 03443</td><td></td></t<>	С	2. 73651	-1.99371	-0. 03443	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	4. 00301	-2.66367	-0. 02561	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	5. 16821	-1.95634	-0. 00386	
C 0.23732 -0.68016 -0.04824 C 0.30118 -2.09718 -0.06406 C 1.52483 -2.72904 -0.05790 C -1.04457 0.04471 -0.04524 C -2.28882 -0.57934 0.11175 C -3.44860 0.18760 -0.03391 0 -0.96954 1.33257 -0.22365 0 -3.41686 1.47539 -0.22465 B -2.14322 2.25599 -0.00167 F -2.1697 2.68118 1.31371 F -2.08259 3.27137 -0.91821 H 7.35028 2.11775 0.6332 H 7.35028 2.11775 0.06332 H 5.19158 3.37152 0.04712 H 3.06241 2.18054 0.00802 H 4.01664 -3.75092 -0.03615 H 6.12427 -2.47506 0.00328 H 1.33990 1.13333 -0.01914 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.02088 0.17841 -0.11129 C -6.29686 1.23498 -0.21947 C -6.21663 -2.03451 0.10491 H -6.22068 1.23498 -0.21947 C -6.47682 -3.07850 0.20383 O -4.89246 -1.75290 0.11426	С	1. 42347	0. 05441	-0. 03074	
C0.30118 -2.09718 -0.06406 C1.52483 -2.72904 -0.05790 C -1.04457 0.04471 -0.04524 C -2.2882 -0.57934 0.11175 C -3.44860 0.18760 -0.03391 0 -0.96954 1.33257 -0.22365 0 -3.41686 1.47539 -0.22465 B -2.14322 2.25599 -0.00167 F -2.11697 2.68118 1.31371 F -2.08259 3.27137 -0.91821 H 7.35028 2.11775 0.06332 H 5.19158 3.37152 0.04712 H 3.06241 2.18054 0.00802 H 4.01664 -3.75092 -0.03615 H 6.12427 -2.47506 0.00328 H 1.33990 1.13333 -0.07540 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.02088 0.17841 -0.1129 C -6.21863 -2.03451 0.104911 H -6.22068 1.23498 -0.21947 H -6.21863 -2.03451 0.10491 H -6.47682 -3.07850 0.20383 O -4.89246 -1.75290 0.21426	С	0. 23732	-0. 68016	-0. 04824	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	0. 30118	-2. 09718	-0. 06406	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	1. 52483	-2. 72904	-0. 05790	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-1.04457	0. 04471	-0. 04524	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-2. 28882	-0. 57934	0. 11175	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-3. 44860	0. 18760	-0. 03391	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	-0. 96954	1. 33257	-0. 22365	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0	-3. 41686	1. 47539	-0. 22465	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	В	-2. 14322	2. 25599	-0. 00167	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	F	-2. 11697	2. 68118	1.31371	
H7. 32761 -0. 36277 0. 03920 H7. 35028 2. 11775 0. 06332 H5. 19158 3. 37152 0. 04712 H3. 06241 2. 18054 0. 00802 H4. 01664 -3. 75092 -0. 03615 H6. 12427 -2. 47506 0. 00328 H1. 33990 1. 13333 -0. 01914 H-0. 60464 -2. 69295 -0. 09637 H1. 57434 -3. 81518 -0. 07540 H2. 37468 -1. 64135 0. 28393 C-4. 77282 -0. 39034 -0. 01858 C-6. 02088 0. 17841 -0. 11129 C-6. 95806 -0. 89062 -0. 03185 H-6. 22068 1. 23498 -0. 21947 C-6. 21863 -2. 03451 0. 10491 H-8. 03656 -0. 82385 -0. 06849 H-6. 47682 -3. 07850 0. 20383 O-4. 89246 -1. 75290 0. 11426	F	-2. 08259	3. 27137	-0. 91821	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	7. 32761	-0.36277	0. 03920	
H $5. 19158$ $3. 37152$ $0. 04712$ H $3. 06241$ $2. 18054$ $0. 00802$ H $4. 01664$ $-3. 75092$ $-0. 03615$ H $6. 12427$ $-2. 47506$ $0. 00328$ H $1. 33990$ $1. 13333$ $-0. 01914$ H $-0. 60464$ $-2. 69295$ $-0. 09637$ H $1. 57434$ $-3. 81518$ $-0. 07540$ H $-2. 37468$ $-1. 64135$ $0. 28393$ C $-4. 77282$ $-0. 39034$ $-0. 01858$ C $-6. 02088$ $0. 17841$ $-0. 11129$ C $-6. 95806$ $-0. 89062$ $-0. 03185$ H $-6. 22068$ $1. 23498$ $-0. 21947$ C $-6. 21863$ $-2. 03451$ $0. 10491$ H $-8. 03656$ $-0. 82385$ $-0. 06849$ H $-6. 47682$ $-3. 07850$ $0. 20383$ O $-4. 89246$ $-1. 75290$ $0. 11426$	H	7.35028	2. 11775	0.06332	
H 3.06241 2.18054 0.00802 H 4.01664 -3.75092 -0.03615 H 6.12427 -2.47506 0.00328 H 1.33990 1.13333 -0.01914 H -0.60464 -2.69295 -0.09637 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.95806 -0.89062 -0.03185 H -6.22068 1.23498 -0.21947 C -6.21863 -2.03451 0.10491 H -8.03656 -0.82385 -0.06849 H -6.47682 -3.07850 0.20383 O -4.89246 -1.75290 0.11426	Н	5. 19158	3. 37152	0. 04712	
H4. 01664 -3.75092 -0.03615 H6. 12427 -2.47506 0.00328 H1. 33990 1.13333 -0.01914 H -0.60464 -2.69295 -0.09637 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.02088 0.17841 -0.11129 C -6.95806 -0.89062 -0.03185 H -6.22068 1.23498 -0.21947 C -6.21863 -2.03451 0.10491 H -8.03656 -0.82385 -0.06849 H -6.47682 -3.07850 0.20383 O -4.89246 -1.75290 0.11426	Н	3. 06241	2. 18054	0.00802	
H 6.12427 -2.47506 0.00328 H 1.33990 1.13333 -0.01914 H -0.60464 -2.69295 -0.09637 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.02088 0.17841 -0.11129 C -6.95806 -0.89062 -0.03185 H -6.22068 1.23498 -0.21947 C -6.21863 -2.03451 0.10491 H -8.03656 -0.82385 -0.06849 H -6.47682 -3.07850 0.20383 0 -4.89246 -1.75290 0.114226	Н	4. 01664	-3.75092	-0.03615	
H 1. 33990 1. 13333 -0. 01914 H -0. 60464 -2. 69295 -0. 09637 H 1. 57434 -3. 81518 -0. 07540 H -2. 37468 -1. 64135 0. 28393 C -4. 77282 -0. 39034 -0. 01858 C -6. 02088 0. 17841 -0. 11129 C -6. 95806 -0. 89062 -0. 03185 H -6. 22068 1. 23498 -0. 21947 C -6. 21863 -2. 03451 0. 10491 H -8. 03656 -0. 82385 -0. 06849 H -6. 47682 -3. 07850 0. 20383 O -4. 89246 -1. 75290 0. 11426	Н	6. 12427	-2. 47506	0.00328	
H -0.60464 -2.69295 -0.09637 H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.02088 0.17841 -0.11129 C -6.95806 -0.89062 -0.03185 H -6.22068 1.23498 -0.21947 C -6.21863 -2.03451 0.10491 H -8.03656 -0.82385 -0.06849 H -6.47682 -3.07850 0.20383 O -4.89246 -1.75290 0.11426	Н	1. 33990	1.13333	-0.01914	
H 1.57434 -3.81518 -0.07540 H -2.37468 -1.64135 0.28393 C -4.77282 -0.39034 -0.01858 C -6.02088 0.17841 -0.11129 C -6.95806 -0.89062 -0.03185 H -6.22068 1.23498 -0.21947 C -6.21863 -2.03451 0.10491 H -8.03656 -0.82385 -0.06849 H -6.47682 -3.07850 0.20383 O -4.89246 -1.75290 0.11426	Н	-0. 60464	-2.69295	-0.09637	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	1. 57434	-3.81518	-0.07540	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-2. 37468	-1.64135	0. 28393	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-4. 77282	-0. 39034	-0. 01858	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-6. 02088	0.17841	-0. 11129	
H -6. 22068 1. 23498 -0. 21947 C -6. 21863 -2. 03451 0. 10491 H -8. 03656 -0. 82385 -0. 06849 H -6. 47682 -3. 07850 0. 20383 0 -4. 89246 -1. 75290 0. 11426	C	-6. 95806	-0.89062	-0. 03185	
C -6. 21863 -2. 03451 0. 10491 H -8. 03656 -0. 82385 -0. 06849 H -6. 47682 -3. 07850 0. 20383 0 -4. 89246 -1. 75290 0. 11426	H	-6. 22068	1.23498	-0. 21947	
H -8. 03656 -0. 82385 -0. 06849 H -6. 47682 -3. 07850 0. 20383 0 -4. 89246 -1. 75290 0. 11426	C	-6. 21863	-2. 03451	0. 10491	
H -6. 47682 -3. 07850 0. 20383 0 -4. 89246 -1. 75290 0. 11426	H	-8. 03656	-0.82385	-0.06849	
0 -4.89246 -1.75290 0.11426	H	-6. 47682	-3.07850	0. 20383	
	0	-4. 89246	-1.75290	0. 11426	

Sum of electronic and zero-point energies = -1258.41789682 Hartree

	Х	Y	Z	
С	6. 39564	0. 18991	0.05616	
С	6. 41097	1. 57271	0. 08645	
С	5. 19307	2. 28228	0. 08062	
С	3. 98434	1. 60486	0. 04514	
С	3.93637	0.19061	0.01438	
С	5. 17274	-0. 52390	0.01975	
С	2. 68727	-0. 56520	-0. 02293	
С	2. 73422	-1.99326	-0. 05298	
С	3.99960	-2.66573	-0. 04718	
С	5. 16616	-1.95980	-0. 01199	
С	1. 42328	0. 05652	-0. 02952	
С	0. 23577	-0. 67822	-0.06059	
С	0. 29856	-2.09629	-0. 09323	
С	1. 52194	-2. 72843	-0.09019	
С	-1.04602	0. 03936	-0. 05529	
С	-2. 28812	-0. 58476	0. 09157	
С	-3. 45263	0. 18005	-0. 02555	
0	-0. 97427	1. 33836	-0. 21716	
0	-3. 41860	1. 47847	-0. 19841	
В	-2. 14615	2. 24328	-0. 03855	
F	-2. 10518	2. 78248	1. 24765	
F	-2.09711	3. 22982	-1.00958	
Н	7. 32761	-0.37056	0. 05992	
Н	7.35480	2.11030	0. 11451	
Н	5. 19857	3.36865	0. 10381	
Н	3.06698	2. 18353	0. 04111	
Н	4. 01165	-3. 75243	-0. 07067	
Н	6. 12116	-2. 47994	-0. 00726	
Н	1.34559	1. 13546	-0. 00357	
Н	-0.60578	-2.69277	-0. 13631	
Н	1. 57044	-3.81390	-0. 12067	
Н	-2.37099	-1.64937	0. 24792	
С	-4. 77100	-0.39434	0. 00622	
С	-6.02595	0. 16937	-0. 06477	
С	-6.95511	-0. 90314	0. 02045	
Н	-6.23970	1. 22420	-0. 16354	
С	-6.20779	-2. 04598	0. 13839	
Н	-8.03415	-0.84156	-0. 00046	
Н	-6.46151	-3. 09150	0. 23290	
0	-4. 88376	-1.75894	0. 13094	

 Table S10. Atom coordinates for the optimized geometry of 3-Phe@F in chloroform.

Sum of electronic and zero-point energies = -1258.44014106 Hartree

C -6.64411 0.09219 -0.04596 C -6.69408 1.47357 -0.06722 C -5.49476 2.21280 -0.05795 C -4.27033 1.56576 -0.02788 C -4.18688 0.15348 -0.00631 C -5.40469 -0.59125 -0.01529 C -2.91934 -0.56973 0.02508 C -2.92947 -1.99797 0.04604 C -4.17749 -2.70178 0.03712 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.46622 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.3317 O 0.68455 1.42615 0.24688 O 3.12506 1.62847 0.23297 B 1.83192 2.77788 0.01460 F 1.78544 2.79817 -1.30194 F 1.78544 2.79817 -0.09082 H -7.56217 -0.49123 -0.05242 H -7.56217 -0.49123 -0.05242 H -7.56217 -0.2103 H -1.61709 3.28990 -0.07244 H -3.36680 2.16575 -0.2103 H -1.6220 -2.57019 -0.00005 H -1.6220 -2.575		Х	Y	Z	
C -6. 69408 1. 47357 -0. 06722 C -5. 49476 2. 21280 -0. 05795 C -4. 27033 1. 56576 -0. 02788 C -4. 18688 0. 15348 -0. 06631 C -5. 40469 -0. 59125 -0. 01529 C -2. 91934 -0. 56973 0. 02508 C -2. 92947 -1. 99797 0. 04604 C -4. 17749 -2. 70178 0. 03712 C -5. 36108 -2. 02604 0. 00725 C -0. 46622 -0. 61767 0. 05879 C -0. 46224 -2. 03573 0. 08342 C -0. 49242 -2. 03573 0. 08342 C -1. 69862 -2. 70033 0. 07781 C -0. 49244 -0. 03417 0. 11620 C 3. 20292 0. 34427 0. 03417 O 0. 68455 1. 42615 0. 24688 O 3. 12506 1. 62847 0. 23297 B 1. 83192 2. 3758 0. 01460 F 1. 78053 3.	С	-6. 64411	0.09219	-0.04596	
C -5.49476 2.21280 -0.05795 C -4.27033 1.56576 -0.02788 C -4.18688 0.15348 -0.06631 C -5.40469 -0.59125 -0.01529 C -2.91934 -0.56973 0.02508 C -2.91934 -0.56973 0.03712 C -4.17749 -2.70178 0.03712 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.01767 0.05879 C -0.46622 -0.01761 0.05879 C -0.46622 -0.01761 0.05879 C -0.49242 -2.03573 0.08342 C -0.49242 -2.03573 0.08342 C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05460 C 2.05474 -0.3417 0.31417 O 0.68455 1.42615 0.24688 O 3.12506 1.62847 0.23297	С	-6.69408	1. 47357	-0.06722	
C -4.27033 1.56576 -0.02788 C -4.18688 0.15348 -0.00631 C -5.40469 -0.59125 -0.01529 C -2.91934 -0.56973 0.02508 C -2.92947 -1.99797 0.04604 C -4.17749 -2.70178 0.03712 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 2.03573 0.08342 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.24888 0 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.75305 3.29406 0.2842 H -7.56217 -0.49123 -0.05242 H -7.55171 3.29890 -0.07424 H -7.55179 1.989760 -0.99082	С	-5. 49476	2. 21280	-0.05795	
C -4.18688 0.15348 -0.00631 C -5.40469 -0.56973 0.02508 C -2.91934 -0.56973 0.02508 C -2.91934 -0.56973 0.03712 C -4.17749 -2.70178 0.03712 C -4.17749 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08540 C -1.69862 -2.70033 0.07781 C -0.49242 -2.03573 0.08540 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 O 0.68455 1.42615 0.24688 O 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.78654 2.79817 -1.30194 F 1.78550 3.39406 0.92842	С	-4. 27033	1.56576	-0. 02788	
C -5.40469 -0.59125 -0.01529 C -2.91934 -0.56973 0.02508 C -2.92947 -1.99797 0.04604 C -4.17749 -2.20178 0.03312 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08342 C -1.99862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 O 0.66455 1.42615 0.24688 O 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.78854 2.9817 -1.30194 F 1.78054 3.9496 0.92842 H -7.56217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082	С	-4. 18688	0. 15348	-0.00631	
C -2.91934 -0.56973 0.02508 C -2.92947 -1.99797 0.04604 C -4.17749 -2.70178 0.03712 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08342 C -0.49242 -2.03573 0.08342 C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 O 0.68455 1.42615 0.24688 O 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.78854 2.79817 -1.30194 F 1.75305 3.39406 0.92842 H -7.56217 -0.49123 -0.05242 H -7.56217 -0.49123 -0.05242 H -7.56217 -0.29890 -0.7424 H -7.56217 -0.0005 H -1.61709 1.16520 O 0.12487 H -2.52701 3.29890 H -4.16200 -3.78892 O 0.12487 H -1.71894 -3.78724 H -1.71894 -3.78724 H -1.71894 -3.78724 H -1.71894 -3.78724 H $-1.$	С	-5.40469	-0. 59125	-0. 01529	
C -2.92947 -1.99797 0.04604 C -4.17749 -2.70178 0.03712 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08342 C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.23297 B 1.83192 2.37758 0.01460 F 1.78854 2.79817 -1.30194 F 1.78854 2.79817 -1.30194 F 1.78854 2.79817 -0.5242 H -7.65119 1.98760 -0.09082 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.5412 H -6.30290 -2.57019 -0.00055 H -1.61709 1.16520 0.01281 H -1.71894 -3.78224 0.10281 H -1.71894 -3.8724 0.10281 H -1.71894 -2.56717 -0.31130 C 6.8912 -0.2537 -0.3437 H 2.14901 -1.50251 -0.31130 C 6.60275 -1.60120 -0.6194 H 7.189899 0.13396 0.06919 H 7.89899 0.13396 0.06919	С	-2. 91934	-0.56973	0. 02508	
C -4.17749 -2.70178 0.03712 C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08342 C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 0 0.66455 1.42615 0.24688 0 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.78854 2.79817 -1.30194 F 1.75305 3.9406 0.92842 H -7.56117 -0.49123 -0.05242 H -7.56119 1.98760 -0.09082 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00055 H -1.61709 1.16520 0.01626 H -0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 6.8912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.0275 -1.60120 -0.06194 H 7.189899 <td>С</td> <td>-2. 92947</td> <td>-1.99797</td> <td>0.04604</td> <td></td>	С	-2. 92947	-1.99797	0.04604	
C -5.36108 -2.02604 0.00725 C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08342 C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 0 0.68455 1.42615 0.24688 0 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.78854 2.79817 -1.30194 F 1.78854 2.79817 -1.30194 F 1.75305 3.39406 0.92842 H -7.56217 -0.49123 -0.05242 H -7.56217 -0.49123 -0.05242 H -7.56217 -0.49123 -0.07424 H -7.56217 -0.2103 H -7.65119 1.98760 -0.09082 H -7.56217 -0.02103 H -1.61709 1.16520 0.01626 H -0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H -1.71894 -3.78724 0.10281 H -1.50251 -0.31130 C 4.5304 -0.19401 0.1620 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C </td <td>С</td> <td>-4. 17749</td> <td>-2. 70178</td> <td>0.03712</td> <td></td>	С	-4. 17749	-2. 70178	0.03712	
C -1.67162 0.08450 0.03395 C -0.46622 -0.61767 0.05879 C -0.49242 -2.03573 0.08342 C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 0 0.68455 1.42615 0.24688 0 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.7854 2.79817 -1.30194 F 1.75305 3.39406 0.92842 H -7.56217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -4.16200 -3.78892 0.05412 H -7.552701 3.29890 -0.07424 H -7.552701 3.29890 -0.07424 H -7.552701 3.29890 -0.017424 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.51791 0.54367 0.09042 H -2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 G 5.72108 0.54367 0.07942 C 6.60275 -1.60120 -0.06194 H 7.99992	С	-5.36108	-2.02604	0.00725	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-1.67162	0. 08450	0. 03395	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-0. 46622	-0. 61767	0.05879	
C -1.69862 -2.70033 0.07781 C 0.79518 0.14283 0.05560 C 2.05474 -0.44417 -0.11620 C 3.20292 0.34427 0.03417 O 0.68455 1.42615 0.24688 O 3.12506 1.62847 0.23297 B 1.83192 2.37758 0.01460 F 1.78854 2.79817 -1.30194 F 1.78545 2.39758 0.01460 F 1.78547 2.39907 -0.05242 H -7.56217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.061919	С	-0. 49242	-2. 03573	0. 08342	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-1. 69862	-2. 70033	0. 07781	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	0. 79518	0. 14283	0.05560	
C 3.20292 0.34427 0.03417 00.684551.426150.246880 3.12506 1.628470.23297B1.83192 2.37758 0.01460F1.78854 2.79817 -1.30194 F1.75305 3.39406 0.92842 H -7.56217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082 H -5.52701 3.29890 -0.07424 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.69919	С	2.05474	-0. 44417	-0. 11620	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	3. 20292	0. 34427	0.03417	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0. 68455	1. 42615	0. 24688	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0	3. 12506	1. 62847	0. 23297	
F1.788542.79817 -1.30194 F1.753053.39406 0.92842 H -7.65217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082 H -5.52701 3.29890 -0.07424 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.6194 H 7.89899 0.13396 0.06919	В	1.83192	2. 37758	0.01460	
F1.753053.394060.92842H -7.56217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082 H -5.52701 3.29890 -0.07424 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	F	1. 78854	2. 79817	-1.30194	
H -7.56217 -0.49123 -0.05242 H -7.65119 1.98760 -0.09082 H -5.52701 3.29890 -0.07424 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	F	1. 75305	3.39406	0. 92842	
H -7.65119 1.98760 -0.09082 H -5.52701 3.29890 -0.07424 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-7. 56217	-0. 49123	-0.05242	
H -5.52701 3.29890 -0.07424 H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-7.65119	1.98760	-0. 09082	
H -3.36680 2.16575 -0.02103 H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-5. 52701	3. 29890	-0.07424	
H -4.16200 -3.78892 0.05412 H -6.30290 -2.57019 -0.00005 H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-3.36680	2. 16575	-0. 02103	
H $-6.\ 30290$ $-2.\ 57019$ $-0.\ 00005$ H $-1.\ 61709$ $1.\ 16520$ $0.\ 01626$ H $0.\ 42837$ $-2.\ 60768$ $0.\ 12487$ H $-1.\ 71894$ $-3.\ 78724$ $0.\ 10281$ H $2.\ 14901$ $-1.\ 50251$ $-0.\ 31130$ C $4.\ 55304$ $-0.\ 19401$ $0.\ 01620$ C $5.\ 72108$ $0.\ 54367$ $0.\ 07942$ C $6.\ 88912$ $-0.\ 25955$ $0.\ 03437$ H $5.\ 71452$ $1.\ 62488$ $0.\ 15123$ C $6.\ 60275$ $-1.\ 60120$ $-0.\ 06194$ H $7.\ 89899$ $0.\ 13396$ $0.\ 06919$	Н	-4. 16200	-3. 78892	0.05412	
H -1.61709 1.16520 0.01626 H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-6. 30290	-2. 57019	-0.00005	
H 0.42837 -2.60768 0.12487 H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-1.61709	1.16520	0.01626	
H -1.71894 -3.78724 0.10281 H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	0. 42837	-2. 60768	0. 12487	
H 2.14901 -1.50251 -0.31130 C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	-1. 71894	-3. 78724	0. 10281	
C 4.55304 -0.19401 0.01620 C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919	Н	2. 14901	-1.50251	-0.31130	
C 5.72108 0.54367 0.07942 C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919 H 7.20802 -2.42054 -0.11222	С	4. 55304	-0. 19401	0.01620	
C 6.88912 -0.25955 0.03437 H 5.71452 1.62488 0.15123 C 6.60275 -1.60120 -0.06194 H 7.89899 0.13396 0.06919 H 7.20802 -2.42054 -0.11222	С	5. 72108	0. 54367	0.07942	
H 5. 71452 1. 62488 0. 15123 C 6. 60275 -1. 60120 -0. 06194 H 7. 89899 0. 13396 0. 06919 H 7. 20802 -2. 42054 -0. 11222	С	6.88912	-0. 25955	0. 03437	
C 6. 60275 -1. 60120 -0. 06194 H 7. 89899 0. 13396 0. 06919 H 7. 20802 -2 42054 -0. 11222	Н	5. 71452	1. 62488	0. 15123	
H 7. 89899 0. 13396 0. 06919	С	6.60275	-1.60120	-0.06194	
	Н	7.89899	0. 13396	0.06919	
11 /. 29003 -Z. 42934 -U. 11322	Н	7. 29803	-2. 42954	-0. 11322	
S 4. 90387 -1. 90599 -0. 09678	S	4. 90387	-1.90599	-0.09678	

 Table S11. Atom coordinates for the optimized geometry of 3-Phe@T in vacuum.

Sum of electronic and zero-point energies = -1581.39478595 Hartree

	Х	Y	Z	
С	6. 64560	0.08717	0.06683	
С	6. 69740	1. 46890	0. 10496	
С	5. 49874	2. 21056	0.09999	
С	4. 27262	1.56560	0. 05758	
С	4. 18736	0. 15333	0. 01872	
С	5. 40429	-0. 59375	0. 02318	
С	2.91872	-0. 56874	-0. 02584	
С	2. 92788	-1.99733	-0.06337	
С	4. 17496	-2. 70327	-0. 05848	
С	5. 35974	-2. 02876	-0. 01677	
С	1.67170	0. 08648	-0. 03202	
С	0. 46516	-0.61609	-0. 06891	
С	0. 49040	-2. 03510	-0. 10904	
С	1.69656	-2.69964	-0. 10713	
С	-0. 79646	0. 13713	-0. 06371	
С	-2.05389	-0. 45024	0. 09877	
С	-3. 20655	0. 33545	-0. 02854	
0	-0. 68865	1. 43148	-0. 24100	
0	-3. 12570	1.63039	-0. 21252	
В	-1.83583	2.36339	-0. 04911	
F	-1.77816	2.88936	1. 24228	
F	-1. 76642	3.35738	-1.01099	
Н	7. 56245	-0.49774	0.06996	
Н	7.65506	1. 98112	0. 13857	
Н	5. 53300	3. 29626	0. 12931	
Н	3. 37080	2. 16813	0.05460	
Н	4. 15821	-3.78977	-0. 08789	
Н	6. 30059	-2. 57403	-0. 01282	
Н	1. 62278	1.16699	-0. 00094	
Н	-0. 42901	-2. 60763	-0.15965	
Н	1.71613	-3.78579	-0. 14423	
Н	-2. 14566	-1.51120	0. 27867	
С	-4. 55122	-0. 19842	0. 00195	
С	-5. 72370	0. 53943	-0. 04592	
С	-6. 88821	-0. 26486	0. 00754	
Н	-5. 72683	1.62090	-0. 11228	
С	-6. 59661	-1.60782	0. 09455	
Н	-7. 89922	0. 12585	-0. 01498	
Н	-7. 28957	-2. 43795	0. 14882	
<u>S</u>	-4. 90003	-1.91300	0. 11118	

Table S12. Atom coordinates for the optimized geometry of 3-Phe@T in chloroform.

Sum of electronic and zero-point energies = -1581.41669452 Hartree

5. ¹H and ¹³C NMR spectra



Figure S3. ¹H NMR spectrum of 1-AcPhe in CDCl₃.



Figure S4. ¹³C NMR spectrum of 1-AcPhe in CDCl₃.



Figure S5. ¹H NMR spectrum of 1-PheDKPh in CDCl₃.



Figure S6. ¹³C NMR spectrum of 1-PheDKPh in CDCl₃.



Figure S7. ¹H NMR spectrum of 2-PheDKPh in CDCl₃.



Figure S8. ¹³C NMR spectrum of 2-PheDKPh in CDCl₃.



Figure S9. ¹H NMR spectrum of 3-PheDKPh in CDCl₃.



Figure S10. ¹³C NMR spectrum of 3-PheDKPh in CDCl₃.



Figure S11. ¹H NMR spectrum of 9-PheDKPh in CDCl₃.



Figure S12. ¹³C NMR spectrum of 9-PheDKPh in CDCl₃.



Figure S13. ¹H NMR spectrum of 3-PheDKF in CDCl₃.



Figure S14. ¹³C NMR spectrum of 3-PheDKF in CDCl₃.



Figure S15. ¹H NMR spectrum of 3-PheDKT in CDCl₃.



Figure S16. ¹³C NMR spectrum of 3-PheDKT in CDCl₃.



Figure S17. ¹H NMR spectrum of 1-Phe@Ph in CDCl₃.



Figure S18. ¹³C NMR spectrum of 1-Phe@Ph in CDCl₃.



Figure S19. ¹H NMR spectrum of 2-Phe@Ph in DMSO-*d*₆.



Figure S20. ¹³C NMR spectrum of 2-Phe@Ph in DMSO- d_6 .



Figure S21. ¹H NMR spectrum of 3-Phe@Ph in DMSO-*d*₆.



Figure S22. ¹³C NMR spectrum of 3-Phe@Ph in DMSO- d_6 .



Figure S23. ¹H NMR spectrum of 9-Phe@Ph in DMSO-*d*₆.



Figure S24. ¹³C NMR spectrum of 9-Phe@Ph in DMSO- d_6 .



Figure S25. ¹H NMR spectrum of 3-Phe@F in DMSO- d_6 .



Figure S26. ¹³C NMR spectrum of 3-Phe@F in DMSO- d_6 . * Benzene.



Figure S27. ¹H NMR spectrum of 3-Phe@T in DMSO- d_6 .



Figure S28. ¹³C NMR spectrum of 3-Phe@T in DMSO- d_6 . * Benzene.

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