**Supporting Information**

# Dihypoiodites Stabilized by 4-ethylpyridine Through an O-I-N Halogen Bond

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## Contents

# Synthesis

## General Considerations

All reagents and solvents were obtained from commercial suppliers and used without further purification. For structural NMR assignments, $^{1}$H NMR and $^{1}$H-$^{15}$N NMR correlation spectra were recorded on a Bruker Avance III 500 MHz spectrometer at 25ºC in $CD_2Cl_2$. Chemical shifts are reported on the δ scale in ppm using the residual solvent signal as internal standard ($CH_2Cl_2$ in $CD_2Cl_2$: $\delta_H$ 5.32), or for $^{1}$H-$^{15}$N NMR spectroscopy, to an external $d_3$-$MeNO_2$ standard. For the $^{1}$H NMR spectroscopy, each resonance was assigned according to the following conventions: chemical shift (δ) measured in ppm, observed multiplicity, number of hydrogens, observed coupling constant (*J* Hz), and assignment. Multiplicities are denoted as: s (singlet), d (doublet), t (triplet), q (quartet), sept (septet), m (multiplet), and br (broad). For the $^{1}$H-$^{15}$N HMBC spectroscopy, spectral windows of 4 ppm ($^{1}$H) and 600 ppm ($^{15}$N) were used, with 1024 points in the direct dimension and 512 increments used in the indirect dimension.

The single crystal X-ray data for **1**, **1F**, and **2** were collected at 120 K using an Agilent SuperNova dual wavelength diffractometer with an Atlas detector using mirror-monochromated Cu-Kα (λ = 1.54184 Å) radiation. The program CrysAlisPro[1] was used for the data collection and reduction on the SuperNova diffractometer, and the intensities were absorption corrected using a gaussian face index absorption correction method. All structures were solved by intrinsic phasing (SHELXT)[2] and refined by full-matrix least squares on $F^2$ using the OLEX2,[3] utilizing the SHELXL-2015 module.[4] Anisotropic displacement parameters were assigned to non-H atoms and isotropic displacement parameters for all H atoms were constrained to multiples of the equivalent displacement parameters of their parent atoms with $U_{iso}(H) = 1.2\ U_{eq}$ (aromatic) or $U_{iso}(H) = 1.5\ U_{eq}$ (alkyl) of their respective parent atoms. The X-ray single crystal data and CCDC numbers of all new structures are included below.

The following abbreviations are used: DCM = dichloromethane, $Et_2O$ = diethylether, TBME = $^{t}$butylmethylether.

# Synthesis of Precursor Silver(I) Salts

**1,2-$(AgO(O)C)_2C_6H_4$**: Phthalic acid (2.0 g, 12.0 mmol) was added to a NaOH solution (961.8 mg, 24.1 mmol in 13.3 mL $H_2O$). After stirring with a magnetic stirrer for 15 minutes, a solution of $AgNO_3$ (4.1 g, 24.1 mmol) in $H_2O$ (16 mL) was added dropwise. A white solid appeared, and the solution was stirred for 1 hour. The precipitate was filtered and then washed with $H_2O$, methanol, and hexane (×3 each). The white solid was dried under vacuum and stored in a vial covered with aluminium foil to protect it from light.

**1,2-$(AgO(O)C)_2C_6F_4$**: Tetrafluorophthalic acid (500 mg, 2.1 mmol) was added to a NaOH solution (168 mg, 4.2 mmol in 2.3 mL $H_2O$). After stirring with a magnetic stirrer for 15 minutes, a solution of $AgNO_3$ (713.5 mg, 4.2 mmol) in $H_2O$ (2.8 mL) was added dropwise. A white/brownish solid appeared, and the solution was stirred for 1 hour. The precipitate was filtered and then washed with $H_2O$, methanol, and hexane (×3 each). The off-white solid was dried under vacuum and stored in a vial covered with aluminium foil to protect it from light.

**1,3-$(AgO(O)C)_2C_6H_4$**: Isophthalic acid (2.0 g, 12.0 mmol) was added to a NaOH solution (961.8 mg, 24.1 mmol in 16.3 mL $H_2O$). After stirring with a magnetic stirrer for 15 minutes and the solution filtered. To this filtered solution, a solution of $AgNO_3$ (4.1 g, 24.1 mmol) in $H_2O$ (16 mL) was added dropwise. A white solid appeared, and the solution was stirred for 1 hour. The precipitate was filtered and then washed with $H_2O$, methanol, and hexane (×3 each). The white solid was dried under vacuum and stored in a vial covered with aluminium foil to protect it from light.

**1,4-$(AgO(O)C)_2C_6H_4$**: Terephthalic acid (2.0 g, 12.0 mmol) was added to a NaOH solution (961.8 mg, 24.1 mmol in 13.3 mL $H_2O$). After stirring with a magnetic stirrer for 15 minutes at room temperature, a solution of $AgNO_3$ (4.1 g, 24.1 mmol) in $H_2O$ (16 mL) was added dropwise. A white solid appeared, and the solution was stirred for 1 hour. The precipitate was filtered and then washed with $H_2O$, methanol, and hexane (×3 each). The white solid was dried under vacuum and stored in a vial covered with aluminium foil to protect it from light.

**(phthaloyl-OI)(4-Etpy)$_2$ (1):** Neat 4-ethylpyridine (21.4 mg, 0.2 mmol) was diluted in DCM (3 mL), and this solution added to 1,2-(AgO(O)C)$_2$C$_6$H$_4$ (38 mg, 0.1 mmol), followed by $I_2$ (50.8 mg, 0.2 mmol) in DCM (2 mL). The mixture was sonicated, centrifuged, and filtered to give a clear red filtrate. The total volume of DCM was lowered under reduced pressure, then $Et_2O$ (18 mL) was added. A white solid appeared and the liquid was decanted off. Additional $Et_2O$ (20 mL) was added to the filtrate and the resulting solution was cooled in the fridge for 10 minutes to give a white precipitate. The solid was decanted and further dried under reduced pressure to leave a white solid. Yield: 71%. $^1$H NMR (500 MHz, $CD_2Cl_2$) δ: 8.58 (d, *J* = 4.3 Hz, 4H), 7.50 (s, 2H), 7.33 (s, 2H), 7.24 (d, *J* = 4.8 Hz, 4H), 2.73 (q, *J* = 7.4 Hz, 4H), 1.25 (t, *J* = 7.6 Hz, 6H). $^{15}$N NMR (500 MHz, $CD_2Cl_2$) δ: –160.7. Analysis Found: C, 41.10; H, 3.44: N, 4.80%. Calculated for $C_{22}H_{22}I_2N_2O_4$·0.5($H_2O$): C, 41.21; H, 3.62: N, 4.37%. Crystals suitable for single crystal X-ray diffraction were obtained from a DCM solution of **1** vapour diffused with TBME. Crystal data for **1**: CCDC-2105108, $C_{22}H_{22}I_2N_2O_4$, M = 632.21, colourless plate, 0.02 x 0.15 x 0.37 mm$^3$, triclinic, space group *P*-1 (No. 2), a = 8.1534(3) Å, b = 9.6858(4) Å, c = 15.4795(8) Å, α = 94.664(4)°, β = 95.181(4)°, γ = 107.477(4)°, V = 1153.66(9) Å$^3$, Z = 2, $D_{calc}$ = 1.820 gcm$^{-3}$, F000 = 612, μ = 21.66 mm$^{-1}$, T = 120.0(1) K, $\theta_{max}$ = 76.6°, 4475 total reflections, 3833 with $I_o > 2\sigma(I_o)$, $R_{int}$ = 0.044, 4475 data, 273 parameters, no restraints, GooF = 1.04, 1.35 < dΔρ < –1.29 eÅ$^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.043, $wR(F^2)$ = 0.127.

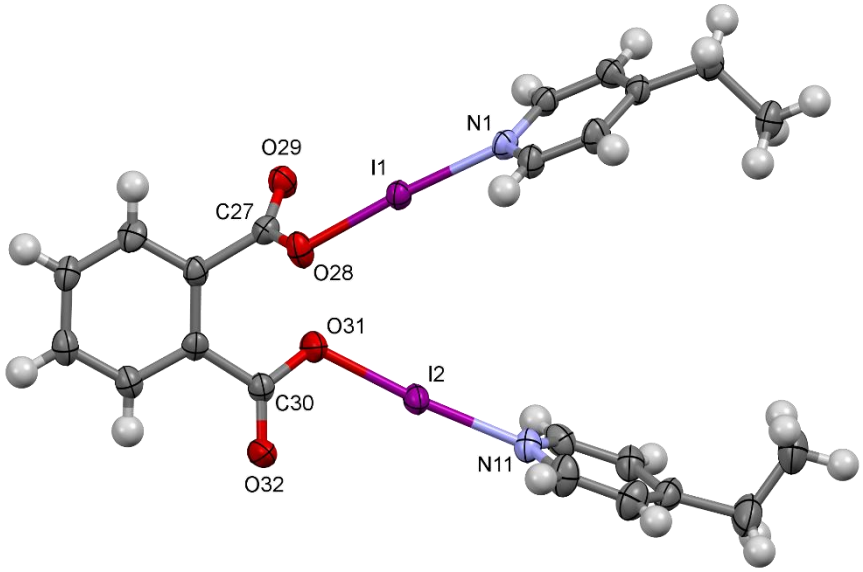



Figure S1: The X-ray crystal structure of **1** (thermal ellipsoids at 50% probability).

**(tetrafluorophthaloyl-OI)(4-Etpy)$_2$** (**1F**): Neat 4-ethylpyridine (21.4 mg, 0.2 mmol) was diluted in DCM (3.8 mL), and this solution added to 1,2-(AgO(O)C)$_2$C$_6$F$_4$ (23.8 mg, 0.1 mmol), followed by $I_2$ (50.8 mg, 0.2 mmol) in DCM (1.2 mL). The mixture was sonicated, centrifuged, and filtered to give a dark red filtrate. $Et_2O$ (15 mL) was added to the filtered solution and the solution was stored in the fridge. After 10 minutes a white precipitate appeared. The solution was filtered, and the recovered solid further dried under reduced pressure to give a white solid. Yield = 80%. $^1$H NMR (500 MHz, $CD_2Cl_2$) δ: 8.59 (d, *J* = 6.1 Hz, 4H), 7.27 (d, *J* = 6.1 Hz, 4H), 2.75 (q, *J* = 7.6 Hz, 4H), 1.25 (t, *J* = 7.6 Hz, 6H). $^{15}$N NMR (500 MHz, $CD_2Cl_2$) δ: −171.2. Analysis Found: C, 36.75; H, 2.45: N, 3.87%. Calculated for $C_{22}H_{18}F_4I_2N_2O_4$·0.75($H_2O$): C, 36.82; H, 2.74: N, 3.90%. Crystals suitable for single crystal X-ray diffraction were obtained from a DCM solution of **1F** vapour diffused with petroleum ether. Crystal data for **1F**: CCDC-2105109, $C_{22}H_{18}F_4I_2N_2O_4$, M = 704.18, colourless plate, 0.03 x 0.14 x 0.32 mm$^3$, monoclinic, space group $P2_1/c$, a = 9.8812(3) Å, b = 32.4911(7) Å, c = 7.4264(2) Å, β = 91.420(2)°, V = 2383.52(11) Å$^3$, Z = 4, $D_{calc}$ = 1.962 gcm$^{-3}$, F000 = 1352, μ = 21.30 mm$^{-1}$, T = 120.0(1) K, $\theta_{max}$ = 76.2°, 4646 total reflections, 4085 with $I_o > 2\sigma(I_o)$, $R_{int}$ = 0.039, 4646 data, 309 parameters, no restraints, GooF = 1.20, 2.36 < dΔρ < −1.23 eÅ$^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.048, $wR(F^2)$ = 0.137.

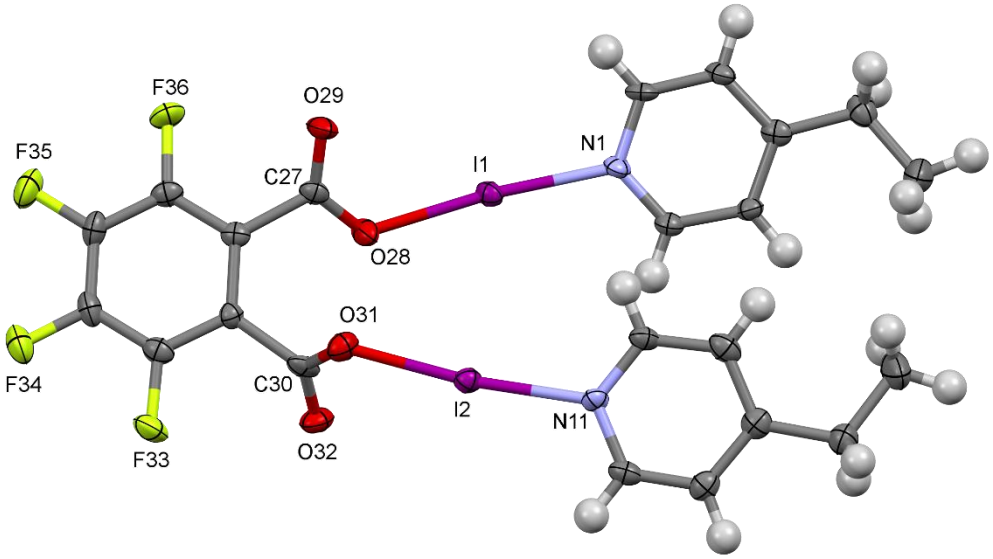



Figure S2: The X-ray crystal structure of **1F** (thermal ellipsoids at 50% probability).

**(isophthaloyl-OI)(4-Etpy)$_2$** (**2**): Neat 4-ethylpyridine (21.4 mg, 0.2 mmol) was diluted in DCM (3.8 mL), and this solution added to 1,3-(AgO(O)C)$_2$C$_6$H$_4$ (38 mg, 0.1 mmol), followed by $I_2$ (50.8 mg, 0.2 mmol) in DCM (1.2 mL). The mixture was sonicated, centrifuged, and filtered to give a dark red filtrate. $Et_2O$ (15mL) was added to the filtrate to immediately give a white precipitate. The solution was filtered and the white precipitate collected and dried under reduced pressure to give a white solid. Yield: 74%. $^1$H NMR (300 MHz, $CD_2Cl_2$) δ: 8.58 (d, *J* = 6.4 Hz, 4H), 8.47 (s, 1H), 8.04 (dd, *J* = 7.6, 1.3 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.26 (d, *J* = 6.4 Hz, 4H), 2.74 (q, *J* = 7.6 Hz, 4H), 1.27 (t, *J* = 7.6 Hz, 6H). $^{15}$N NMR (300 MHz, $CD_2Cl_2$) δ: −159.5. Analysis Found: C, 40.92; H, 3.37: N, 4.26%. Calculated for $C_{22}H_{22}I_2N_2O_4$·0.5($H_2O$): C, 41.21; H, 3.62: N, 4.37%. Crystals suitable for single crystal X-ray diffraction were obtained by evaporation of a concentrated DCM solution of **2**. Crystal data for **2**: CCDC-2105110, $C_{22}H_{22}I_2N_2O_4$, M = 632.21, colourless plate, 0.01 x 0.06 x 0.17 mm$^3$, triclinic, space group *P*-1 (No. 2), a = 8.0109(5) Å, b = 9.0287(6) Å, c = 16.548(2) Å, α = 84.321(8)°, β = 87.332(8)°, γ = 71.188(6)°, V = 1127.23(18) Å$^3$, Z = 2, $D_{calc}$ = 1.863 gcm$^{-3}$, F000 = 612, μ = 22.17 mm$^{-1}$, T = 120.0(1) K, $\theta_{max}$ = 75.0°, 4411 total reflections, 3134 with $I_o > 2\sigma(I_o)$, $R_{int}$ = 0.120, 4411 data, 323 parameters, 222 restraints, GooF = 1.01, 2.11 < dΔρ < −1.52 eÅ$^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.082, $wR(F^2)$ = 0.244.

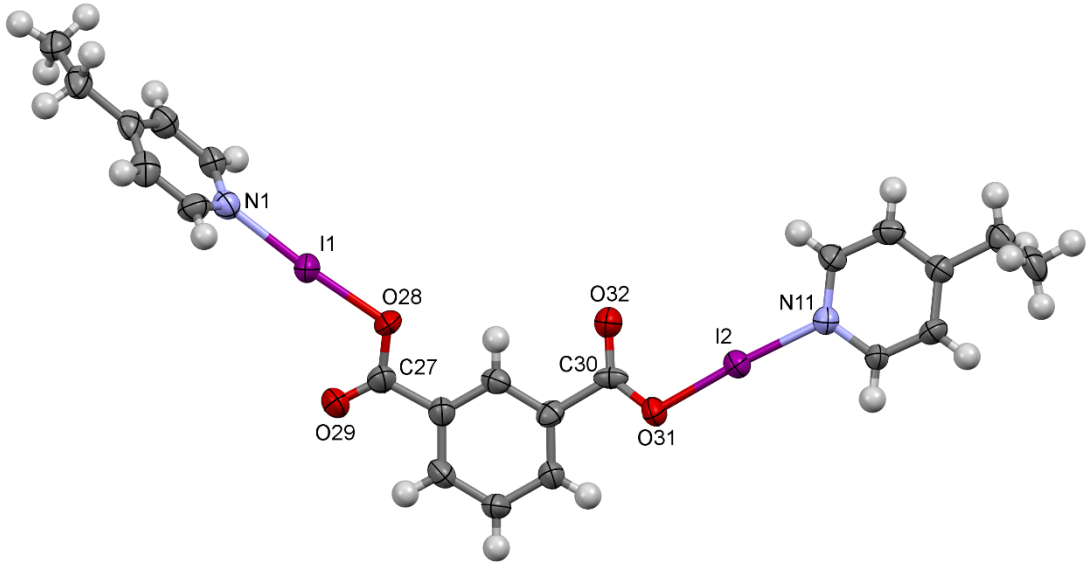



Figure S3: The X-ray crystal structure of **2** (Disordered atoms omitted for clarity; thermal ellipsoids at 50% probability).

**(terephthaloyl-OI)(4-Etpy)$_2$** (**3**): Neat 4-ethylpyridine (21.4 mg, 0.2 mmol) was diluted in DCM (3.8 mL), and this solution added to 1,4-(AgO(O)C)$_2$C$_6$H$_4$ (38 mg, 0.1 mmol), followed by $I_2$ (50.8 mg, 0.2 mmol) in DCM (1.2 mL). The mixture was sonicated, centrifuged, and filtered to give a dark red filtrate. $Et_2O$ (15mL) was added to the filtered solution and immediately a white precipitate appeared. The solution was filtered and the white precipitate collected and dried under reduced pressure to give a white solid. Yield: 70%. $^1$H NMR (500 MHz, $CD_2Cl_2$) δ: 8.57 (d, *J* = 5.7 Hz, 4H), 7.91 (s, 4H), 7.26 (d, *J* = 5.3 Hz, 4H), 2.74 (q, *J* = 7.4 Hz, 4H), 1.26 (t, *J* = 7.6 Hz, 6H). $^{15}$N NMR (500 MHz, $CD_2Cl_2$) δ: –162.9. Analysis Found: C, 40.93; H, 3.27: N, 4.31%. Calculated for $C_{22}H_{22}I_2N_2O_4$·0.75($H_2O$): C, 40.92; H, 3.67: N, 4.34%.

**(benzoyl)(OI(4-Etpy))** (**4**)**:** Neat 4-ethylpyridine (3.2 mg, 0.03 mmol) was diluted in $CD_2Cl_2$ (832 µL), and this solution added to (AgO(O)C)C$_6$H$_5$ (6.9 mg, 0.03 mmol),[5] followed by $I_2$ (7.6 mg, 0.03 mmol) in $CD_2Cl_2$ (167.9 µL). The mixture was sonicated, centrifuged, and filtered to give a red filtrate, which was immediately used for NMR spectroscopy. $^1$H NMR (500 MHz, $CD_2Cl_2$) δ: 8.55 (br, 2H), 7.94 (br, 2H), 7.45 (br, 1H), 7.36 (br, 2H), 7.25 (d, *J* = 4.4 Hz, 2H), 2.74 (br. d, *J* = 7.3 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). $^{15}$N NMR (500 MHz, $CD_2Cl_2$) δ: –161.6.

## Comparison Table of $^{15}$N NMR Chemical Shifts

Table S1: Comparison of $^{15}$N NMR Chemical Shifts in $CD_2Cl_2$ for Compounds **1-4**.

| **Compound** | **$^{15}$N NMR Chemical Shifts in $CD_2Cl_2$ (ppm)** |
|---|---|
| **1** | –160.7 |
| **1F** | –171.2 |
| **2** | –159.5 |
| **3** | –162.9 |
| **4** | –161.6 |

# NMR Spectra

Figure S4: The $^{1}H$ NMR spectrum of compound **1** in $CD_2Cl_2$.

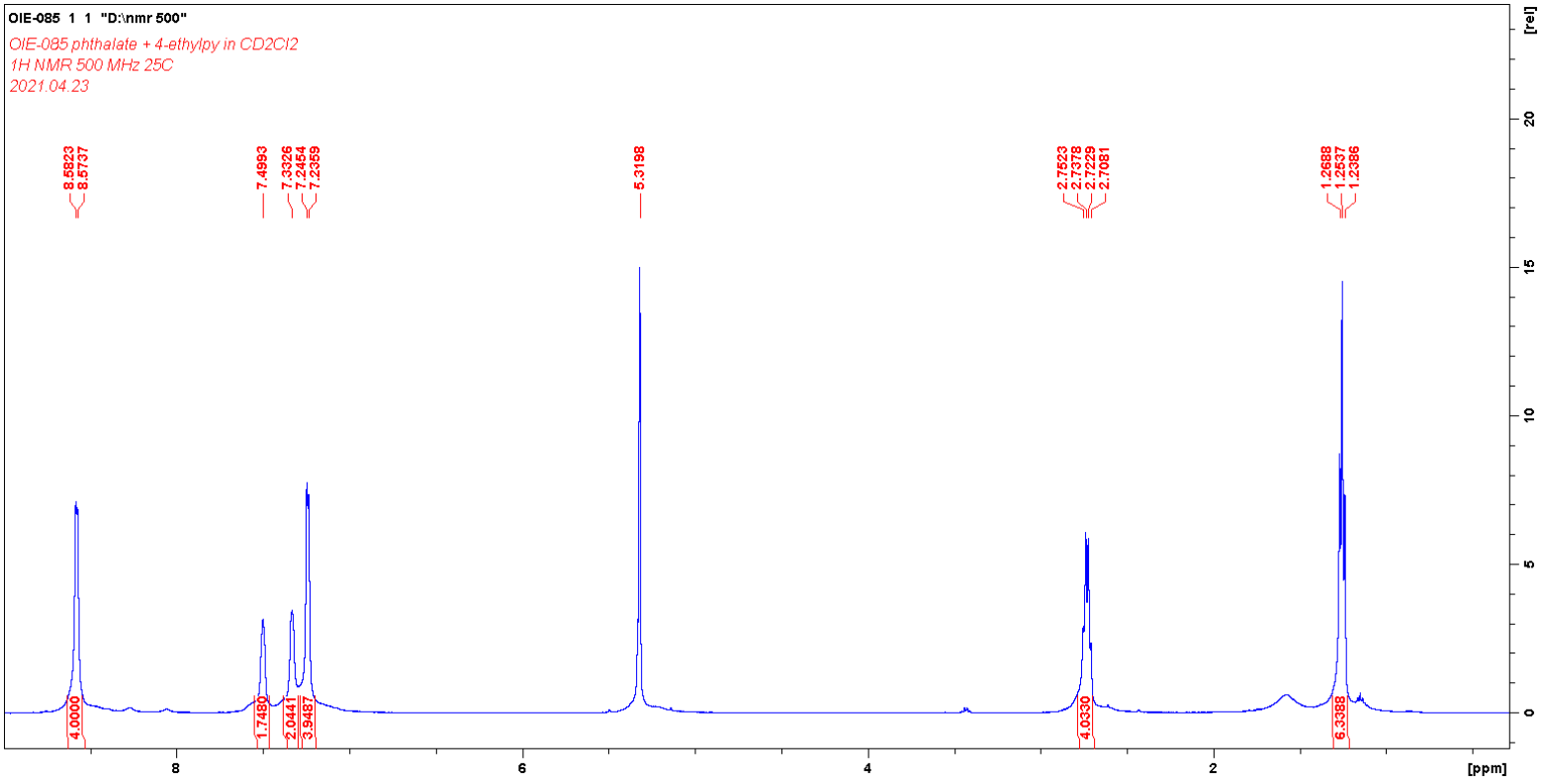


Figure S5: The $^{1}H$-$^{15}N$ HMBC spectrum of compound **1** in $CD_2Cl_2$.

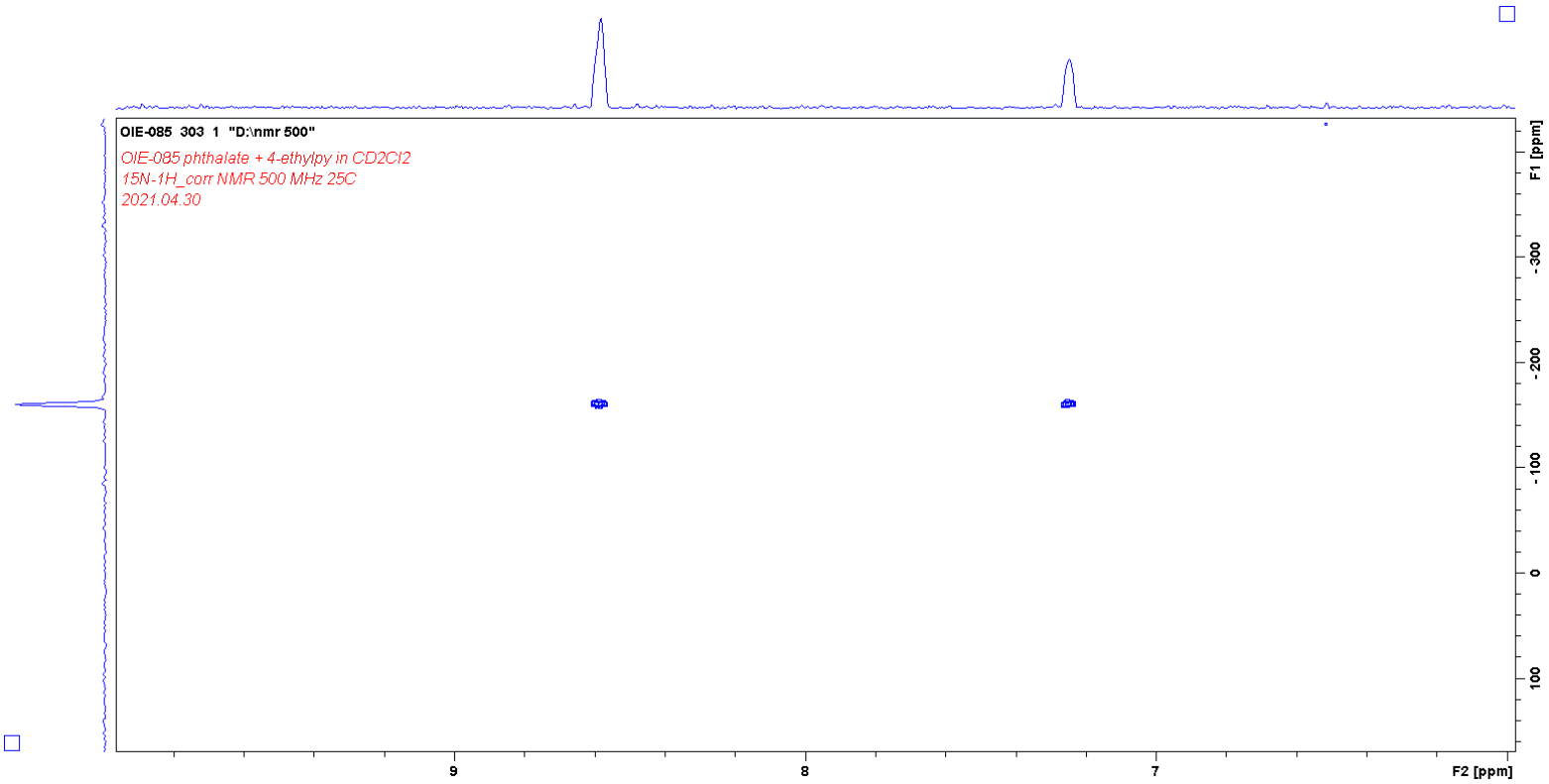


Figure S6: The $^{1}H$ NMR spectrum of compound **1F** in $CD_2Cl_2$.

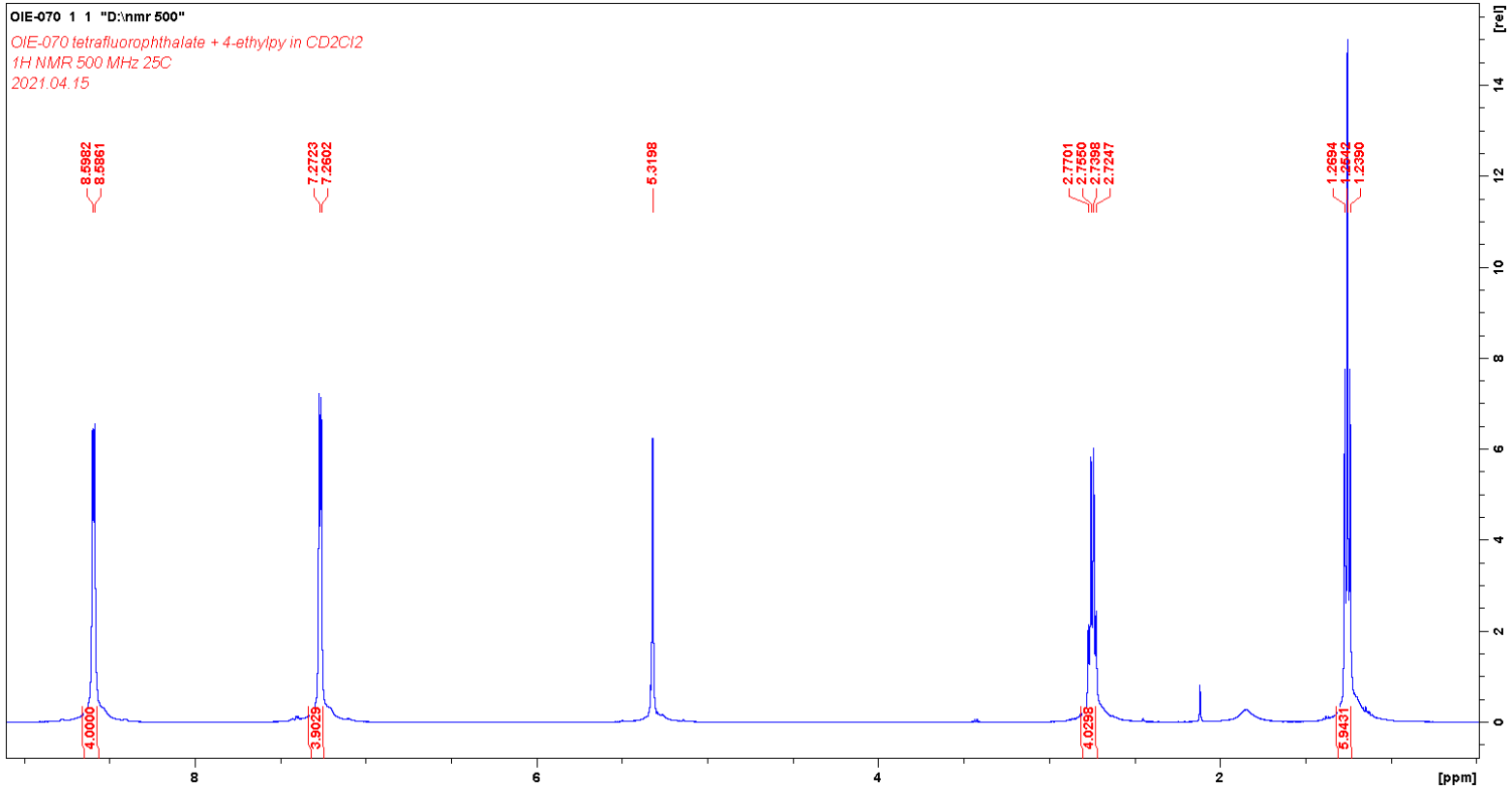


Figure S7: The $^{1}H$-$^{15}N$ HMBC spectrum of compound **1F** in $CD_2Cl_2$.

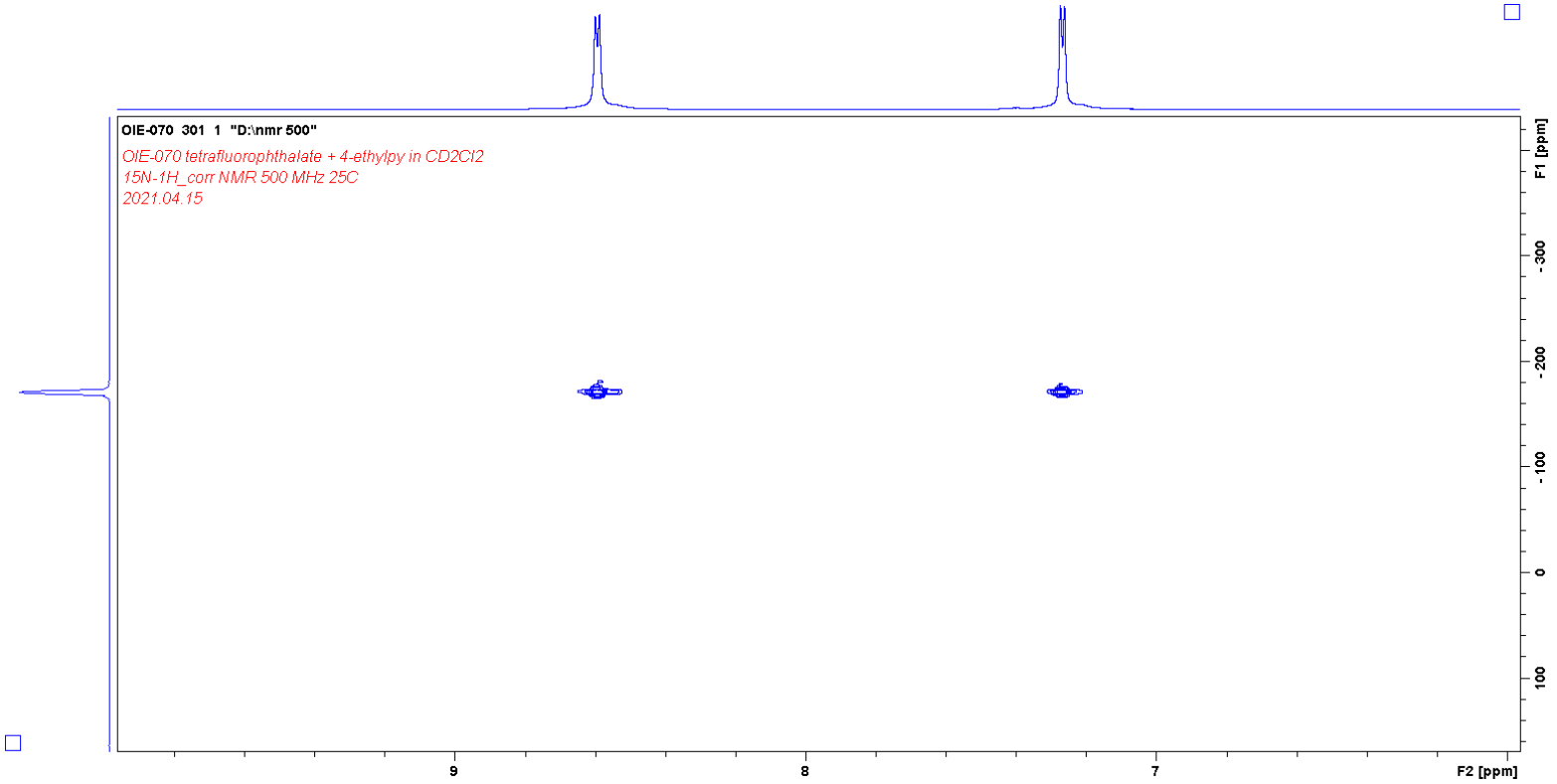


Figure S8: The $^{1}H$ NMR spectrum of compound **2** in $CD_2Cl_2$.

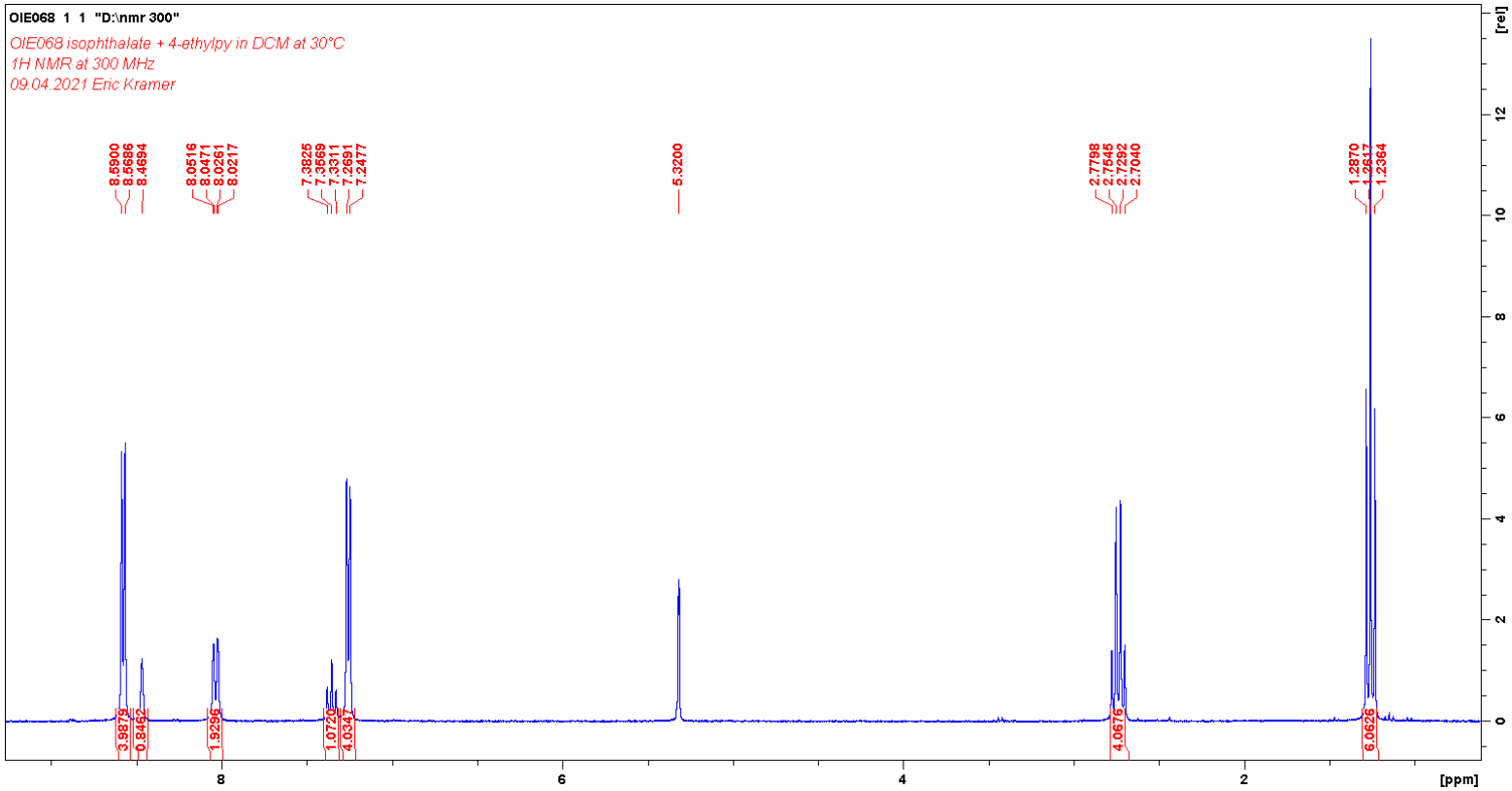


Figure S9: The $^{1}H$-$^{15}N$ HMBC spectrum of compound **2** in $CD_2Cl_2$.

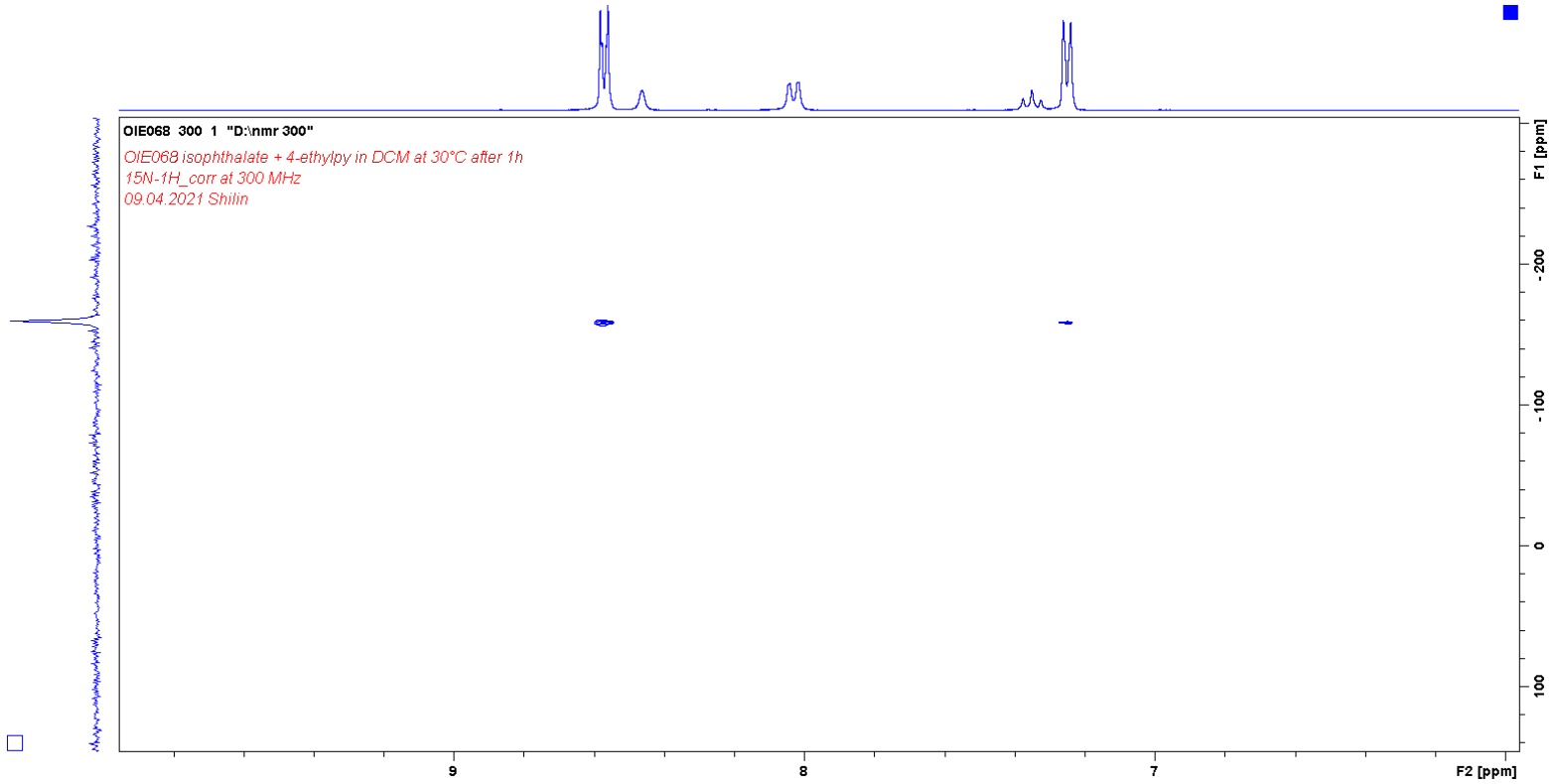


Figure S10: The $^{1}H$ NMR spectrum of compound **3** in $CD_2Cl_2$.

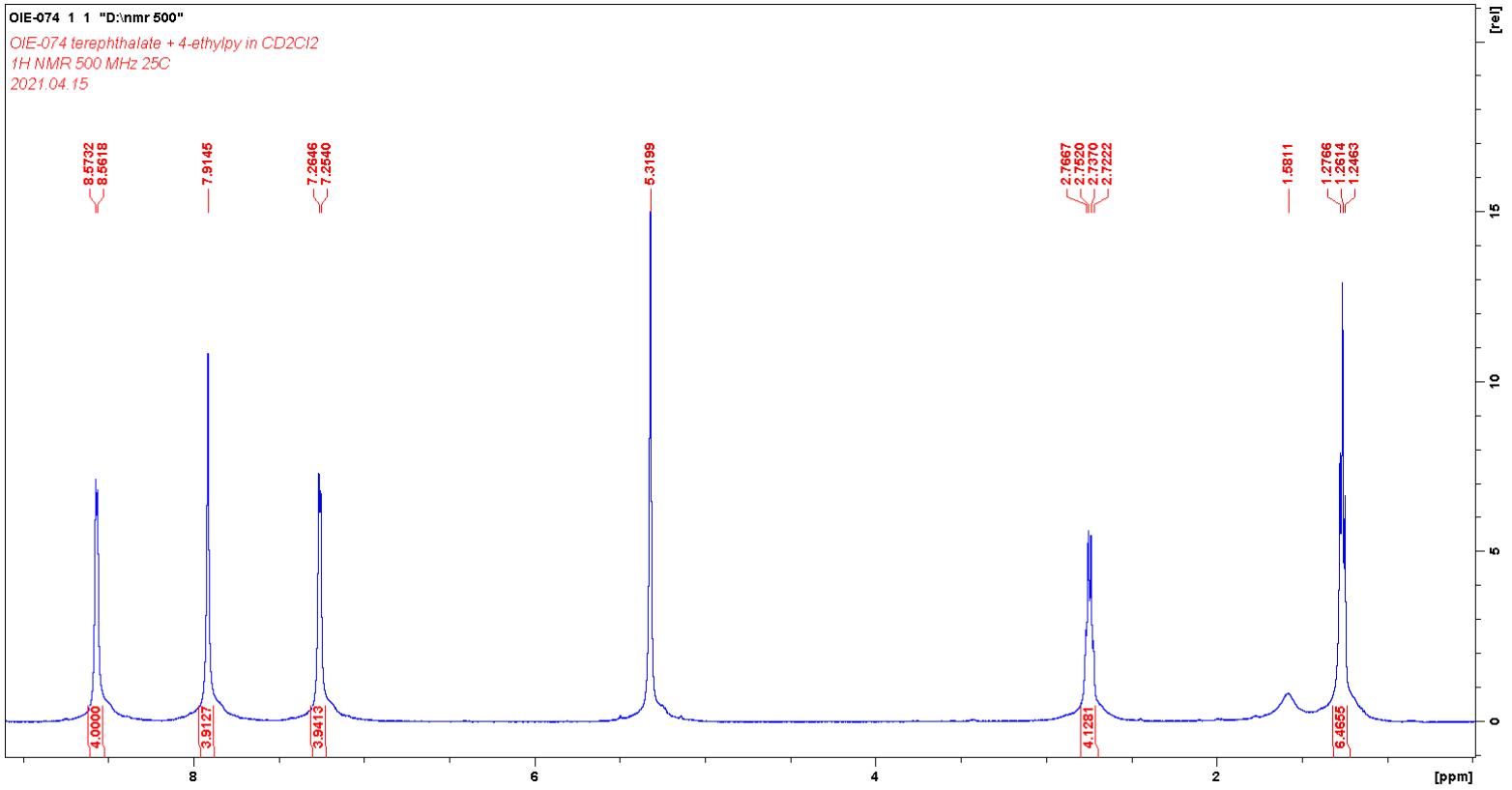


Figure S11: The $^{1}H$-$^{15}N$ HMBC spectrum of compound **3** in $CD_2Cl_2$.

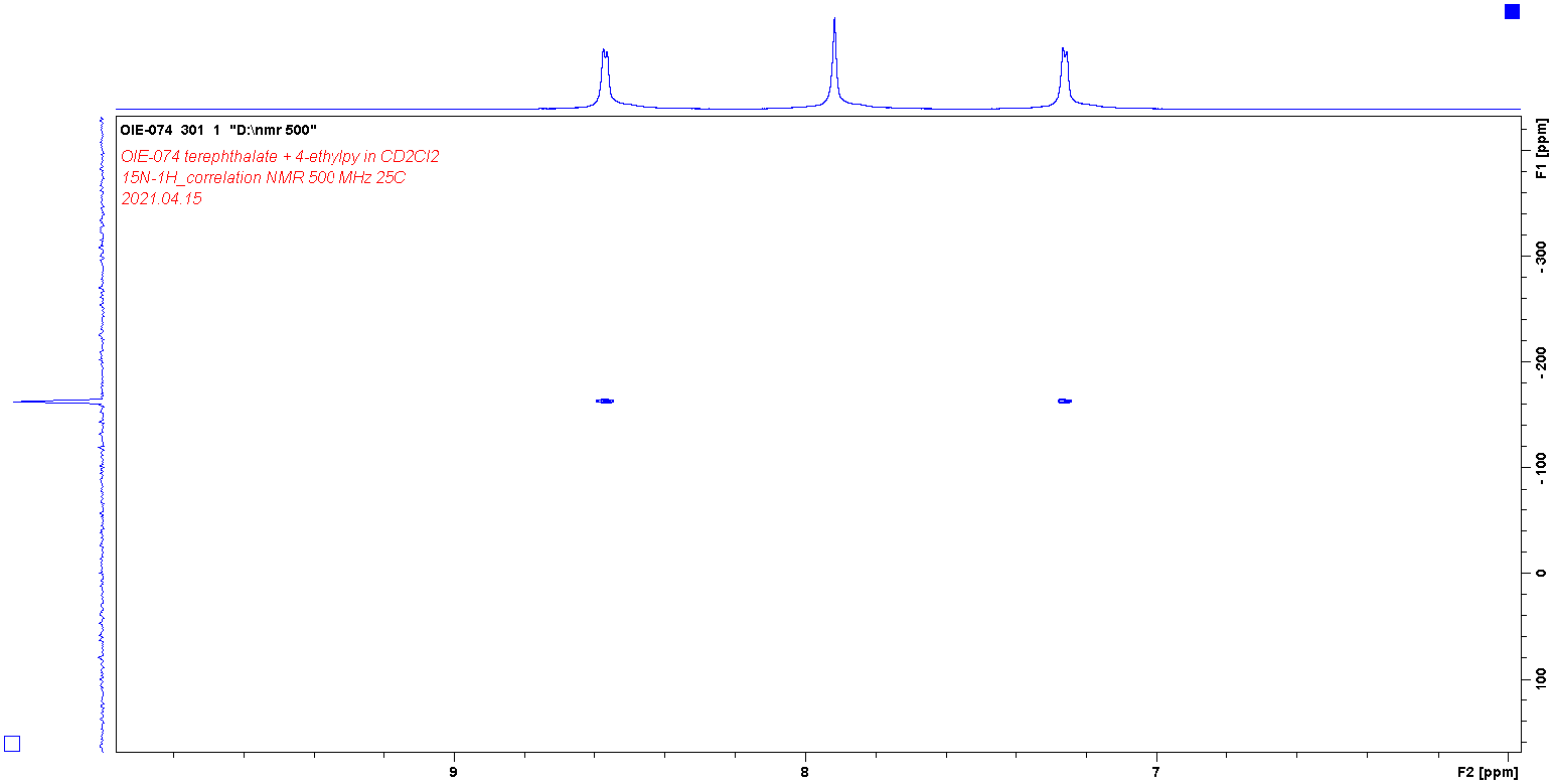


Figure S12: The $^{1}H$ NMR spectrum of compound **4** in $CD_2Cl_2$.

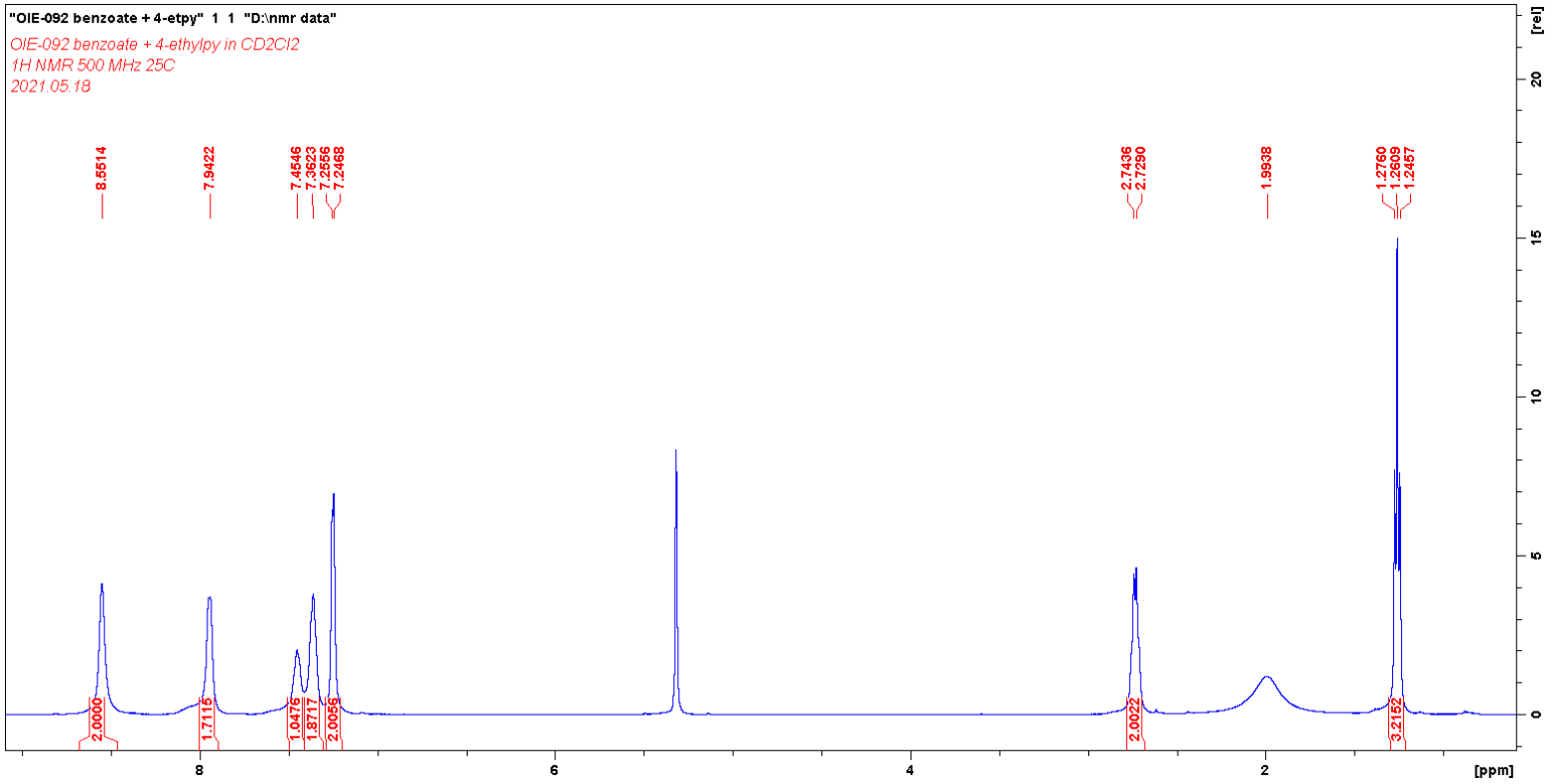
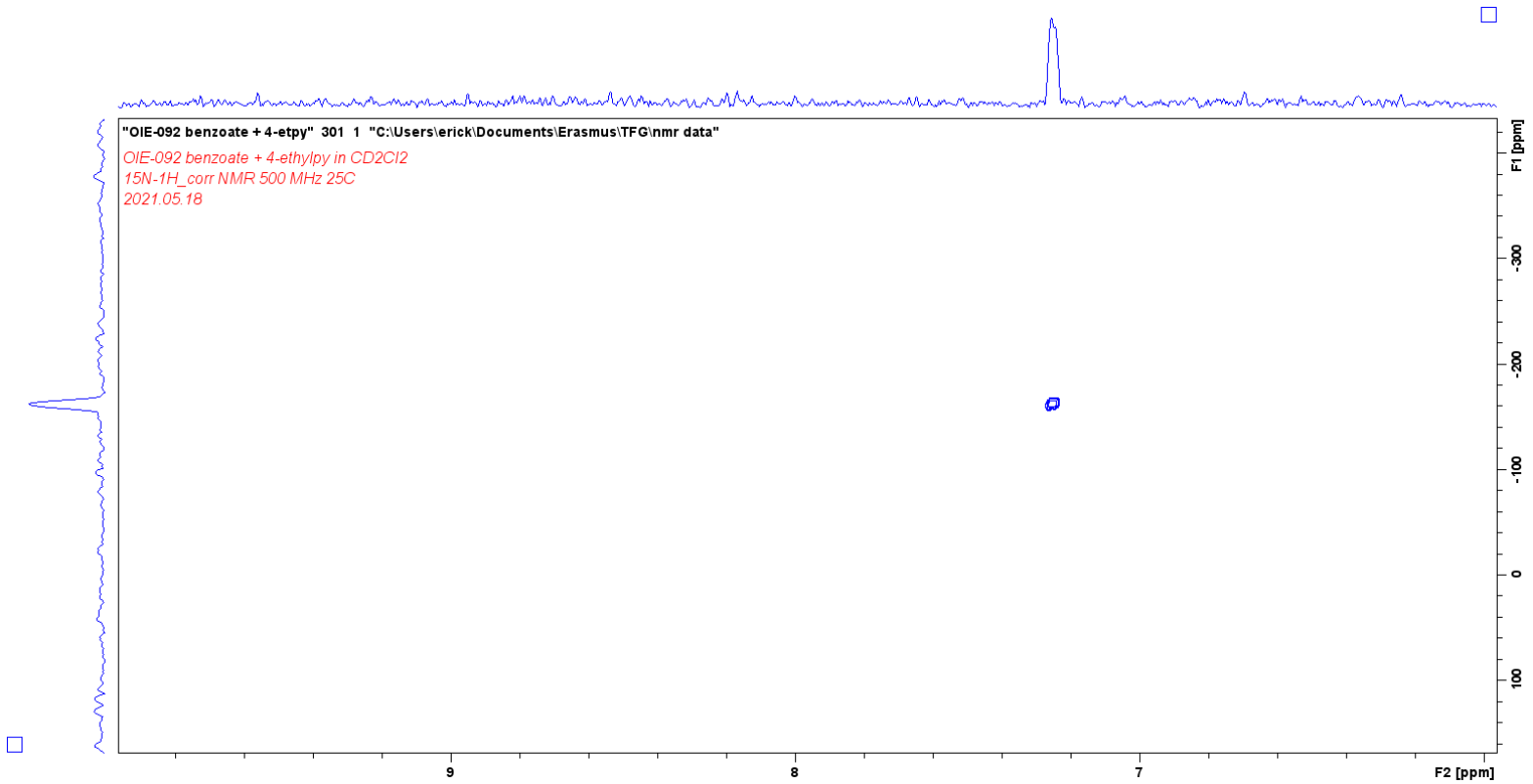


Figure S13: The $^{1}H$-$^{15}N$ HMBC spectrum of compound **4** in $CD_2Cl_2$.



# Computational Details

## General Considerations

The geometry calculations for the complexes were done at the M06-2X/def2-TZVP level of theory[6] using the SPARTAN18 program[7] with dichloromethane (dielectric = 8.82) as the solvent using the conductor like polarizable continuum model (C-PCM).[8,9] The initial models were built using SPARTAN18 and optimized at the MM-level before the DFT calculations. The hypoiodite complexes **1**, **1F**, **2**, **3** and **BZPRIB** (CCDC refcode) were built up from the corresponding MM-level optimized carboxyl dihypoiodites and 4-ethylpyridine so that the N···O distance was ca. 4.7 Å and the O–I···N angle ca. 170 - 175º and then optimized with the given DFT method.

## XRD Comparison Table

Table S2: Comparison of Experimental (XRD) Versus Computational (DFT) Bond Lengths and Angles.

| **Compound** | **1** | **1F** | **2** | **3** | **(phthaloyl-OI)(pyridine)$_2$ (BZPRIB)**‡[5] |
|---|---|---|---|---|---|
| **O–I (Å)** | 2.153(5) | 2.213(6) | 2.17(1) | - | 2.136 |
| **(XRD)** | 2.173(4) | 2.223(6) | 2.18(1) | | 2.183 |
| **O–I (Å)** | 2.143 | 2.172 | 2.141 | 2.144 | 2.131 |
| **(DFT)** | 2.146 | 2.175 | 2.145 | 2.148 | 2.133 |
| **I–N (Å)** | 2.275(4) | 2.208(6) | 2.25(2) | - | 2.282 |
| **(XRD)** | 2.305(5) | 2.223(6) | 2.29(1) | | 2.324 |
| **I–N (Å)** | 2.283 | 2.260 | 2.287 | 2.282 | 2.301 |
| **(DFT)** | 2.294 | 2.260 | 2.288 | 2.287 | 2.305 |
| **C=O (Å)** | 1.212(8) | 1.212(9) | 1.19(2) | - | 1.181 |
| **(XRD)** | 1.214(8) | 1.214(9) | 1.23(1) | | 1.219 |
| **C=O (Å)** | 1.216 | 1.216 | 1.219 | 1.220 | 1.216 |
| **(DFT)** | 1.219 | 1.216 | 1.219 | 1.220 | 1.217 |
| **C–O (Å)** | 1.299(8) | 1.276(9) | 1.25(1) | - | 1.293 |
| **(XRD)** | 1.310(8) | 1.30(1) | 1.31(1) | | 1.305 |
| **C–O (Å)** | 1.300 | 1.288 | 1.301 | 1.300 | 1.301 |
| **(DFT)** | 1.301 | 1.290 | 1.301 | 1.300 | 1.302 |
| **O–I–N (°)** | 173.6(2) | 173.2(2) | 175.6(4) | - | 174.50 |
| **(XRD)** | 175.4(2) | 174.1(2) | 176.2(6) | | 175.69 |
| **O–I–N (°)** | 176.5 | 176.4 | 176.2 | 176.0 | 176.1 |
| **(DFT)** | 176.6 | 176.5 | 176.2 | 176.4 | 176.3 |

‡ There were no esds available for (phthaloyl-OI)(pyridine)2 (BZPRIB) on the CSD.[10]

## Computational structures

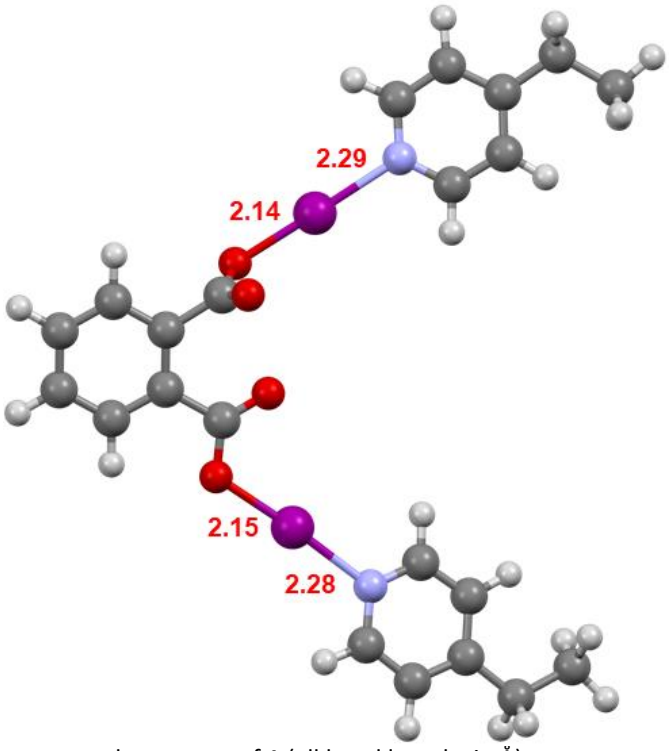



Figure S14: The computationally generated geometry of **1** (all bond lengths in Ă).

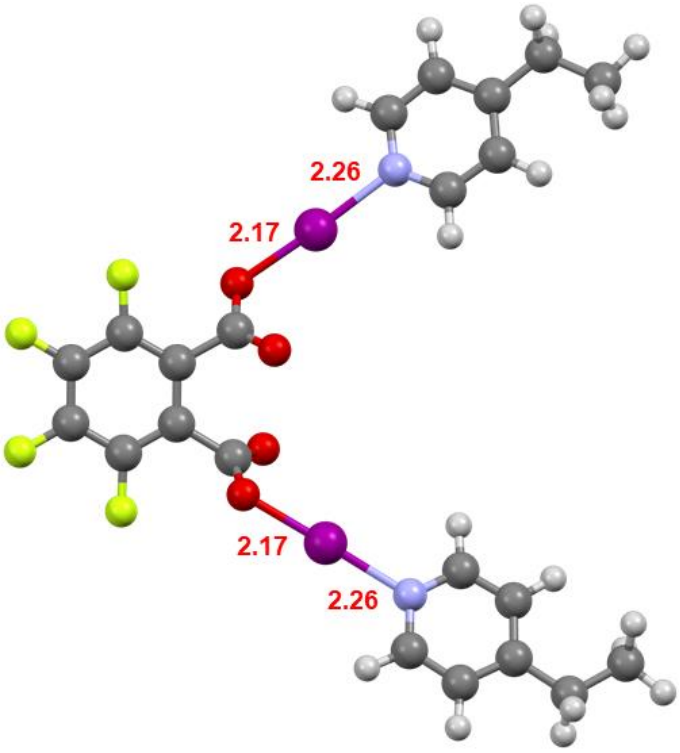



Figure S15: The computationally generated geometry of **1F** (all bond lengths in Å).

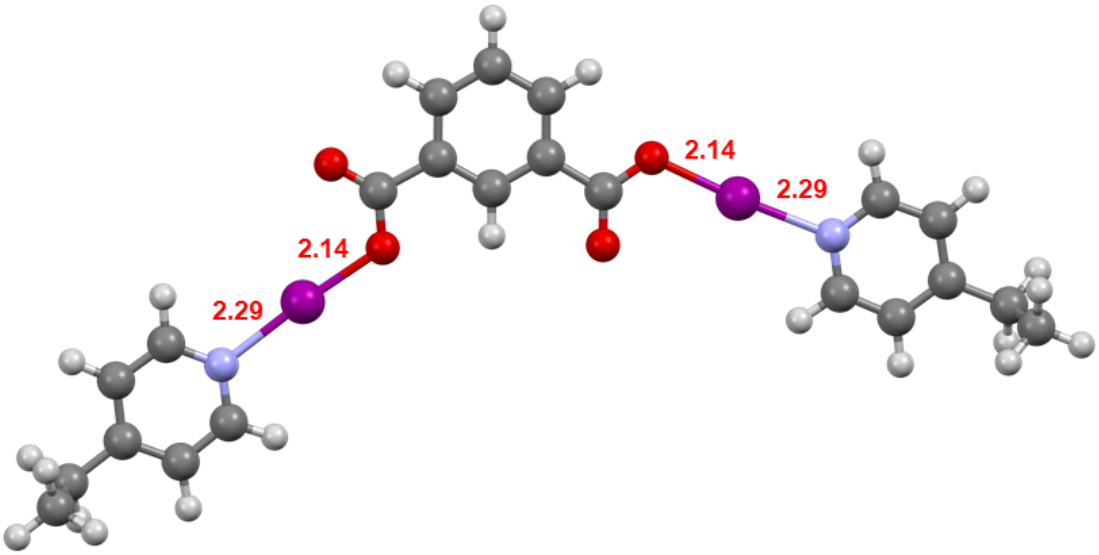



Figure S16: The computationally generated geometry of **2** (all bond lengths in Å).

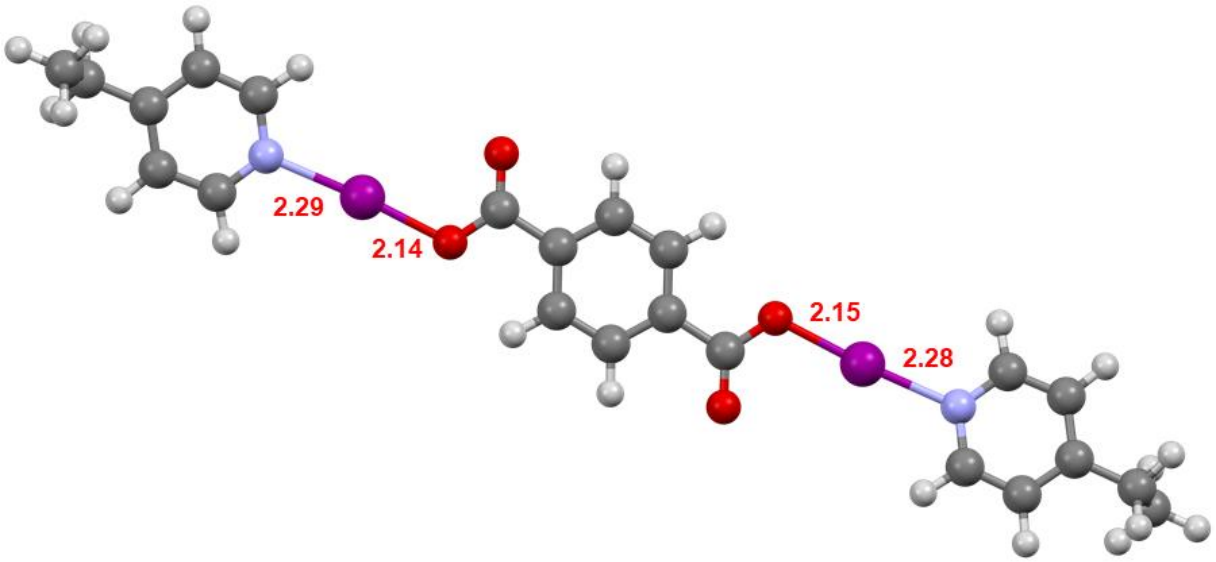



Figure S17: The computationally generated geometry of **3** (all bond lengths in Å).

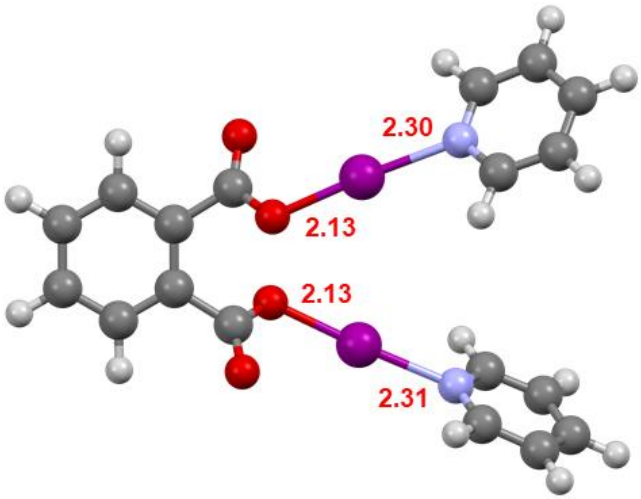



Figure S18: The computationally generated geometry of (phthaloyl-OI)(pyridine)$_2$ (**BZPRIB**; all bond lengths in Å), the synthesis of which has been previously described.[5]

# Cartesian Coordinates

**Compound 1**

| | | | |
|---|---|---|---|
| H | 1.579205 | -7.146650 | -3.723734 |
| C | 1.256492 | -6.141611 | -3.483377 |
| C | 0.443213 | -3.650978 | -2.768311 |
| C | 1.083171 | -5.191397 | -4.491790 |
| C | 1.016876 | -5.804027 | -2.170352 |
| N | 0.616338 | -4.575290 | -1.824455 |
| C | 0.666118 | -3.922009 | -4.106177 |
| H | 1.141564 | -6.516222 | -1.364561 |
| H | 0.509768 | -3.134512 | -4.829578 |
| H | 0.118161 | -2.673770 | -2.433555 |
| C | -0.524076 | -2.320927 | 4.327477 |
| C | -1.078600 | -2.072919 | 7.047062 |
| C | -0.811759 | -3.446075 | 5.097016 |
| C | -0.511210 | -1.063078 | 4.932250 |
| C | -0.789652 | -0.946786 | 6.289704 |
| C | -1.089941 | -3.326375 | 6.449514 |
| H | -0.819531 | -4.416521 | 4.620130 |
| H | -0.777043 | 0.032375 | 6.753505 |
| H | -1.316105 | -4.207837 | 7.035197 |
| H | -1.294195 | -1.969992 | 8.103020 |
| C | -0.249301 | -2.455550 | 2.853998 |
| O | -0.164105 | -1.473303 | 2.137519 |
| O | -0.124894 | -3.685543 | 2.449304 |
| I | 0.236345 | -4.053433 | 0.366352 |
| C | 1.349765 | -5.569617 | -5.923322 |
| H | 0.723339 | -6.434897 | -6.156866 |
| H | 2.380839 | -5.929494 | -5.980892 |
| C | 1.122659 | -4.467649 | -6.945517 |
| H | 1.770111 | -3.610349 | -6.755139 |
| H | 0.088021 | -4.121467 | -6.932364 |
| H | 1.340679 | -4.838348 | -7.946220 |
| C | -0.160753 | 0.205807 | 4.193090 |
| O | 0.994192 | 0.574041 | 4.096220 |
| O | -1.208687 | 0.862312 | 3.793117 |
| I | -0.919176 | 2.655967 | 2.658286 |
| H | 0.350060 | 5.572669 | -1.573281 |
| C | -0.085408 | 5.667215 | -0.588703 |
| C | -1.163982 | 5.746814 | 1.909439 |
| C | -0.218626 | 4.532773 | 0.191820 |
| C | -0.509643 | 6.896111 | -0.095465 |
| C | -1.060578 | 6.914575 | 1.187351 |
| N | -0.746080 | 4.576348 | 1.413845 |
| H | 0.103531 | 3.560818 | -0.160820 |
| H | -1.407812 | 7.842531 | 1.623561 |
| H | -1.584815 | 5.726017 | 2.906711 |
| C | -0.396870 | 8.178774 | -0.873664 |

| | | | |
|---|---|---|---|
| H | 0.183819 | 8.879482 | -0.267347 |
| H | -1.399036 | 8.610651 | -0.942949 |
| C | 0.216932 | 8.052616 | -2.258500 |
| H | 1.232274 | 7.656265 | -2.206655 |
| H | 0.261624 | 9.030342 | -2.736400 |
| H | -0.373217 | 7.392125 | -2.895491 |

**Compound 1F**

| | | | |
|---|---|---|---|
| H | 1.540394 | -7.110681 | -3.713330 |
| C | 1.267101 | -6.089441 | -3.480967 |
| C | 0.576312 | -3.555398 | -2.785937 |
| C | 1.112087 | -5.146379 | -4.499223 |
| C | 1.071366 | -5.725332 | -2.168529 |
| N | 0.730926 | -4.474825 | -1.833407 |
| C | 0.758791 | -3.854700 | -4.123385 |
| H | 1.182615 | -6.430499 | -1.354874 |
| H | 0.621888 | -3.070487 | -4.854157 |
| H | 0.299579 | -2.561322 | -2.458198 |
| C | -0.662176 | -2.357633 | 4.317023 |
| C | -0.992161 | -2.051872 | 7.064096 |
| C | -0.959239 | -3.443264 | 5.119736 |
| C | -0.538369 | -1.095769 | 4.901320 |
| C | -0.700106 | -0.959263 | 6.263489 |
| C | -1.129209 | -3.298048 | 6.487474 |
| C | -0.540187 | -2.505373 | 2.816548 |
| O | -1.102303 | -1.710012 | 2.087533 |
| O | 0.185056 | -3.509015 | 2.456158 |
| I | 0.417105 | -3.927234 | 0.336510 |
| C | 1.327020 | -5.558224 | -5.929686 |
| H | 0.647287 | -6.389678 | -6.136009 |
| H | 2.334206 | -5.977800 | -6.002629 |
| C | 1.140147 | -4.460742 | -6.964601 |
| H | 1.842157 | -3.640795 | -6.805147 |
| H | 0.128408 | -4.053552 | -6.932844 |
| H | 1.310672 | -4.860072 | -7.963441 |
| C | -0.163531 | 0.110789 | 4.063524 |
| O | 0.912871 | 0.145327 | 3.501311 |
| O | -1.078106 | 1.019144 | 4.056802 |
| I | -0.803910 | 2.770091 | 2.797089 |
| H | 0.402234 | 5.527282 | -1.521821 |
| C | -0.034022 | 5.647055 | -0.540513 |
| C | -1.109196 | 5.794769 | 1.957736 |
| C | -0.127878 | 4.541222 | 0.284087 |
| C | -0.499512 | 6.880140 | -0.096401 |
| C | -1.045427 | 6.933741 | 1.187710 |
| N | -0.655787 | 4.619237 | 1.505508 |
| H | 0.222304 | 3.566141 | -0.030109 |
| H | -1.423348 | 7.866064 | 1.586991 |
| H | -1.527480 | 5.799721 | 2.955992 |

| | | | |
|---|---|---|---|
| C | -0.440286 | 8.130386 | -0.930597 |
| H | 0.121118 | 8.877684 | -0.362904 |
| H | -1.458352 | 8.522489 | -1.005294 |
| C | 0.160109 | 7.965822 | -2.317388 |
| H | 1.193045 | 7.618289 | -2.265016 |
| H | 0.153078 | 8.921032 | -2.840742 |
| H | -0.409165 | 7.250981 | -2.913646 |
| F | -1.131983 | -4.661793 | 4.611104 |
| F | -1.429288 | -4.348045 | 7.242260 |
| F | -1.140605 | -1.906867 | 8.374177 |
| F | -0.556251 | 0.226707 | 6.856618 |

**Compound 2**

| | | | |
|---|---|---|---|
| C | 0.543210 | 3.009452 | -3.692489 |
| C | 0.462789 | 2.895637 | -0.916834 |
| C | 0.430858 | 1.778634 | -3.051164 |
| C | 0.614981 | 4.178144 | -2.949436 |
| C | 0.575905 | 4.123340 | -1.562672 |
| C | 0.390410 | 1.725481 | -1.663674 |
| C | 0.354876 | 0.528796 | -3.886703 |
| O | 0.390356 | 0.582420 | -5.104439 |
| O | 0.251342 | -0.564950 | -3.190754 |
| C | 0.416617 | 2.798078 | 0.584603 |
| O | 0.298507 | 1.720959 | 1.143090 |
| O | 0.513541 | 3.945775 | 1.190222 |
| I | 0.110166 | -2.444808 | -4.206332 |
| I | 0.486411 | 4.001059 | 3.333684 |
| H | 0.302742 | 0.775786 | -1.155198 |
| H | 0.632114 | 5.030357 | -0.976542 |
| H | 0.702006 | 5.133574 | -3.450337 |
| H | 0.572941 | 3.036657 | -4.773802 |
| N | 0.476234 | 4.209162 | 5.611286 |
| C | 0.482558 | 4.453494 | 8.372868 |
| C | 0.406015 | 3.120286 | 6.381056 |
| C | 0.549131 | 5.416412 | 6.177569 |
| C | 0.553249 | 5.574037 | 7.548472 |
| C | 0.405832 | 3.206084 | 7.758541 |
| H | 0.352408 | 2.168670 | 5.867474 |
| H | 0.607776 | 6.262619 | 5.504733 |
| H | 0.616535 | 6.568908 | 7.970293 |
| H | 0.351117 | 2.300525 | 8.348876 |
| C | 0.434837 | 4.590084 | 9.865226 |
| H | 1.021998 | 5.458366 | 10.167009 |
| H | 0.881313 | 3.706651 | 10.323494 |
| C | -1.009797 | 4.749954 | 10.348755 |
| H | -1.466275 | 5.637410 | 9.908042 |
| H | -1.038173 | 4.849975 | 11.433402 |
| H | -1.607727 | 3.882587 | 10.066032 |
| H | -0.188422 | -5.947863 | -8.171605 |

| | | | |
|---|---|---|---|
| C | -0.170740 | -5.884328 | -7.091103 |
| C | -0.111553 | -5.608371 | -4.384619 |
| C | -0.232184 | -7.035211 | -6.308463 |
| C | -0.080582 | -4.648268 | -6.484603 |
| N | -0.051847 | -4.520080 | -5.155281 |
| C | -0.203153 | -6.875434 | -4.925815 |
| H | -0.026970 | -3.732131 | -7.059079 |
| H | -0.247055 | -7.733882 | -4.268103 |
| H | -0.082345 | -5.444846 | -3.314650 |
| C | -0.379600 | -8.389838 | -6.934878 |
| H | 0.188867 | -8.419645 | -7.865639 |
| H | 0.033338 | -9.144941 | -6.265068 |
| C | -1.852521 | -8.698548 | -7.220391 |
| H | -2.275029 | -7.959710 | -7.902707 |
| H | -2.434255 | -8.682672 | -6.297743 |
| H | -1.952749 | -9.683849 | -7.674602 |

**Compound 3**

| | | | |
|---|---|---|---|
| C | 0.056480 | 0.118256 | -1.434701 |
| C | -0.101512 | -0.056087 | 1.331693 |
| C | -0.147450 | -1.116834 | -0.826885 |
| C | 0.181676 | 1.262527 | -0.663576 |
| C | 0.102883 | 1.178946 | 0.723973 |
| C | -0.225874 | -1.200376 | 0.560747 |
| C | -0.277806 | -2.340747 | -1.695417 |
| O | -0.188939 | -2.264537 | -2.908913 |
| O | -0.488138 | -3.437673 | -1.029504 |
| C | 0.232179 | 2.402418 | 1.593858 |
| O | 0.132210 | 2.324110 | 2.806605 |
| O | 0.453506 | 3.499216 | 0.932233 |
| I | -0.687942 | -5.289624 | -2.091791 |
| I | 0.665846 | 5.344746 | 2.009064 |
| H | -0.384111 | -2.161312 | 1.030041 |
| H | 0.340518 | 2.223495 | -1.132681 |
| H | 0.115523 | 0.170195 | -2.513567 |
| N | 0.912302 | 7.371290 | 3.028993 |
| C | 1.205763 | 9.829813 | 4.275509 |
| C | 1.283803 | 8.441484 | 2.321701 |
| C | 0.682839 | 7.490249 | 4.339264 |
| C | 0.820422 | 8.698623 | 4.991155 |
| C | 1.440081 | 9.680013 | 2.910995 |
| H | 1.453235 | 8.286279 | 1.263672 |
| H | 0.381524 | 6.590324 | 4.860395 |
| H | 0.623039 | 8.756447 | 6.053896 |
| H | 1.740241 | 10.524569 | 2.304373 |
| C | 1.415554 | 11.146922 | 4.960847 |
| H | 0.715080 | 11.236395 | 5.792306 |
| H | 1.209999 | 11.956533 | 4.259448 |
| C | 2.851992 | 11.264416 | 5.479857 |

| | | | |
|---|---|---|---|
| H | 3.067952 | 10.470075 | 6.195648 |
| H | 2.999403 | 12.224091 | 5.974321 |
| H | 3.564907 | 11.186136 | 4.657879 |
| H | -1.088817 | -8.712117 | -6.121926 |
| C | -1.073136 | -8.666135 | -5.040495 |
| C | -1.015161 | -8.435660 | -2.329878 |
| C | -1.171866 | -9.826961 | -4.276364 |
| C | -0.947112 | -7.443078 | -4.414358 |
| N | -0.918736 | -7.337576 | -3.083026 |
| C | -1.143428 | -9.690484 | -2.891176 |
| H | -0.863369 | -6.519916 | -4.973736 |
| H | -1.214921 | -10.557541 | -2.247383 |
| H | -0.984623 | -8.290009 | -1.257420 |
| C | -1.356145 | -11.166632 | -4.924850 |
| H | -0.786815 | -11.197432 | -5.855023 |
| H | -0.965834 | -11.943601 | -4.266467 |
| C | -2.836471 | -11.429734 | -5.217594 |
| H | -3.236509 | -10.669545 | -5.890008 |
| H | -3.419787 | -11.410979 | -4.295999 |
| H | -2.962989 | -12.405188 | -5.686212 |
| H | -0.161468 | -0.107789 | 2.410478 |

**BZPRIB**

| | | | |
|---|---|---|---|
| I | 0.282693 | -2.253703 | 0.247950 |
| O | 1.701183 | -1.182743 | 1.427132 |
| O | 3.429665 | -1.788042 | 0.135883 |
| C | 2.948302 | -1.152587 | 1.055914 |
| C | 2.001287 | 1.526627 | 2.014939 |
| O | 1.854072 | 1.588378 | 0.722900 |
| O | 1.207266 | 1.937460 | 2.839715 |
| I | 0.000941 | 2.283338 | -0.066899 |
| C | 3.798736 | -0.268294 | 1.926525 |
| C | 5.065420 | -0.714635 | 2.282176 |
| H | 5.416561 | -1.660702 | 1.890760 |
| C | 5.858551 | 0.035476 | 3.139601 |
| H | 6.841917 | -0.322050 | 3.417003 |
| C | 5.385262 | 1.239363 | 3.644892 |
| H | 5.999869 | 1.828154 | 4.313715 |
| C | 4.122699 | 1.691866 | 3.288875 |
| H | 3.749175 | 2.634030 | 3.669473 |
| C | 3.328557 | 0.947838 | 2.425288 |
| N | -1.353812 | -3.356303 | -0.936091 |
| C | -3.311170 | -4.677400 | -2.343902 |
| C | -1.041672 | -4.007568 | -2.058396 |
| C | -2.613425 | -3.344808 | -0.495205 |
| C | -3.624285 | -3.997530 | -1.176109 |
| C | -1.998816 | -4.682736 | -2.793005 |
| H | -0.002672 | -3.978277 | -2.360821 |
| H | -2.799686 | -2.799240 | 0.421257 |

| | | | |
|---|---|---|---|
| H | -4.633834 | -3.968621 | -0.791307 |
| H | -1.712411 | -5.200780 | -3.697312 |
| H | -4.081752 | -5.197574 | -2.897668 |
| N | -1.942971 | 3.014965 | -1.065958 |
| C | -4.245263 | 3.919585 | -2.264854 |
| C | -1.931003 | 3.358566 | -2.355695 |
| C | -3.069605 | 3.108475 | -0.356820 |
| C | -4.246754 | 3.558844 | -0.925344 |
| C | -3.068800 | 3.817573 | -2.992557 |
| H | -0.984982 | 3.259408 | -2.872821 |
| H | -3.011184 | 2.814934 | 0.683607 |
| H | -5.141728 | 3.622859 | -0.322888 |
| H | -3.024926 | 4.088649 | -4.037770 |
| H | -5.151406 | 4.277206 | -2.736185 |

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