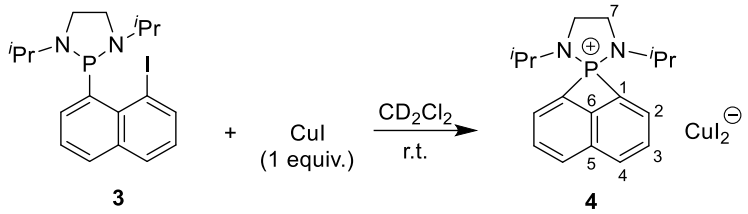
Supporting Information

1. Materials and Methods

Unless otherwise stated, all reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques or in a glovebox under an inert atmosphere. Dry, oxygen-free solvents were employed. Solution ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on a Bruker Avance 300 and 500 spectrometers at 298 K. Chemical shifts (δ) are expressed with a positive sign, in parts per million. ^{1}H and ^{13}C chemical shifts reported are referenced internally to residual protio (^{1}H) or deutero (^{13}C) solvent, while ^{31}P chemical shifts are relative to 85% H_3PO_4. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; hept, heptuplet. The ^{1}H and ^{13}C resonance signals were attributed by means of 2D COSY, HSQC and HMBC. Mass spectra were recorded on a Waters UPLC Xevo G2 Q TOF apparatus. Elemental analyses were performed by the in-house service at the *Laboratoire de Chimie de Coordination* (205, Route de Narbonne, 31077, Toulouse, France) on a PerkinElmer 2400 Series II system. Melting points were determined with a Stuart SMP40 apparatus. ICPMS analysis was performed using a quadrupole ICPMS (Agilent 7500Ce). Introduction was performed in wet plasma (nebulizer at 125µl/min, 1200W plasma) using a peltier effect and a collision cell to reduce oxides and interferences. The machine was calibrated every 2 hours using an in house standard and a geostandard was used to control precision and drift every 2 hours. For mineralization a sample of **2b** (0.9 mg) was dissolved in 70% HNO_3 (TraceMetal Grade, Fisher Chemical, 2 mL), then the solution was diluted with deionized water (98 mL). All starting materials were purchased from Aldrich and used as received unless otherwise stated. 1-Iodo-8-diisopropylphosphinonaphthalene **1-I,** 1-bromo-8-diisopropylphosphinonaphthalene **1-Br**, 1-chloro-8-diisopropylphosphinonaphthalene **1-Cl**,[1] *peri*-bridged naphthyl-phosphonium **2a**,[2] 1-iodo-8-*N*,*N*-isopropyldiazaphospholidinonaphthalene **3**,[3] 1-iodo-8-diphenylphosphinonaphthalene **5**,[4] (P,C)-cyclometallated gold(III) di-iodide complex **8**[5] and dimethylsulfide gold bromide[6] were prepared according to the reported procedures.

2. Synthesis of phosphoniums

i. Synthesis of phosphonium **4**



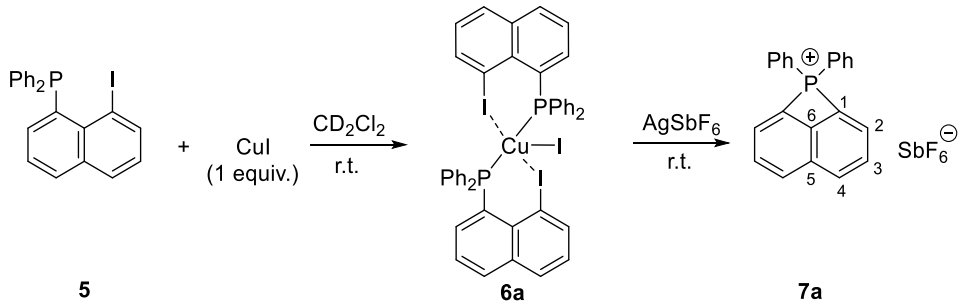
3 **4**

In a J Young valve NMR tube CuI (6.7 mg, 0.035 mmol) was suspended in 0.3 mL of CD_2Cl_2 and a solution of 1-iodo-8-*N*,*N*-isopropyldiazaphospholidinonaphthalene **3** (15.0 mg, 0.035 mmol) in 0.3 mL of CD_2Cl_2 was added. Color evolved from light yellow to colorless within a few minutes along with consumption of CuI. NMR analysis revealed complete conversion to the phosphonium **4**.

^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.28 (dd, 2H, $^3J_{HH}$ = 8.3 Hz, J_{PH} = 5.3 Hz, $H_{2\text{ or }4}$), 8.11 (dd, 2H, $^3J_{HH}$ = 7.0 Hz, J_{PH} = 14.0 Hz, $H_{2\text{ or }4}$), 8.03-7.92 (m, 2H, H_3) 3.94 (s, 2H, H_7), 3.92 (s, 2H, H_7), 3.38-3.27 (m, 2H, CH*i*Pr), 1.22 (d, 12H, $^3J_{HH}$ = 6.7 Hz, CH_3*i*Pr); **^{13}C{^{1}H} NMR** (126 MHz, CD_2Cl_2): δ 153.7 (d, $^3J_{PC}$ = 12.7 Hz, C_6), 139.0 (d, $^1J_{PC}$ = 104.7 Hz, C_1), 132.8 (d, $^2J_{PC}$ = 15.2 Hz, C_3), 129.5 (d, J_{PC} = 4.9 Hz, $C_{2\text{ or }4}$), 127.9 (d, $^3J_{PC}$ = 23.1 Hz, C_5), 127.2 (s, $C_{2\text{ or }4}$), 47.0 (d, $^2J_{PC}$ = 8.0 Hz, CH*i*Pr), 42.5 (d, $^2J_{PC}$ = 7.2 Hz, C_7), 20.9 (d, $^3J_{PC}$ = 3.5 Hz, CH_3*i*Pr); **^{31}P{^{1}H} NMR** (202 MHz, CD_2Cl_2): δ 53.9. **HRMS (DCI-CH_4)**: calcd for $[M]^+ = C_{18}H_{24}N_2P^+$: 299.1677. Found: 299.1675; **HRMS (DCI-CH_4)**: calcd for $[M]^- = CuI_2^-$: 316.7386. Found: 316.7387.

ii. Synthesis of phosphoniums **7a** and **7b**

Procedure A:



5 **6a** **7a**

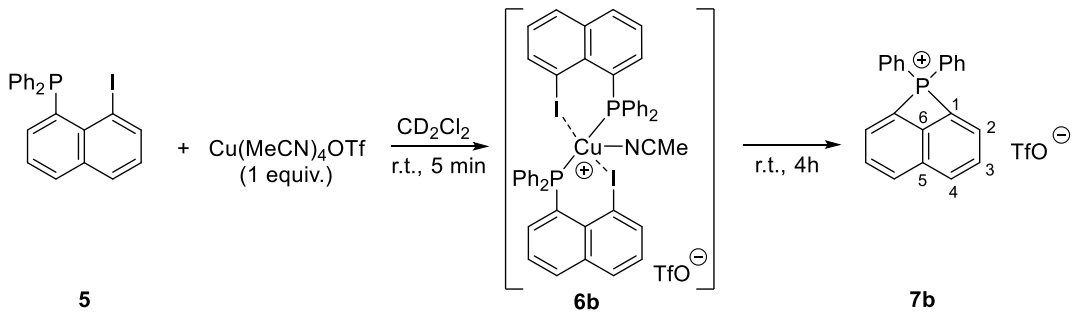
NMR experiment: In a J Young valve NMR tube, CuI (6.5 mg, 0.034 mmol) was suspended in 0.3 mL of CD_2Cl_2 and a solution of 1-iodo-8-diphenylphosphinonaphthalene **5** (15.0 mg, 0.034 mmol) in 0.3 mL of CD_2Cl_2 was added. After a few minutes, ^{31}P NMR analysis revealed formation of a single species in solution (δ -12.0 ppm). A white crystalline material started to precipitate and a crystal suitable for X-ray diffraction analysis could be extracted to reveal the

formation of the diphosphine Cu(I) complex **6a**. [**HRMS (ESI+)**: calcd for $[M\text{-}I]^+$ = $C_{44}H_{32}P_2CuI_2^+$: 938.9365. Found: 938.9367.] $AgSbF_6$ (11.7 mg, 0.034 mmol) in 0.3 mL of CD_2Cl_2 was then added to the mixture. NMR analysis showed immediate and complete conversion to phosphonium **7a**.

Preparative manipulation: In a glove-box, a vial was charged with CuI (43.5 mg, 0.228 mmol). A solution of 1-iodo-8-diphenylphosphinonaphthalene **5** (100.0 mg, 0.228 mmol) in 3.5 mL of CH_2Cl_2 was added and the mixture was stirred for 30 minutes during which a pale yellow precipitate appeared. $AgSbF_6$ (78.4 mg, 0.228 mmol) was then added to the mixture and stirring was continued for another 30 minutes with the persistence of the white precipitate. Filtration over a Celite® pad and evaporation of the solvent afforded compound **7a** as a beige powder (85.0 mg, 68%).

MP: 138 °C; **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 8.32 (dd, $^3J_{HH}$ = 8.5 Hz, J_{PH} = 4.3 Hz, 2H, $H_{2\text{ or }4}$), 8.13 (dd, $^3J_{HH}$ = 7.0 Hz, J_{PH} = 11,3 Hz, 2H, $H_{2\text{ or }4}$), 8,01 (ddd, $^3J_{HH}$ = 8.5 Hz, $^3J_{HH}$ = 7.0 Hz, $^4J_{PH}$ = 7.1 Hz, 2H, H_3), 7.95-7.90 (m, 6H, $H_{ortho\ Ph}$ + $H_{para\ Ph}$), 7.77-7.72 (m, 4H, $H_{meta\ Ph}$); **^{13}C{^{1}H} NMR** (126 MHz, CD_2Cl_2): δ 153.0 (s, C_6), 137.2 (d, $^4J_{PC}$ = 3.4 Hz, $C_{para\ Ph}$), 133,8 (d, $^2J_{PC}$ = 13.2 Hz, $C_{ortho\ Ph}$), 132,6 (d, $^3J_{PC}$ = 13.9 Hz, C_3), 131.0 (d, $^4J_{PC}$ = 13.8 Hz, $C_{meta\ Ph}$), 130,7 (d, J_{PC} = 4.1 Hz, $C_{2\text{ or }4}$), 128.6 (d, $^3J_{PC}$ = 16.0 Hz, C_5), 128.4 (d, $^3J_{PC}$ = 92.9 Hz, C_1), 126.9 (s, $C_{2\text{ or }4}$), 118.5 (d, $^1J_{PC}$ = 70.2 Hz, C_{ipso}); **^{31}P{^{1}H} NMR** (202 MHz, CD_2Cl_2): δ 71.8; **HRMS (DCI-CH_4)**: calcd for $[M]^+ = C_{22}H_{16}P^+$: 311.0990. Found: 311.0990; **HRMS (ESI-)**: calcd for $[M]^- = SbF_6^-$: 234.8942. Found: 234.8944; **Elemental Analysis**: calcd for $C_{22}H_{16}F_6PSb$: C 48.30, H 2.95. Found: C 47.73, H 2.49.

Procedure B:

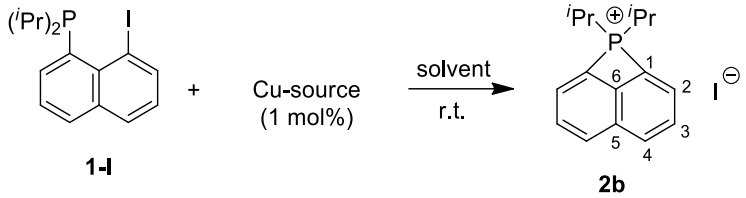


5 **6b** **7b**

NMR experiment: In a J Young valve NMR tube, $Cu(MeCN)_4OTf$ (12.9 mg, 0.034 mmol) was suspended in 0.3 mL of CD_2Cl_2 and a solution of 1-iodo-8-diphenylphosphinonaphthalene **5** (15.0 mg, 0.034 mmol) in 0.3 mL of CD_2Cl_2 was added. After a few minutes, ^{31}P NMR analysis revealed formation of a single species in solution (δ -7.5 ppm, complex **6b**). This was accompanied by the formation of a white crystalline material. This species gradually evolved

to phosphonium **7b** after 4h at room temperature. ^{1}H and ^{31}P spectra of **7b** are similar to those of **7a** (see above). **HRMS (ESI-)**: calcd for $[M]^- = CF_3SO_3^-$: 148.9520. Found: 148.9522.

iii. Optimized catalytic conditions for the synthesis of phosphonium **2b**



NMR experiment: In a J. Young valve NMR tube, the copper source (1 mol%) was suspended in 0.3 mL of solvent (see Table 2) and a solution of 1-iodo-8-diisopropylphosphinonaphthalene **1-I** (15.0 mg, 0.041 mmol) in 0.3 mL of the same solvent was added. Color evolved from light yellow to light red within a few minutes. The formation of the phosphonium **2b** was monitored by NMR spectroscopy.

Preparative manipulations:

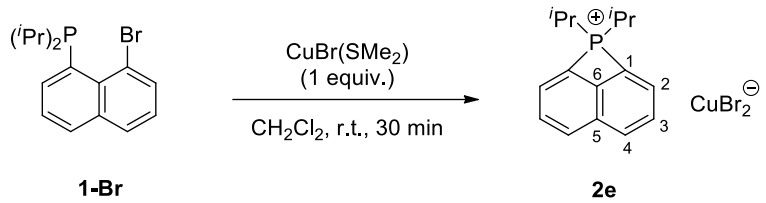
Conditions A *(Table 1, entry 3)***:** In a glove-box, $Cu(MeCN)_4OTf$ (1.2 mg, 0.0031 mmol) was suspended in 2 mL of THF and a solution of 1-iodo-8-diisopropylphosphinonaphthalene **1-I** (113.0 mg, 0.31 mmol) in 1 mL of THF was added. Color evolved from light yellow to red within a few minutes. A white precipitate appeared during the reaction corresponding to the phosphonium **2b**. NMR analysis revealed complete conversion to the phosphonium species after 30 min. The precipitated solid was filtered and dried. The solution was concentrated to dryness *in vacuo*. The residue was washed with 1 mL of THF. The 2 crops were combined and dried to obtain a light yellow solid (101 mg, 89 %).

Conditions B *(Table 1, entry 4)***:** In a glove-box, CuI (0.5 mg, 0.0027 mmol) was suspended in 2.0 mL of MeCN and a solution of 1-iodo-8-diisopropylphosphinonaphthalene **1-I** (100.0 mg, 0.27 mmol) in 3.0 mL of MeCN was added. Color evolved from light yellow to red within a few seconds. NMR analysis revealed complete conversion to the phosphonium **2b** after 5 min. Volatiles were removed *in vacuo*. The crude product was washed with 2.0 mL of THF, filtrated and dried to obtain a light yellow solid (91 mg, 91 %).

MP : 216 °C. **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.22 (dd, J_{PH} = 9.0 Hz, $^{3}J_{HH}$ = 7.0 Hz, 2H, H_4), 8.13 (dd, J_{PH} = 8.5 Hz, $^{3}J_{HH}$ = 3.8 Hz, 2H, H_2),7.85 (td, J_{PH} = 8.5 Hz, $^{3}J_{HH}$ = 6.5 Hz, 2H, H_3), 4.27 (hept d , $^{2}J_{PH}$ = 9.5 Hz, $^{3}J_{HH}$ = 7.1 Hz, 2H, CH*i*Pr), 1.41 (d, $^{3}J_{PH}$ = 21.0 Hz, $^{3}J_{HH}$ = 7.1 Hz, 12H, CH_3*i*Pr); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, CD_2Cl_2): δ 151.5 (s, C_6), 131.4 (d, $^{1}J_{PC}$ = 11.7 Hz,

C_3), 129.2 (d, $^2J_{PC}$ = 3.5 Hz, C_2), 128.9 (s, C_4), 127.1 (d, $^2J_{PC}$ = 14.3 Hz, C_5), 126 (d, $^2J_{PC}$ = 82.1 Hz, C_1), 29.3 (d, $^2J_{PC}$ = 28.9 Hz, CH*i*Pr), 18.3 (d, $^2J_{PC}$ = 1.5 Hz, CH_3*i*Pr); **$^{31}P\{^1H\}$ NMR** (121 MHz, CD_2Cl_2): δ 117.5. **HRMS (ESI+)**: calcd for $[M]^+$ = $C_{16}H_{20}P^+$: 243.1303. Found: 243.1310; **HRMS (ESI-)**: calcd for $[M]^-$ = I^-: 126.9050. Found: 126.9046. **Elemental Analysis**: calcd for $C_{16}H_{20}PI$: C 51.91, H 5.45. Found: C 52.07, H 5.57. **ICP-MS**: calcd 1706 ppm (based on 1 mol% CuI_2^- in **2b**), found: 1865 ppm.

iv. Synthesis of phosphonium **2e**

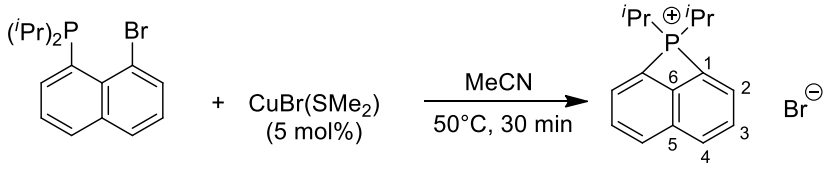


1-Br **2e**

NMR experiment: In a J. Young valve NMR tube, $CuBr(SMe)_2$ (9.5 mg, 0.0464 mmol) was suspended in 0.3 mL of CH_2Cl_2 and a solution of 1-bromo-8-diisopropylphosphinonaphthalene **1-Br** (15.0 mg, 0.0464 mmol) in 0.3 mL of CH_2Cl_2 was added. Color evolved from yellow to light yellow within a few minutes. NMR analysis revealed complete conversion to the phosphonium species in 30 min at room temperature.

HRMS (ESI-): calcd for $[M]^-$ = $CuBr_2^-$: 222.7643. Found: 222.7648;

v. Optimized conditions for the synthesis of phosphonium **2c**



1-Br **2c**

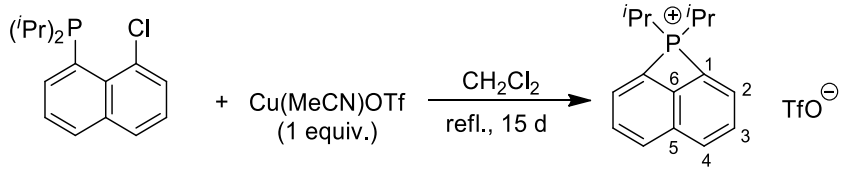
NMR experiment: In a J. Young valve NMR tube, $CuBr(SMe_2)$ (0.47 mg, 0.00232 mmol) was suspended in 0.3 mL of MeCN and a solution of 1-bromo-8-diisopropylphosphinonaphthalene **1-Br** (15.0 mg, 0.0464 mmol) in 0.3 mL of MeCN was added. Color evolved from yellow to light yellow within a few minutes. NMR analysis revealed complete conversion to the phosphonium species in 30 min at 50°C.

Preparative manipulation: 1-bromo-8-diisopropylphosphinonaphthalene **1-Br** (100.0 mg, 0.309 mmol) was suspended in 7 mL of MeCN and a solution of $CuBr(SMe_2)$ (2.8 mg, 0.0155 mmol) in 2 mL of MeCN was added. Color evolved from light yellow to orange and NMR analysis revealed complete conversion to the phosphonium **2c** after 30 min at 50°C. Volatiles

were removed under *vacuo*. The crude product was washed with 3 mL of THF, filtered and dried to afford a beige solid (82.7 mg, 82 %).

MP : 202 °C. **^{1}H NMR** (300 MHz, CD_2Cl_2): δ 8.15 (dd, J_{PH} = 9.0 Hz, $^{3}J_{HH}$ = 6.8 Hz 2H, H_4), 8.09 (dd, J_{PH} = 8.4 Hz, $^{3}J_{HH}$ = 8.4 Hz 2H, H_2),7.81 (td, J_{PH} = 8.5 Hz, $^{3}J_{HH}$ = 6.5 Hz, 2H, H_3), 4.18 (hept d, $^{3}J_{HH}$ = 7.1 Hz, $^{2}J_{PH}$ = 3.7 Hz, 2H, CH*i*Pr), 1.38 (dd, $^{3}J_{PH}$ = 20.15 Hz, $^{3}J_{HH}$ = 7.1 Hz, 12H, CH_3*i*Pr); **^{13}C{^{1}H} NMR** (126 MHz, CD_2Cl_2): δ 151.8 (d, J_{PC} = 4.1 Hz, C_6), 131.3 (d, J_{PC} = 11.4 Hz, C_3), 128.8 (d, J_{PC} = 3.7 Hz, C_2), 128.7 (s, C_4), 127.5 (d, J_{PC} = 83.2 Hz, C_1), 127.1 (d, J_{PC} = 14.9 Hz, C_5), 29.8 (d, $^{1}J_{PC}$ = 30.3 Hz, CH*i*Pr), 18.2 (d, $^{2}J_{PC}$ = 1.3 Hz, CH_3*i*Pr); **^{31}P{^{1}H} NMR** (121 MHz, CD_2Cl_2): δ 113.9. **HRMS (ESI+)**: calcd for $[M]^+ = C_{16}H_{20}P^+$: 243.1303. Found: 243.1314; **MS (DCI-NH_3)**: calcd for $[^{79}Br]^-$ = 78.92 (100%); for $[^{81}Br]^-$ = 80.92 (97.3%). Found: 79.0 (95%); 81.0 (100%). **Elemental Analysis**: calcd for $C_{16}H_{20}PBr$: C 59.46, H 6.24. Found: C 59.86, H 6.58.

vi. Synthesis of phosphonium **2d**



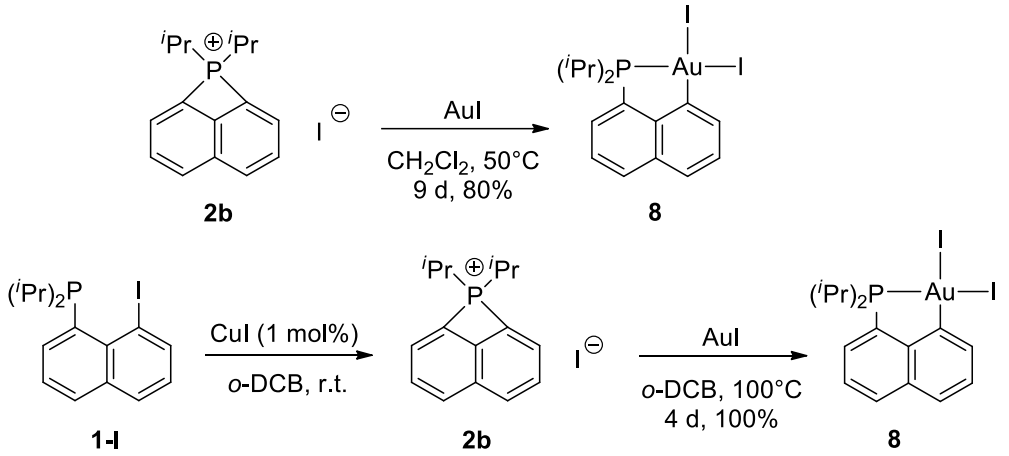
1-Cl **2d**

NMR experiment: In a J. Young valve NMR tube, $Cu(MeCN)_4OTf$ (20.3 mg, 0.0538 mmol) was suspended in 0.3 mL of CH_2Cl_2 and a solution of 1-chloro-8-diisopropylphosphinonaphthalene **1-Cl** (15.0 mg, 0.0538 mmol) in 0.3 mL of CH_2Cl_2 was added. After 15 days of reflux in CH_2Cl_2, ^{31}P NMR spectroscopy revealed complete conversion to the phosphonium **2d**.

^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.15 (dd, J_{PH} = 8.4 Hz, $^{3}J_{HH}$ = 3.7 Hz, 2H, H_4), 8.01 (dd, J_{PH} = 9.2 Hz, $^{3}J_{HH}$ = 6.9 Hz 2H, H_2),7.87 (m, 2H, H_3), 3.57 (hept d, $^{2}J_{PH}$ = 7.1 Hz, $^{3}J_{HH}$ = 1.8 Hz 2H, CH*i*Pr), 1.40 (d, $^{3}J_{PH}$ = 20.7 Hz, $^{3}J_{HH}$ = 7.1 Hz, 12H, CH_3*i*Pr); **^{31}P{^{1}H} NMR** (121 MHz, CD_2Cl_2): δ 118.2. **HRMS (ESI-)**: calcd for $[M]^- = CF_3SO_3^-$: 148.9520 Found : 148.9519.

3. Synthesis of Au(III) complexes

i. Synthesis of (P,C)AuI_2 **8** starting from the phosphonium **2b**

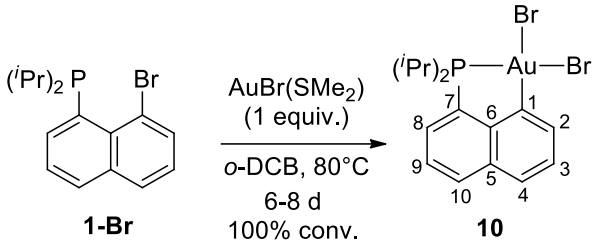


NMR experiment: In a J Young NMR tube, AuI (13 mg, 0.0405 mmol) was suspended in CH_2Cl_2 (0.3 mL) and a solution of phosphonium **2b** (15 mg, 0.0405 mmol) in CH_2Cl_2 (0.3 mL) was added. The reaction mixture was stirred at 50°C. ^{31}P NMR spectroscopy revealed 80% conversion to the gold(III) complex **8**[5] after 9 days.

NMR experiment: In a J. Young valve NMR tube, CuI (1 mol%) was suspended in 0.1 mL of *o*-DCB and a solution of 1-iodo-8-diisopropylphosphinonaphthalene **1-I** (20 mg, 0.054 mmol) in 0.4 mL of *o*-DCB was added. Conversion to the phosphonium **2b** was monitored by ^{31}P NMR spectroscopy. After complete conversion, AuI (17.5 mg, 0.054 mmol) was added in 0.2 mL of *o*-DCB and the reaction mixture was stirred at 100°C. NMR monitoring revealed complete conversion after 4 days.

Preparative manipulation: In a J. Young valve NMR tube, CuI (1 mol%) was suspended in 0.1 mL of *o*-DCB and a solution of 1-iodo-8-diisopropylphosphinonaphthalene **1-I** (100 mg, 0.27 mmol) in 0.4 mL of *o*-DCB was added. Conversion to the phosphonium **2b** was monitored by ^{31}P NMR spectroscopy. After complete conversion, AuI (87.4 mg, 0.27 mmol) was added in 0.2 mL of *o*-DCB and the reaction mixture was stirred at 100°C. NMR monitoring revealed complete conversion after 4 days. The reaction mixture was filtered, concentrated under vacuum and dried to afford the product **8** as an orange powder (154.2 mg, 82 %).

ii. Synthesis of (P,C)$AuBr_2$ **10** starting from the *peri*-bromo phosphine **1-Br**

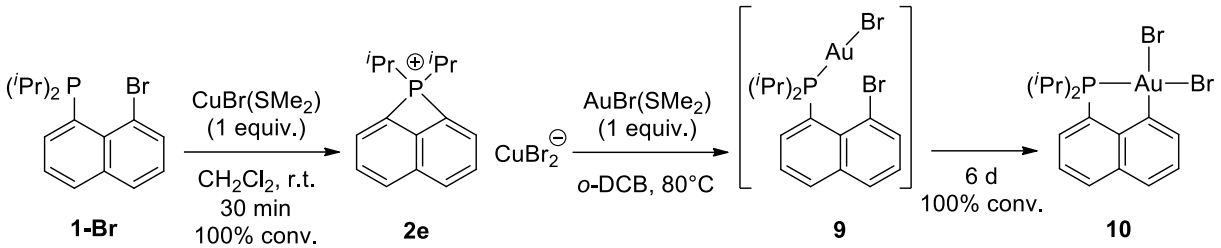


NMR experiment: In a J. Young valve NMR tube, $AuBr(SMe_2)$ (15.7 mg, 0.0464 mmol) was suspended in 0.2 mL of *o*-DCB and a solution of 1-bromo-8-diisopropylphosphinonaphthalene **1-Br** (15 mg, 0.0464 mmol) in 0.4 mL of *o*-DCB was added. The mixture was warmed to 80°C and NMR analysis revealed complete conversion to the product **10** after 6 days.

Preparative manipulation: In a Schlenk tube, $AuBr(SMe_2)$ (52 mg, 0.153 mmol) was suspended in 1 mL of *o*-DCB and a solution of 1-bromo-8-diisopropylphosphinonaphthalene **1-Br** (50 mg, 0.153 mmol) in 1.5 mL of *o*-DCB was added. The mixture was stirred for 8 days at 80°C. Volatiles were removed under vacuum to afford the product **10** as a white solid (86 mg; 93 %).

MP : 250 °C (dec.) **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 9.00 (ddd, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 0.86 Hz, J_{PH} = 2.3 Hz, 1H, H_2), 8.11 (dd, $^3J_{HH}$ = 7.9 Hz, J_{PH} = 3.4 Hz, 1H, H_6), 7.87 (ddd, , $^3J_{HH}$ = 8.1 Hz, $^4J_{HH}$ = 0.55 Hz, J_{PH} = 2.9 Hz, 1H, H_4), 7.80 (ddd, , $^3J_{HH}$ = 7.2 Hz, $^4J_{HH}$ = 0.75 Hz, J_{PH} = 9.9 Hz, 1H, H_{10}), 7.65 (ddd, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 7.4 Hz, J_{PH} = 3.6 Hz, 1H, H_9), 7.51 (dd, $^3J_{HH}$ = 7.9 Hz, 1H, H_3), 3.36 (heptd, $^3J_{HH}$ = 7.1 Hz, $^2J_{PH}$ = 2.3 Hz, 2H, CH*i*Pr), 1.45 (dd, $^3J_{HH}$ = 7.0 Hz, $^2J_{PH}$ = 20.0 Hz, 6H, CH_3*i*Pr), 1.35 (dd, $^3J_{HH}$ = 7.0 Hz, $^2J_{PH}$ = 18.6 Hz, 6H, CH_3*i*Pr); **^{13}C{^{1}H} NMR** (126 MHz, CD_2Cl_2): δ 150.4 (d, J_{PC} = 6.6 Hz, C_1), 147.0 (d, J_{PC} = 24.2 Hz, C_6), 135.8 (d, J_{PC} = 2.3 Hz, C_2), 134.9 (d, J_{PC} = 15.2 Hz, C_5), 133.6 (d, J_{PC} = 2.6 Hz, C_8), 131.2 (d, J_{PC} = 2.3 Hz, C_{10}), 128.7 (s, C_3), 127.6 (s, C_4), 126.4 (d, J_{PC} = 9.7 Hz, C_9), 126.3 (d, J_{PC} = 53.6 Hz, C_7), 29.2 (d, $^1J_{PC}$ = 3.4 Hz, CH*i*Pr), 18.3 (s, CH_3*i*Pr), 17.8 (d, $^2J_{PC}$ = 2.2 Hz, CH_3*i*Pr); **^{31}P{^{1}H} NMR** (121 MHz, CD_2Cl_2): δ 106.1. **HRMS (ESI+)**: calcd for $[M\text{-}Br]^+ = C_{16}H_{20}PAuBr^+$: 519.0152. Found: 519.0148. **Elemental Analysis**: calcd for $C_{16}H_{20}PAuBr_2$: C 32.02, H 3.36. Found: C 32.00, H 3.49.

iii. Synthesis of (P,C)$AuBr_2$ **10** starting from the phosphonium **2e**



NMR experiment: In a J. Young valve NMR tube, the phosphonium **2e** was prepared freshly prior to use: $CuBr(SMe_2)$ (9.5 mg, 0.0464 mmol) was suspended in 0.1 mL of CH_2Cl_2 and a solution of 1-bromo-8-diisopropylphosphinonaphthalene **1-Br** (15 mg, 0.0464 mmol) in 0.4 mL of CH_2Cl_2 was added. After 30 min at r.t., ^{31}P NMR spectroscopy revealed complete conversion to the phosphonium **2e**. Then CH_2Cl_2 was removed and $AuBr(SMe_2)$ (15.7 mg, 0.0464 mmol) was added in 0.5 mL of *o*-DCB and the reaction mixture was stirred at 80°C. NMR analysis that was performed after 1 hour, showed complete consumption of the starting phosphonium **2e**. It also revealed the formation of intermediate **9** (^{31}P NMR resonance signal at δ 53.5 ppm) along with the product **10**. The reaction was continued and complete conversion to complex **10** was reached after 6 days at 80°C.

4. Crystallographic data for complex 6a

Crystallographic data were collected at low temperature (193 K) on a Bruker-AXS APEX II CCD diffractometer equipped with a 30 W air-cooled microfocus source, using MoKα radiation (λ = 0.71073Å). Phi- and omega- scans were used. The data were integrated with SAINT, and an empirical absorption correction with SADABS was applied.[7] The structures were solved using an intrinsic phasing method (SHELXT)[8] and refined using the least-squares method on F^2.[9] All non-H atoms were refined with anisotropic displacement parameters. The H atoms were refined isotropically at calculated positions using a riding model. Some residual electron density due to the presence of disordered solvent were difficult to modelize. Therefore the SQUEEZE function of PLATON[10] was used to eliminate the contribution of the electron density in the solvent region from the intensity data, and the solvent-free model was employed for the final refinement.

CCDC-1998316 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.a-c.uk/data_request/cif.

Selected data for complex 6a : $C_{44}H_{32}CuI_3P_2$, M = 1066.89, monoclinic, space group $P2_1/n$, a = 10.971(2) Å, b = 18.180(3) Å, c = 20.965(3) Å, β = 102.961(7)°, V = 4075.0(12) Å^3, Z = 4, crystal size 0.08 x 0.04 x 0.02 mm^3, 34032 reflections collected (8600 independent, R*int* = 0.0766), 451 parameters, $R1$ [I>2σ(I)] = 0.0414, $wR2$ [all data] = 0.0819, largest diff. peak and hole: 0.624 and –0.566 eÅ^{-3}.

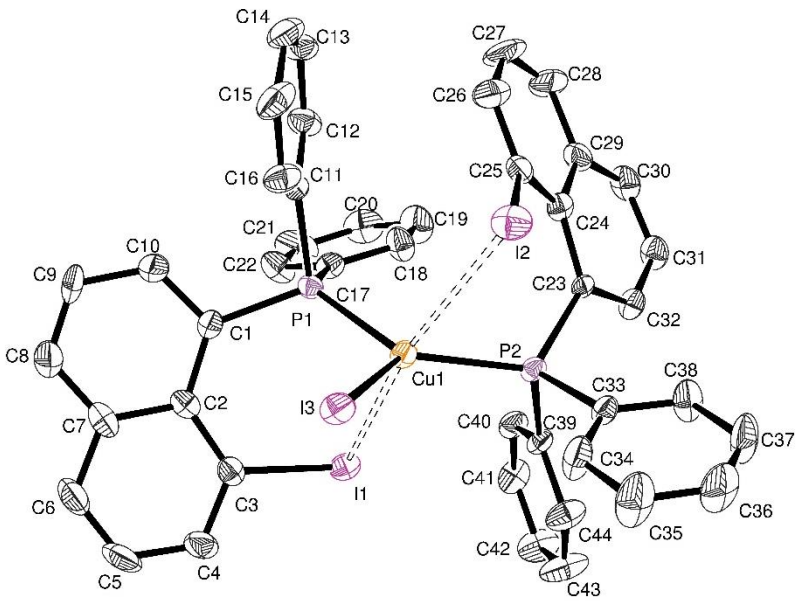


Table S1. Crystal data and structure refinement for complex **6a**.

Identification code	CHB148	
Empirical formula	C44 H32 Cu I3 P2	
Formula weight	1066.89	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.971(2) Å	α= 90°.
	b = 18.180(3) Å	β= 102.961(7)°.
	c = 20.965(3) Å	γ = 90°.
Volume	4075.0(12) $Å^3$	
Z	4	
Density (calculated)	1.739 Mg/m^3	
Absorption coefficient		2.917 mm^{-1}
F(000)	2056	
Crystal size	0.080 x 0.040 x 0.020 mm^3	
Theta range for data collection	4.097 to 26.732°.	
Index ranges	-13<=h<=13, -23<=k<=20, -26<=l<=26	
Reflections collected	34032	
Independent reflections	8600 [R(int) = 0.0766]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6710	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8600 / 0 / 451	
Goodness-of-fit on F^2	0.948	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0705	
R indices (all data)	R1 = 0.0808, wR2 = 0.0819	
Largest diff. peak and hole	0.624 and -0.566 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CHB148. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-96(5)	1093(3)	7003(2)	24(1)
C(2)	-891(5)	489(3)	7092(2)	22(1)
C(3)	-817(5)	45(3)	7660(2)	25(1)
C(4)	-1634(6)	-518(3)	7691(3)	38(2)
C(5)	-2593(6)	-676(4)	7151(3)	54(2)
C(6)	-2692(6)	-298(3)	6590(3)	44(2)
C(7)	-1854(5)	270(3)	6543(3)	33(1)
C(8)	-1951(6)	590(4)	5926(3)	49(2)
C(9)	-1108(7)	1104(4)	5832(3)	57(2)
C(10)	-210(6)	1362(3)	6379(3)	39(2)
C(11)	1045(5)	2514(3)	7249(2)	20(1)
C(12)	2063(5)	2773(3)	7029(3)	31(1)
C(13)	2074(6)	3478(3)	6785(3)	39(2)
C(14)	1073(7)	3940(3)	6746(3)	43(2)
C(15)	29(6)	3686(3)	6957(3)	41(2)
C(16)	21(5)	2986(3)	7206(3)	32(1)
C(17)	2532(5)	1236(3)	7618(2)	24(1)
C(18)	3552(5)	1467(3)	8087(3)	33(1)
C(19)	4761(5)	1248(4)	8085(3)	42(2)
C(20)	4956(6)	776(3)	7601(3)	43(2)
C(21)	3960(6)	524(3)	7135(3)	48(2)
C(22)	2755(5)	754(3)	7140(3)	35(2)
C(23)	3327(5)	2299(3)	9736(2)	19(1)
C(24)	3585(5)	2846(3)	9288(2)	22(1)
C(25)	2706(5)	3329(3)	8884(2)	27(1)
C(26)	3026(6)	3764(3)	8414(3)	41(2)
C(27)	4239(7)	3769(4)	8325(3)	52(2)
C(28)	5152(6)	3384(4)	8734(3)	45(2)
C(29)	4855(5)	2941(3)	9229(3)	30(1)
C(30)	5830(5)	2581(3)	9682(3)	33(1)
C(31)	5575(5)	2149(3)	10167(3)	32(1)
C(32)	4324(5)	1999(3)	10173(2)	24(1)
C(33)	1148(5)	2177(3)	10332(2)	23(1)
C(34)	-113(6)	2142(3)	10287(3)	40(2)
C(35)	-620(6)	2337(4)	10820(3)	59(2)
C(36)	144(6)	2591(4)	11379(3)	51(2)
C(37)	1389(6)	2637(4)	11426(3)	48(2)
C(38)	1908(5)	2430(3)	10912(3)	40(2)
C(39)	2277(5)	902(3)	9939(2)	22(1)
C(40)	3099(5)	500(3)	9654(2)	27(1)
C(41)	3396(5)	-213(3)	9837(3)	32(1)
C(42)	2882(6)	-551(3)	10293(3)	40(2)
C(43)	2044(6)	-169(3)	10572(3)	50(2)
C(44)	1761(5)	555(3)	10397(3)	36(2)
P(1)	1008(1)	1613(1)	7642(1)	19(1)
P(2)	1790(1)	1839(1)	9654(1)	19(1)
Cu(1)	529(1)	1760(1)	8636(1)	22(1)
I(1)	664(1)	101(1)	8493(1)	27(1)
I(2)	923(1)	3518(1)	9057(1)	37(1)
I(3)	-1844(1)	1988(1)	8424(1)	29(1)

Table S3. Bond lengths [Å] and angles [°] for CHB148.

C(1)-C(10)	1.377(7)	C(32)-H(32)	0.9500
C(1)-C(2)	1.441(7)	C(33)-C(34)	1.367(7)
C(1)-P(1)	1.850(5)	C(33)-C(38)	1.389(7)
C(2)-C(3)	1.425(7)	C(33)-P(2)	1.829(5)
C(2)-C(7)	1.434(7)	C(34)-C(35)	1.401(7)
C(3)-C(4)	1.372(7)	C(34)-H(34)	0.9500
C(3)-I(1)	2.104(5)	C(35)-C(36)	1.360(8)
C(4)-C(5)	1.391(8)	C(35)-H(35)	0.9500
C(4)-H(4)	0.9500	C(36)-C(37)	1.350(8)
C(5)-C(6)	1.346(8)	C(36)-H(36)	0.9500
C(5)-H(5)	0.9500	C(37)-C(38)	1.380(7)
C(6)-C(7)	1.400(7)	C(37)-H(37)	0.9500
C(6)-H(6)	0.9500	C(38)-H(38)	0.9500
C(7)-C(8)	1.399(8)	C(39)-C(44)	1.372(7)
C(8)-C(9)	1.361(8)	C(39)-C(40)	1.396(7)
C(8)-H(8)	0.9500	C(39)-P(2)	1.844(5)
C(9)-C(10)	1.413(8)	C(40)-C(41)	1.370(7)
C(9)-H(9)	0.9500	C(40)-H(40)	0.9500
C(10)-H(10)	0.9500	C(41)-C(42)	1.361(7)
C(11)-C(12)	1.383(7)	C(41)-H(41)	0.9500
C(11)-C(16)	1.402(7)	C(42)-C(43)	1.382(8)
C(11)-P(1)	1.837(5)	C(42)-H(42)	0.9500
C(12)-C(13)	1.381(8)	C(43)-C(44)	1.384(8)
C(12)-H(12)	0.9500	C(43)-H(43)	0.9500
C(13)-C(14)	1.371(8)	C(44)-H(44)	0.9500
C(13)-H(13)	0.9500	P(1)-Cu(1)	2.2763(14)
C(14)-C(15)	1.395(8)	P(2)-Cu(1)	2.2723(14)
C(14)-H(14)	0.9500	Cu(1)-I(3)	2.5749(8)
C(15)-C(16)	1.376(7)	Cu(1)-I(2)	3.319(10)
C(15)-H(15)	0.9500	Cu(1)-I(1)	3.0372(9)
C(16)-H(16)	0.9500		
C(17)-C(18)	1.379(7)	C(10)-C(1)-C(2)	117.7(5)
C(17)-C(22)	1.393(7)	C(10)-C(1)-P(1)	114.3(4)
C(17)-P(1)	1.819(5)	C(2)-C(1)-P(1)	127.8(4)
C(18)-C(19)	1.386(7)	C(3)-C(2)-C(7)	114.1(5)
C(18)-H(18)	0.9500	C(3)-C(2)-C(1)	128.1(5)
C(19)-C(20)	1.383(8)	C(7)-C(2)-C(1)	117.8(5)
C(19)-H(19)	0.9500	C(4)-C(3)-C(2)	123.1(5)
C(20)-C(21)	1.370(8)	C(4)-C(3)-I(1)	112.8(4)
C(20)-H(20)	0.9500	C(2)-C(3)-I(1)	123.7(4)
C(21)-C(22)	1.389(8)	C(3)-C(4)-C(5)	119.9(6)
C(21)-H(21)	0.9500	C(3)-C(4)-H(4)	120.1
C(22)-H(22)	0.9500	C(5)-C(4)-H(4)	120.1
C(23)-C(32)	1.374(6)	C(6)-C(5)-C(4)	120.3(6)
C(23)-C(24)	1.438(7)	C(6)-C(5)-H(5)	119.9
C(23)-P(2)	1.855(5)	C(4)-C(5)-H(5)	119.9
C(24)-C(25)	1.433(7)	C(5)-C(6)-C(7)	120.8(6)
C(24)-C(29)	1.436(7)	C(5)-C(6)-H(6)	119.6
C(25)-C(26)	1.369(7)	C(7)-C(6)-H(6)	119.6
C(25)-I(2)	2.097(5)	C(6)-C(7)-C(8)	117.2(5)
C(26)-C(27)	1.385(8)	C(6)-C(7)-C(2)	121.6(5)
C(26)-H(26)	0.9500	C(8)-C(7)-C(2)	121.1(5)
C(27)-C(28)	1.358(8)	C(9)-C(8)-C(7)	120.4(6)
C(27)-H(27)	0.9500	C(9)-C(8)-H(8)	119.8
C(28)-C(29)	1.409(7)	C(7)-C(8)-H(8)	119.8
C(28)-H(28)	0.9500	C(8)-C(9)-C(10)	118.9(6)
C(29)-C(30)	1.421(7)	C(8)-C(9)-H(9)	120.5
C(30)-C(31)	1.361(7)	C(10)-C(9)-H(9)	120.5
C(30)-H(30)	0.9500	C(1)-C(10)-C(9)	123.5(6)
C(31)-C(32)	1.403(7)	C(1)-C(10)-H(10)	118.3
C(31)-H(31)	0.9500	C(9)-C(10)-H(10)	118.3

C(12)-C(11)-C(16)	117.7(5)	C(32)-C(31)-H(31)	120.5
C(12)-C(11)-P(1)	123.6(4)	C(23)-C(32)-C(31)	123.4(5)
C(16)-C(11)-P(1)	118.5(4)	C(23)-C(32)-H(32)	118.3
C(11)-C(12)-C(13)	121.0(5)	C(31)-C(32)-H(32)	118.3
C(11)-C(12)-H(12)	119.5	C(34)-C(33)-C(38)	118.4(5)
C(13)-C(12)-H(12)	119.5	C(34)-C(33)-P(2)	119.4(4)
C(14)-C(13)-C(12)	121.1(6)	C(38)-C(33)-P(2)	122.1(4)
C(14)-C(13)-H(13)	119.4	C(33)-C(34)-C(35)	120.7(5)
C(12)-C(13)-H(13)	119.4	C(33)-C(34)-H(34)	119.7
C(13)-C(14)-C(15)	118.8(6)	C(35)-C(34)-H(34)	119.7
C(13)-C(14)-H(14)	120.6	C(36)-C(35)-C(34)	119.7(6)
C(15)-C(14)-H(14)	120.6	C(36)-C(35)-H(35)	120.1
C(16)-C(15)-C(14)	120.1(6)	C(34)-C(35)-H(35)	120.1
C(16)-C(15)-H(15)	119.9	C(37)-C(36)-C(35)	120.1(6)
C(14)-C(15)-H(15)	119.9	C(37)-C(36)-H(36)	120.0
C(15)-C(16)-C(11)	121.2(5)	C(35)-C(36)-H(36)	120.0
C(15)-C(16)-H(16)	119.4	C(36)-C(37)-C(38)	121.0(6)
C(11)-C(16)-H(16)	119.4	C(36)-C(37)-H(37)	119.5
C(18)-C(17)-C(22)	117.4(5)	C(38)-C(37)-H(37)	119.5
C(18)-C(17)-P(1)	118.0(4)	C(37)-C(38)-C(33)	120.1(5)
C(22)-C(17)-P(1)	124.5(4)	C(37)-C(38)-H(38)	119.9
C(17)-C(18)-C(19)	122.3(5)	C(33)-C(38)-H(38)	119.9
C(17)-C(18)-H(18)	118.9	C(44)-C(39)-C(40)	117.8(5)
C(19)-C(18)-H(18)	118.9	C(44)-C(39)-P(2)	121.1(4)
C(20)-C(19)-C(18)	119.1(6)	C(40)-C(39)-P(2)	120.9(4)
C(20)-C(19)-H(19)	120.4	C(41)-C(40)-C(39)	120.8(5)
C(18)-C(19)-H(19)	120.4	C(41)-C(40)-H(40)	119.6
C(21)-C(20)-C(19)	120.0(6)	C(39)-C(40)-H(40)	119.6
C(21)-C(20)-H(20)	120.0	C(42)-C(41)-C(40)	120.9(5)
C(19)-C(20)-H(20)	120.0	C(42)-C(41)-H(41)	119.6
C(20)-C(21)-C(22)	120.2(6)	C(40)-C(41)-H(41)	119.6
C(20)-C(21)-H(21)	119.9	C(41)-C(42)-C(43)	119.4(5)
C(22)-C(21)-H(21)	119.9	C(41)-C(42)-H(42)	120.3
C(21)-C(22)-C(17)	121.0(6)	C(43)-C(42)-H(42)	120.3
C(21)-C(22)-H(22)	119.5	C(42)-C(43)-C(44)	119.7(5)
C(17)-C(22)-H(22)	119.5	C(42)-C(43)-H(43)	120.1
C(32)-C(23)-C(24)	117.8(5)	C(44)-C(43)-H(43)	120.1
C(32)-C(23)-P(2)	117.0(4)	C(39)-C(44)-C(43)	121.4(5)
C(24)-C(23)-P(2)	124.0(4)	C(39)-C(44)-H(44)	119.3
C(25)-C(24)-C(29)	114.4(5)	C(43)-C(44)-H(44)	119.3
C(25)-C(24)-C(23)	127.2(5)	C(17)-P(1)-C(11)	102.2(2)
C(29)-C(24)-C(23)	118.4(5)	C(17)-P(1)-C(1)	104.1(2)
C(26)-C(25)-C(24)	122.2(5)	C(11)-P(1)-C(1)	102.0(2)
C(26)-C(25)-I(2)	115.4(4)	C(17)-P(1)-Cu(1)	118.09(17)
C(24)-C(25)-I(2)	121.9(4)	C(11)-P(1)-Cu(1)	109.82(16)
C(25)-C(26)-C(27)	120.6(6)	C(1)-P(1)-Cu(1)	118.29(17)
C(25)-C(26)-H(26)	119.7	C(33)-P(2)-C(39)	101.1(2)
C(27)-C(26)-H(26)	119.7	C(33)-P(2)-C(23)	106.1(2)
C(28)-C(27)-C(26)	120.5(6)	C(39)-P(2)-C(23)	101.3(2)
C(28)-C(27)-H(27)	119.8	C(33)-P(2)-Cu(1)	119.48(18)
C(26)-C(27)-H(27)	119.8	C(39)-P(2)-Cu(1)	108.46(17)
C(27)-C(28)-C(29)	120.0(6)	C(23)-P(2)-Cu(1)	117.73(15)
C(27)-C(28)-H(28)	120.0	P(2)-Cu(1)-P(1)	130.58(6)
C(29)-C(28)-H(28)	120.0	P(2)-Cu(1)-I(3)	122.07(4)
C(28)-C(29)-C(30)	119.4(5)	P(1)-Cu(1)-I(3)	107.01(4)
C(28)-C(29)-C(24)	121.4(5)	P(2)-Cu(1)-I(1)	97.08(4)
C(30)-C(29)-C(24)	119.2(5)	P(1)-Cu(1)-I(1)	76.55(4)
C(31)-C(30)-C(29)	120.9(5)	I(3)-Cu(1)-I(1)	102.29(2)
C(31)-C(30)-H(30)	119.5	C(3)-I(1)-Cu(1)	94.84(14)
C(29)-C(30)-H(30)	119.5	I(1)-Cu-I(2)	167.49(4)
C(30)-C(31)-C(32)	119.0(5)		
C(30)-C(31)-H(31)	120.5		

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for CHB148. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(3)	27(3)	19(3)	0(2)	4(2)	1(2)
C(2)	16(3)	23(3)	30(3)	-6(3)	10(2)	1(2)
C(3)	23(3)	27(3)	25(3)	-6(3)	8(2)	-2(2)
C(4)	43(4)	42(4)	34(4)	-11(3)	22(3)	-20(3)
C(5)	51(5)	61(5)	54(5)	-13(4)	22(4)	-40(4)
C(6)	32(4)	55(4)	42(4)	-13(3)	4(3)	-20(3)
C(7)	25(3)	31(4)	40(4)	-8(3)	1(3)	-5(3)
C(8)	56(5)	46(4)	35(4)	6(3)	-12(3)	-15(4)
C(9)	76(5)	60(5)	20(3)	7(3)	-18(3)	-22(4)
C(10)	57(4)	29(4)	28(3)	2(3)	4(3)	-14(3)
C(11)	22(3)	23(3)	15(3)	0(2)	6(2)	-3(2)
C(12)	32(3)	29(3)	36(3)	-4(3)	16(3)	-7(3)
C(13)	51(4)	38(4)	35(4)	-1(3)	23(3)	-17(3)
C(14)	82(5)	26(4)	24(3)	3(3)	18(3)	-4(4)
C(15)	68(5)	33(4)	25(3)	4(3)	17(3)	12(3)
C(16)	37(4)	34(4)	31(3)	5(3)	18(3)	-1(3)
C(17)	20(3)	28(3)	25(3)	2(3)	10(2)	2(2)
C(18)	21(3)	45(4)	34(3)	-11(3)	9(3)	-5(3)
C(19)	18(3)	64(5)	46(4)	-5(4)	9(3)	-1(3)
C(20)	23(3)	50(4)	59(4)	12(4)	13(3)	11(3)
C(21)	42(4)	41(4)	69(5)	-12(4)	35(4)	2(3)
C(22)	29(3)	34(4)	46(4)	-12(3)	17(3)	-5(3)
C(23)	19(3)	26(3)	14(2)	-2(2)	9(2)	-4(2)
C(24)	21(3)	27(3)	21(3)	-4(2)	10(2)	1(2)
C(25)	29(3)	29(3)	25(3)	-7(3)	9(2)	-11(3)
C(26)	46(4)	37(4)	38(4)	12(3)	9(3)	-6(3)
C(27)	56(5)	65(5)	40(4)	25(4)	21(4)	-16(4)
C(28)	41(4)	59(5)	40(4)	10(3)	22(3)	-18(3)
C(29)	24(3)	34(3)	31(3)	-4(3)	8(2)	-10(3)
C(30)	16(3)	46(4)	37(3)	-7(3)	5(3)	-3(3)
C(31)	20(3)	42(4)	30(3)	-2(3)	0(2)	0(3)
C(32)	20(3)	32(3)	21(3)	1(2)	3(2)	6(3)
C(33)	25(3)	29(3)	17(3)	0(2)	7(2)	1(2)
C(34)	33(4)	65(5)	22(3)	-6(3)	5(3)	3(3)
C(35)	34(4)	109(7)	39(4)	-16(4)	16(3)	2(4)
C(36)	40(4)	87(6)	36(4)	-16(4)	26(3)	1(4)
C(37)	46(4)	73(5)	26(3)	-21(3)	10(3)	-1(4)
C(38)	20(3)	71(5)	31(3)	-20(3)	15(3)	-8(3)
C(39)	20(3)	27(3)	17(3)	6(2)	4(2)	2(2)
C(40)	25(3)	36(4)	24(3)	2(3)	11(2)	0(3)
C(41)	36(4)	33(4)	30(3)	1(3)	10(3)	14(3)
C(42)	48(4)	24(3)	52(4)	15(3)	17(3)	18(3)
C(43)	68(5)	39(4)	57(4)	18(3)	43(4)	10(4)
C(44)	48(4)	30(4)	37(4)	6(3)	27(3)	12(3)
P(1)	17(1)	20(1)	21(1)	0(1)	5(1)	-1(1)
P(2)	16(1)	25(1)	17(1)	3(1)	5(1)	1(1)
Cu(1)	17(1)	30(1)	20(1)	2(1)	5(1)	0(1)
I(1)	31(1)	24(1)	28(1)	6(1)	8(1)	3(1)
I(2)	30(1)	33(1)	46(1)	10(1)	6(1)	7(1)
I(3)	17(1)	39(1)	32(1)	8(1)	7(1)	2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for CHB148.

	x	y	z	U(eq)
H(4)	-1544	-800	8080	45
H(5)	-3181	-1051	7179	64
H(6)	-3339	-417	6221	53
H(8)	-2610	446	5571	59
H(9)	-1123	1287	5406	68
H(10)	345	1741	6312	46
H(12)	2765	2462	7047	37
H(13)	2788	3645	6641	47
H(14)	1089	4424	6578	52
H(15)	-677	3997	6929	49
H(16)	-692	2821	7351	39
H(18)	3422	1789	8423	40
H(19)	5447	1419	8413	51
H(20)	5781	626	7590	52
H(21)	4093	191	6809	57
H(22)	2072	581	6812	42
H(26)	2409	4066	8146	49
H(27)	4434	4044	7976	63
H(28)	5992	3413	8686	54
H(30)	6672	2642	9646	40
H(31)	6235	1953	10496	38
H(32)	4158	1671	10497	29
H(34)	-651	1983	9891	48
H(35)	-1493	2292	10791	71
H(36)	-199	2736	11738	62
H(37)	1916	2814	11819	58
H(38)	2787	2461	10954	47
H(40)	3458	723	9330	33
H(41)	3967	-476	9642	39
H(42)	3099	-1044	10419	49
H(43)	1663	-403	10883	60
H(44)	1198	818	10597	43

5. NMR Spectra

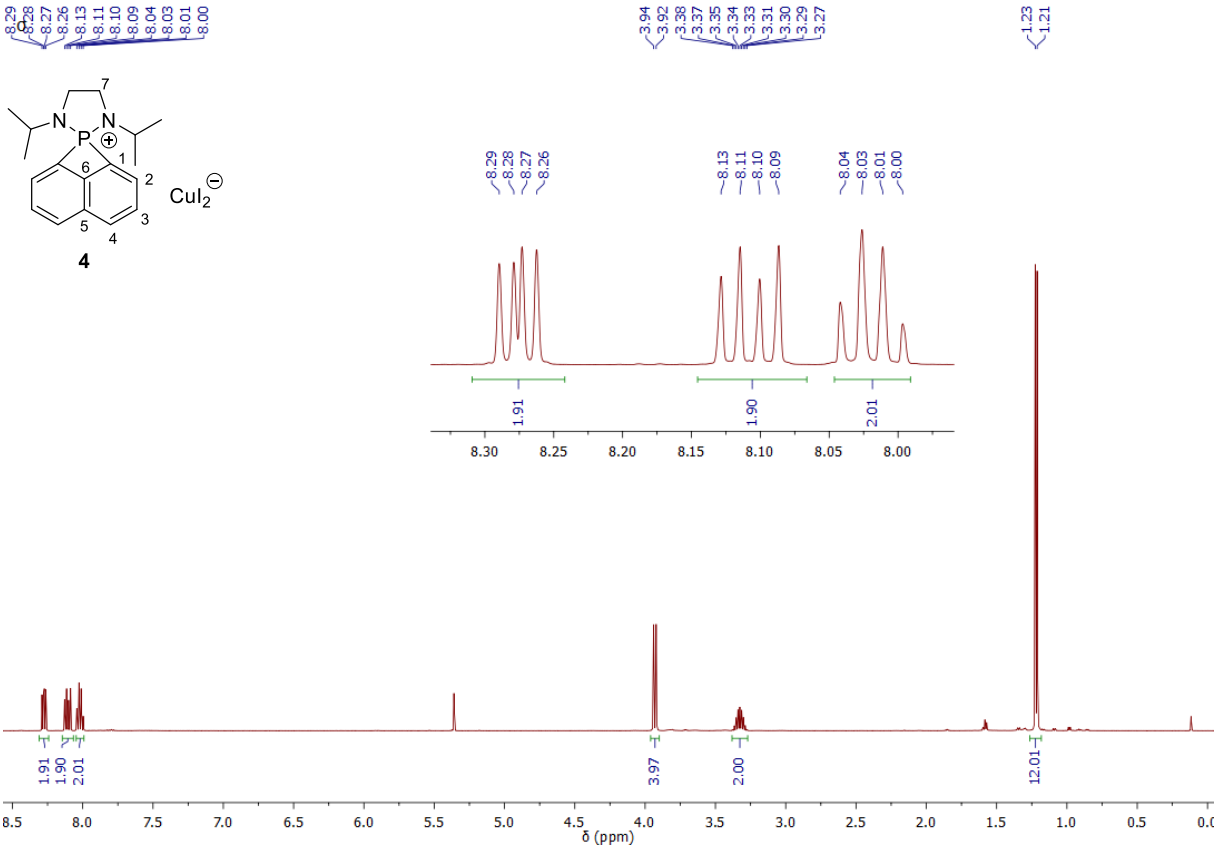


Figure S1: ^{1}H NMR spectrum of **4** in CD_2Cl_2

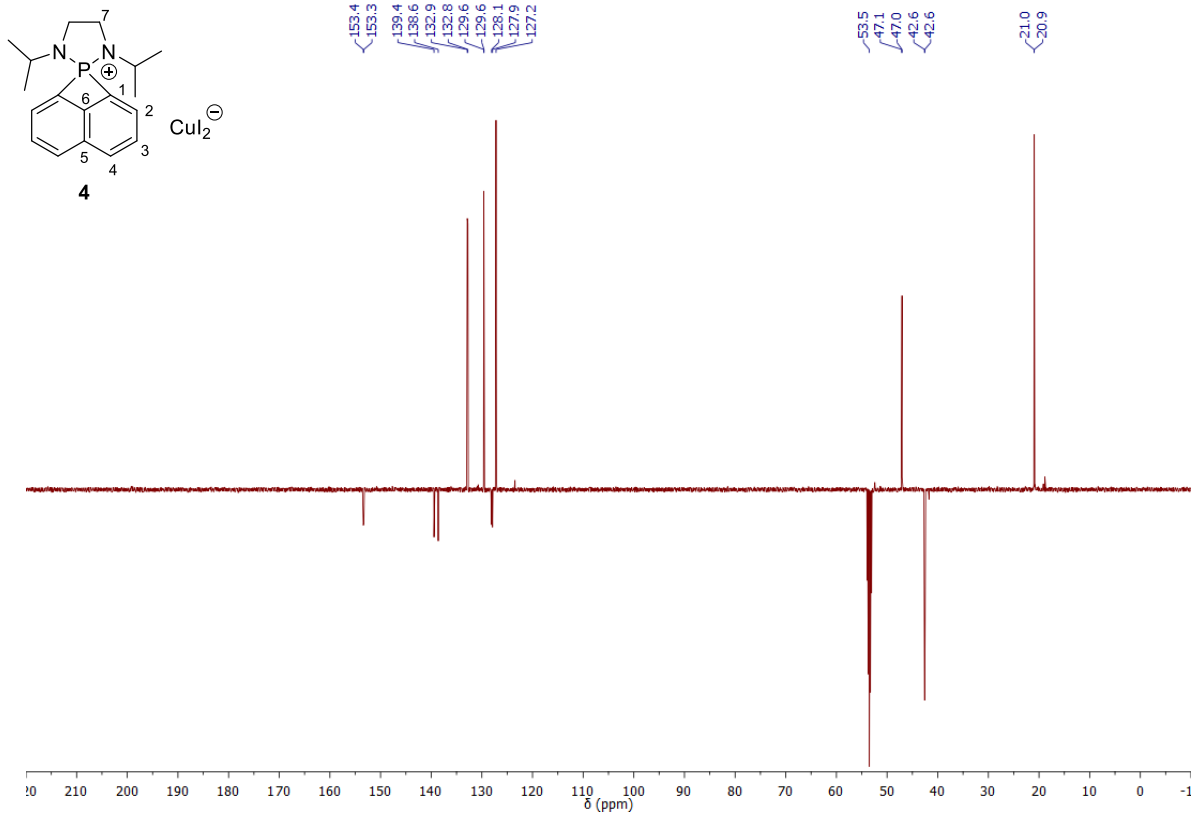


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2

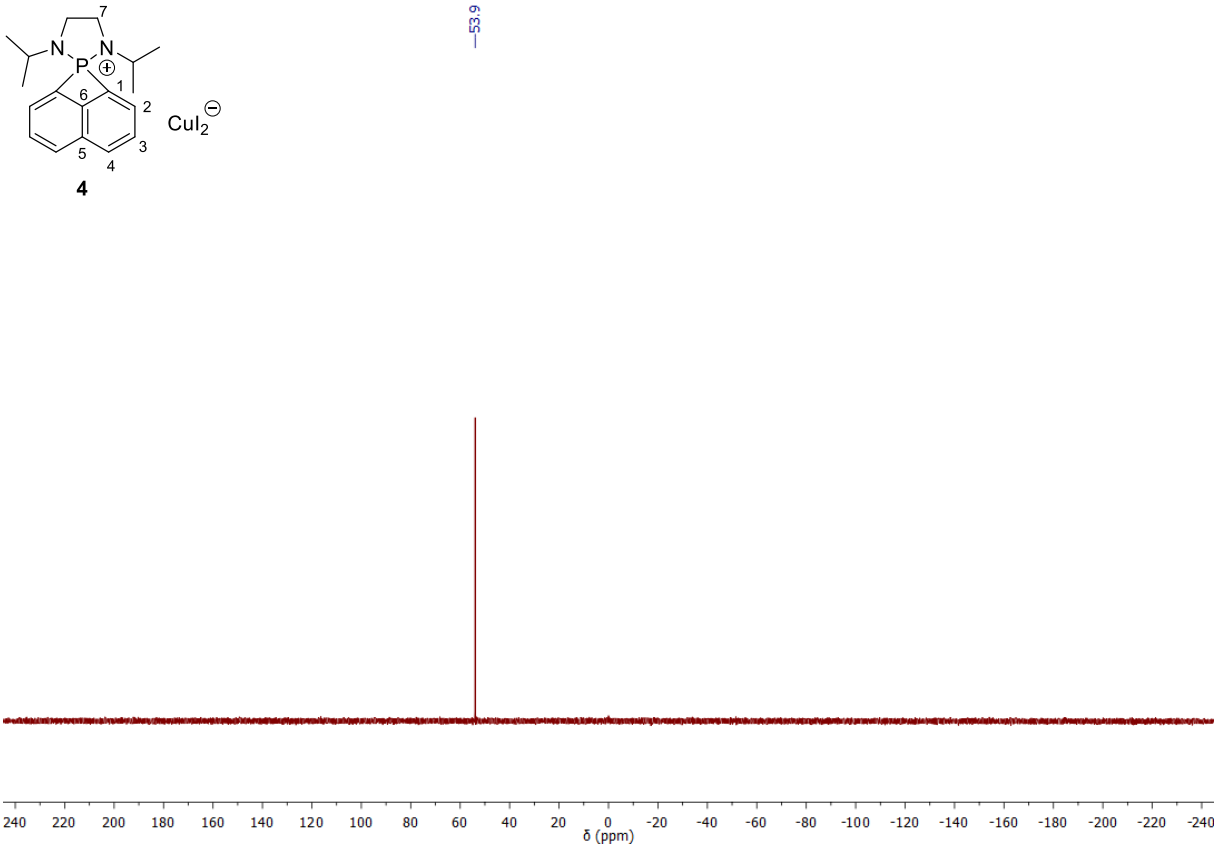
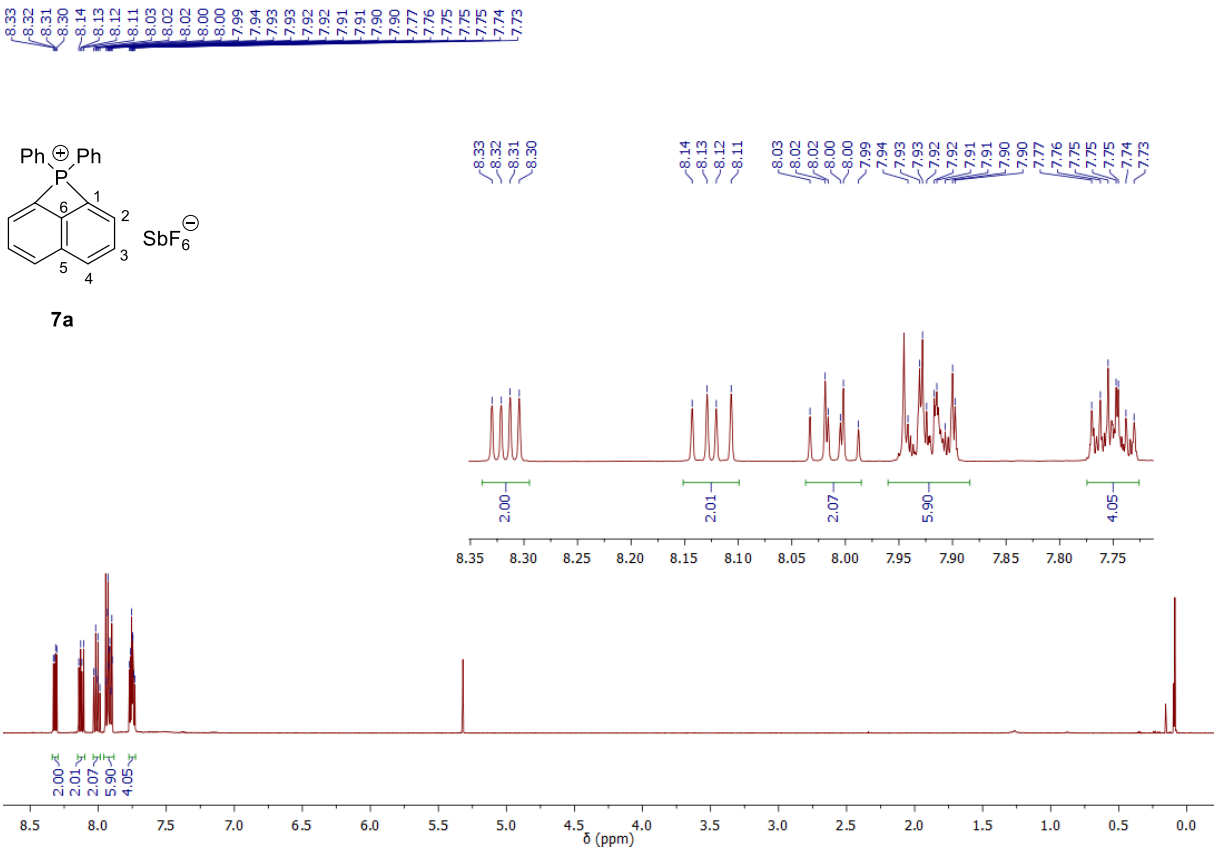


Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2



7a

Figure S4: ^{1}H NMR spectrum of **7a** in CD_2Cl_2

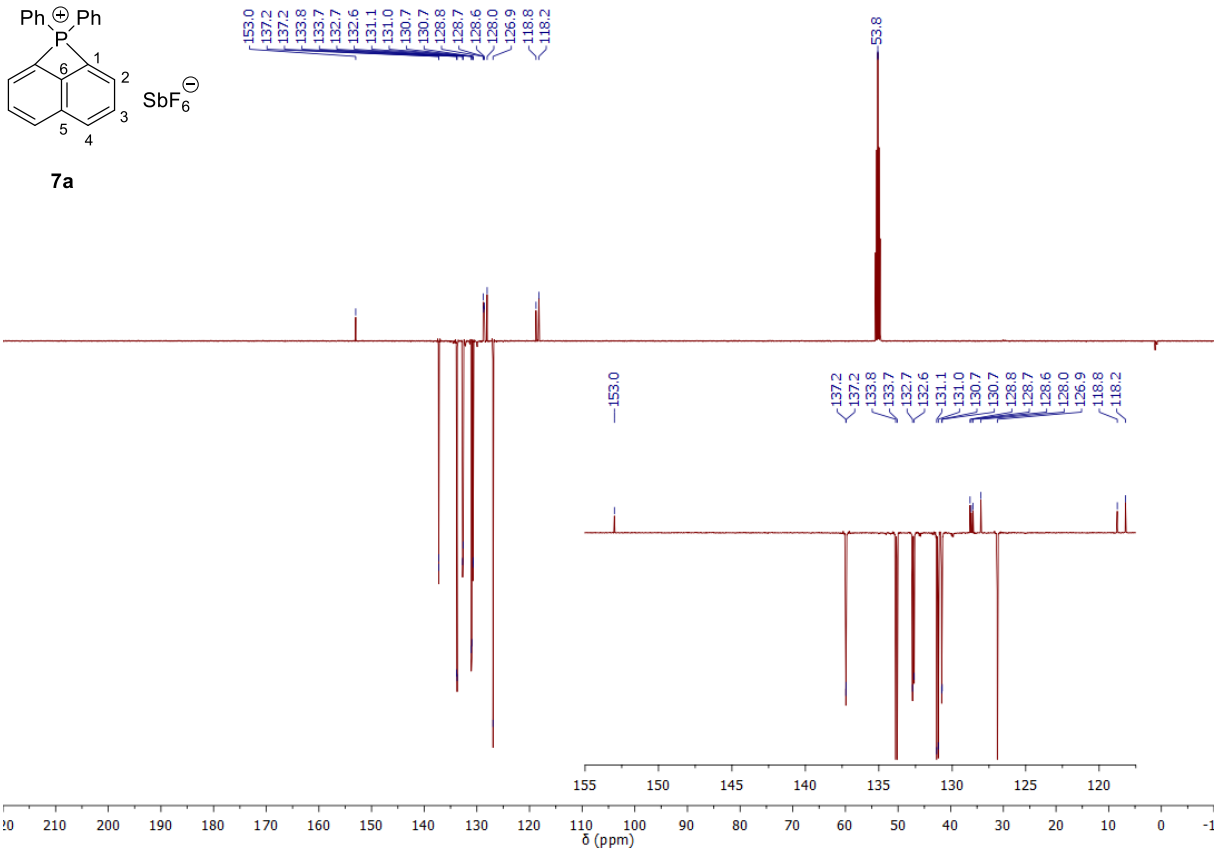


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **7a** in CD_2Cl_2

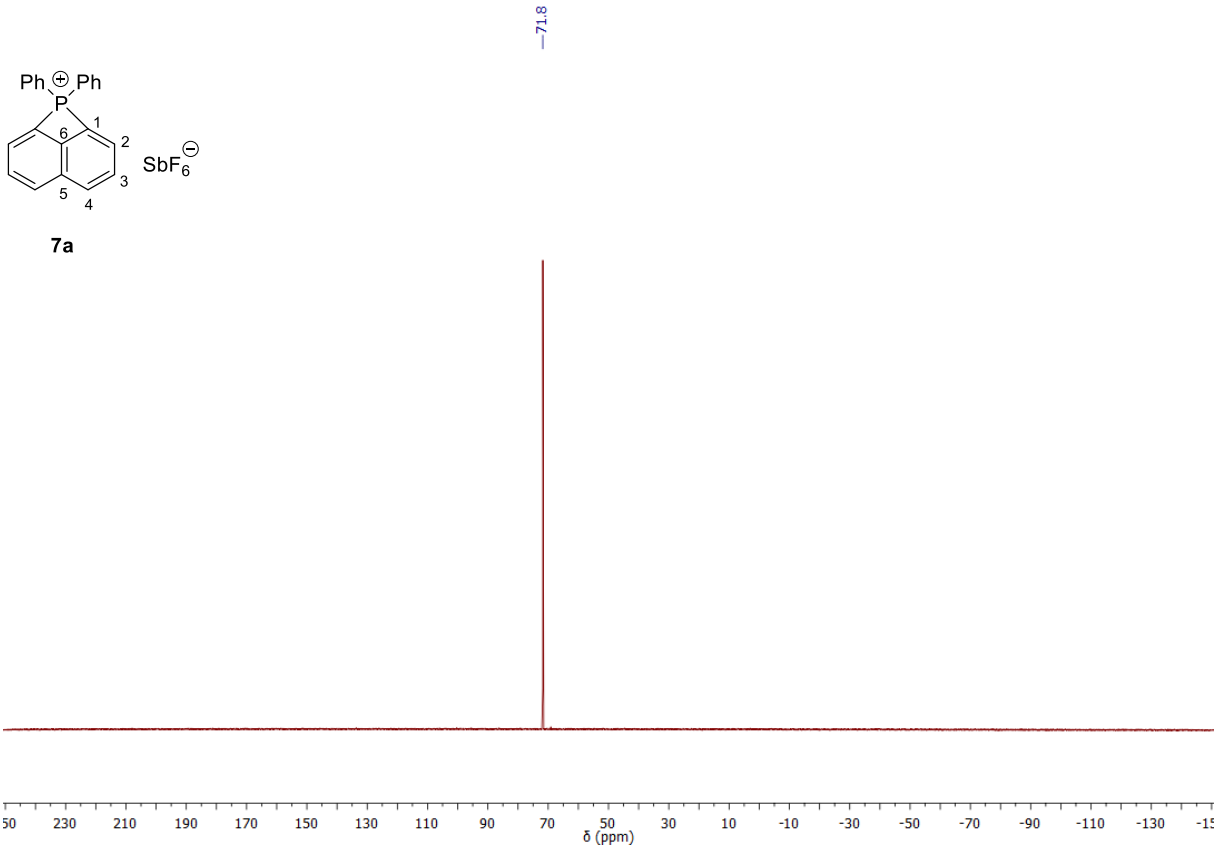


Figure S6: $^{31}P\{^{1}H\}$ NMR spectrum of **7a** in CD_2Cl_2

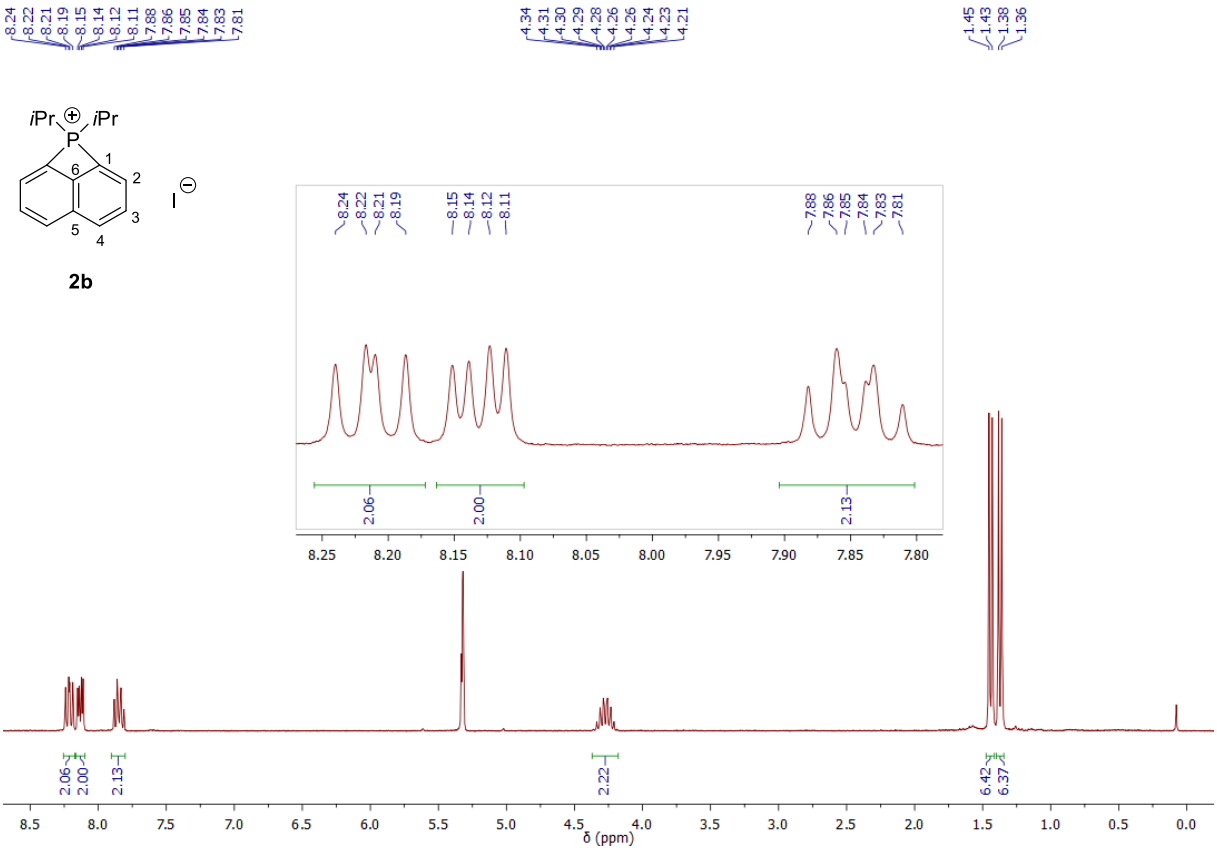


Figure S7: ^{1}H NMR spectrum of **2b** in CD_2Cl_2

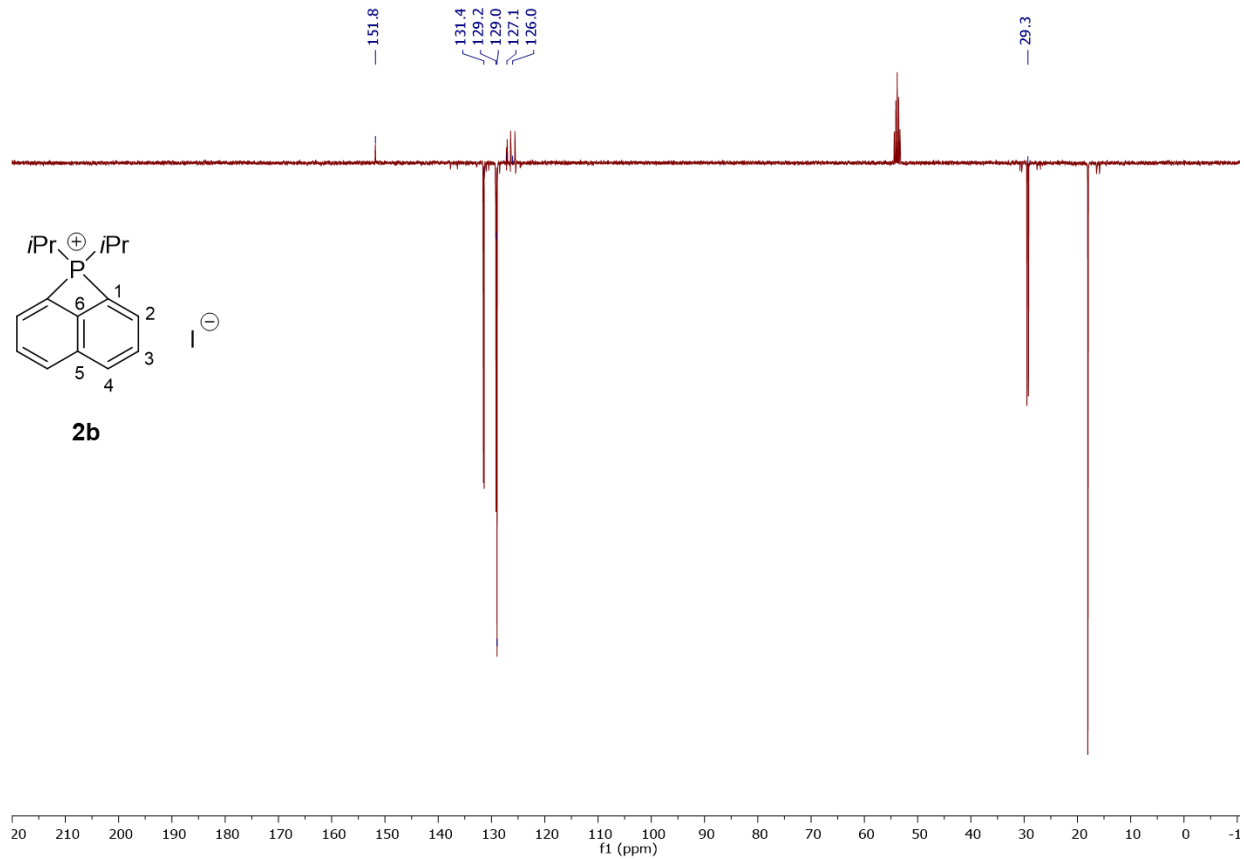


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of **2b** in CD_2Cl_2

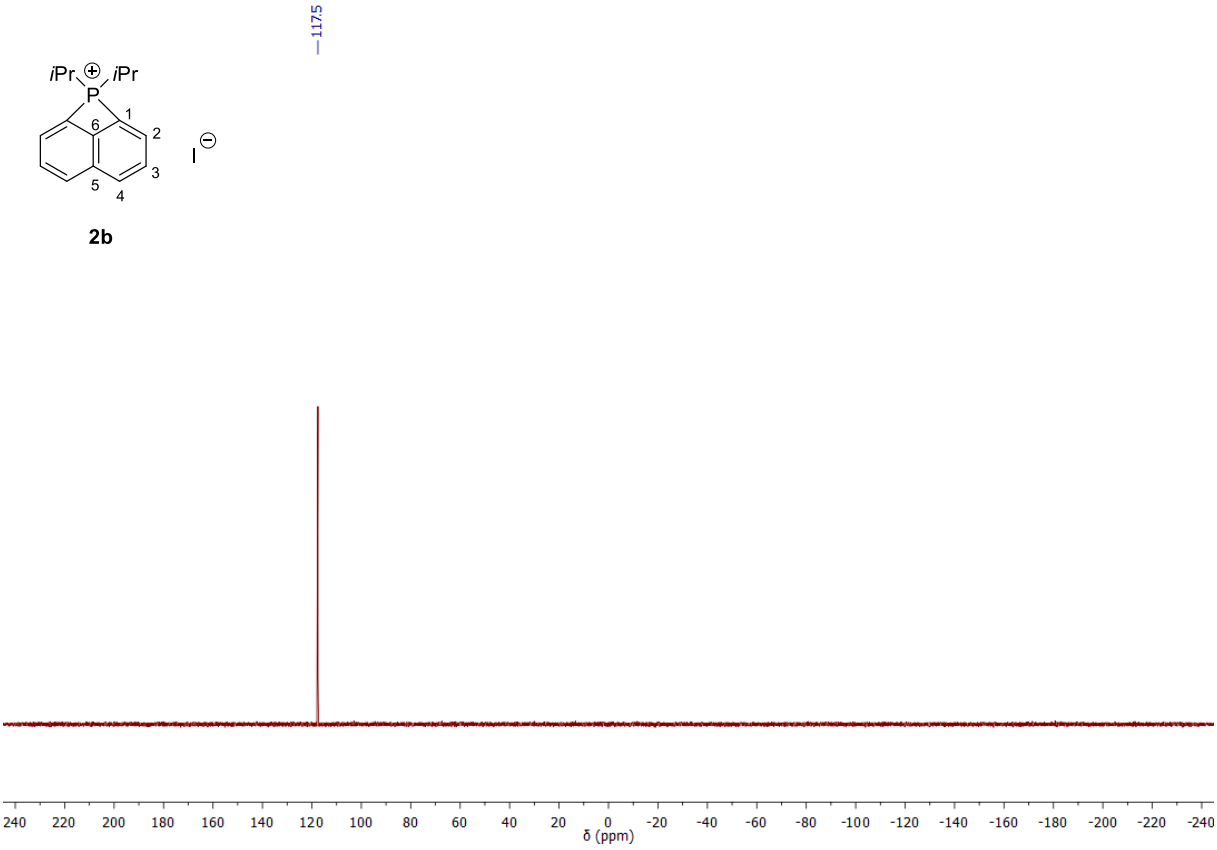


Figure S9: $^{31}P\{^{1}H\}$ NMR spectrum of **2b** in CD_2Cl_2

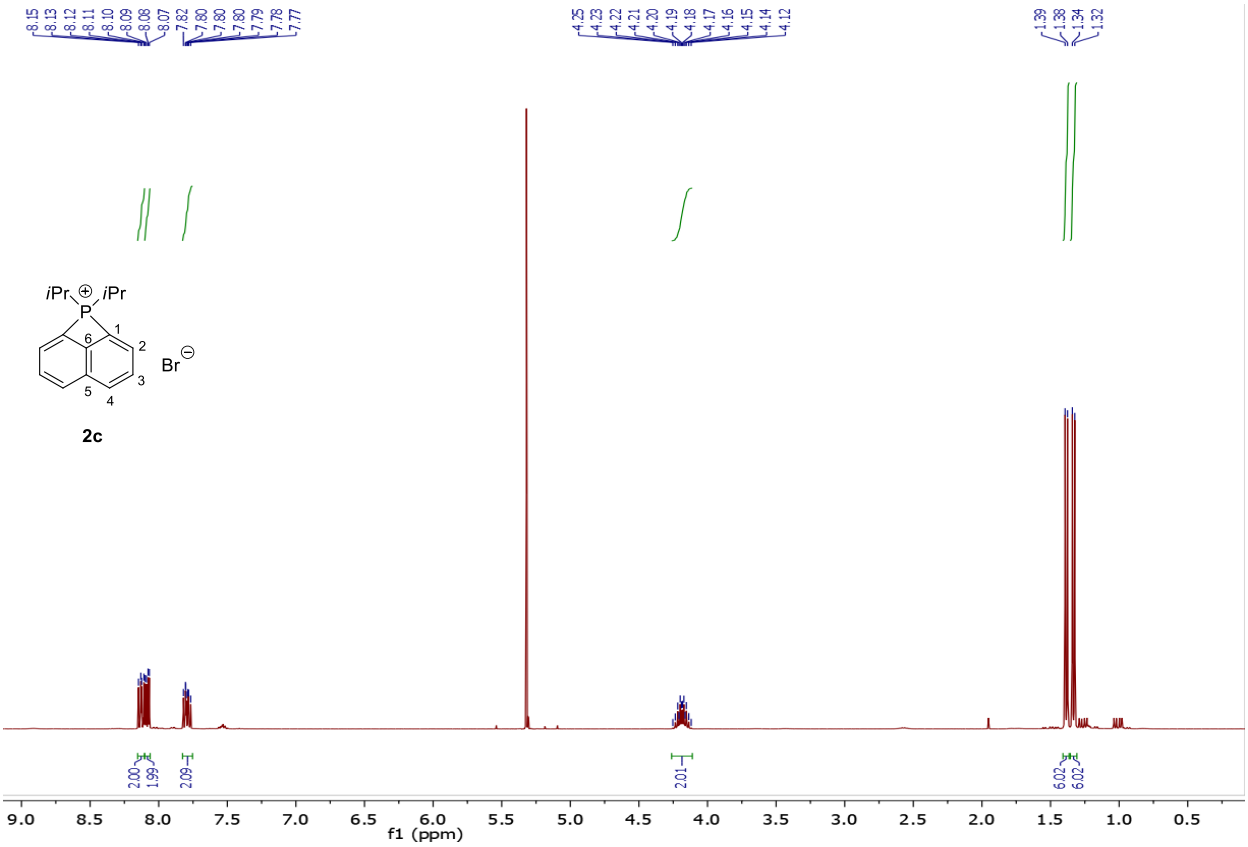


Figure S10: ^{1}H NMR spectrum of **2c** in CD_2Cl_2

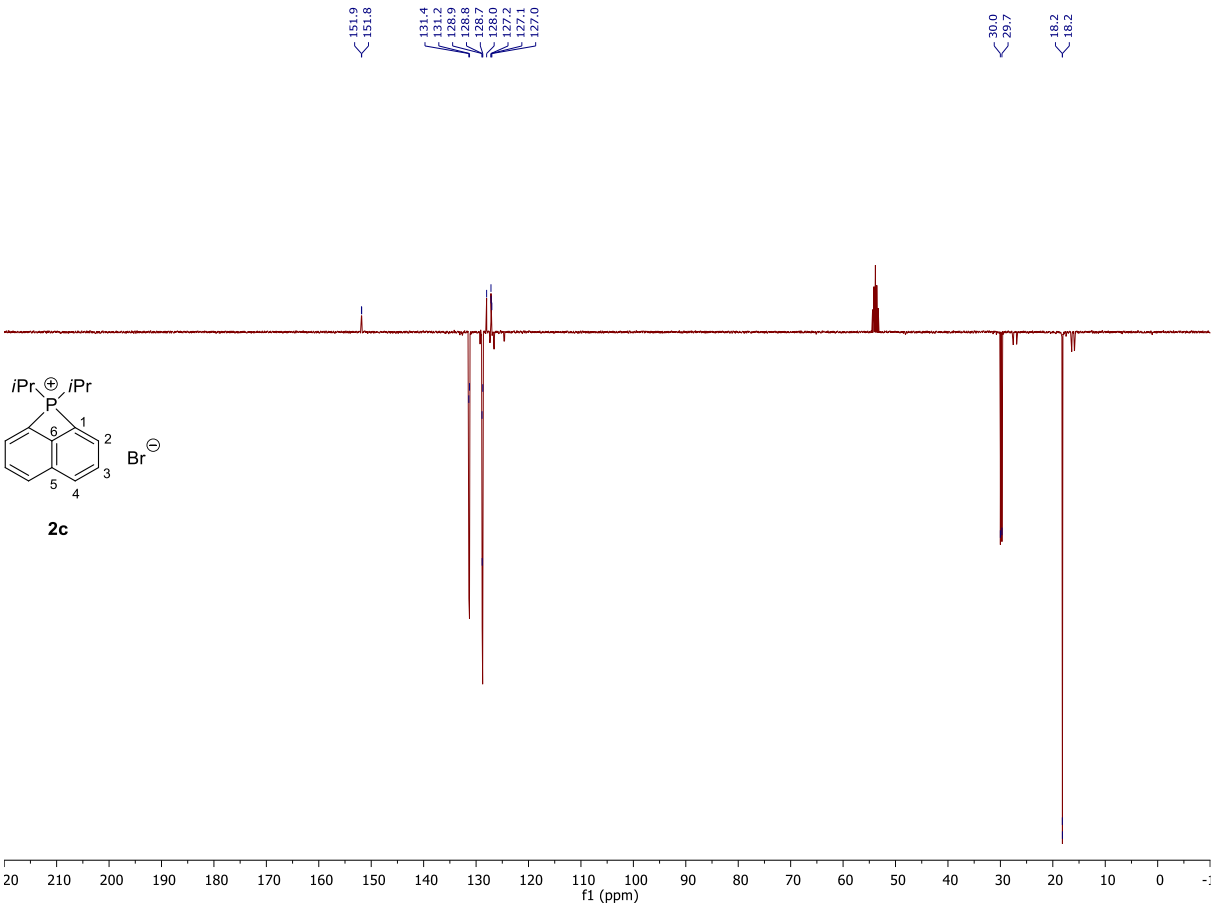


Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum of **2c** in CD_2Cl_2

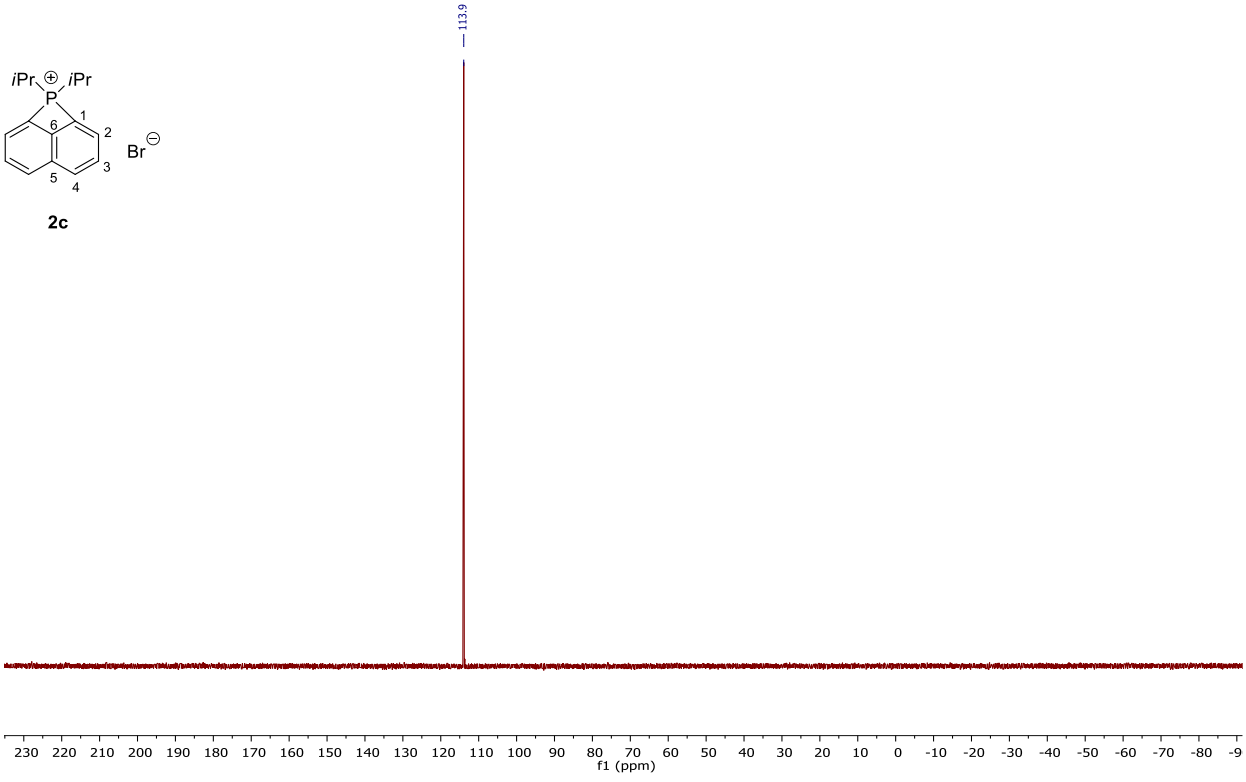


Figure S12: $^{31}P\{^{1}H\}$ NMR spectrum of **2c** in CD_2Cl_2

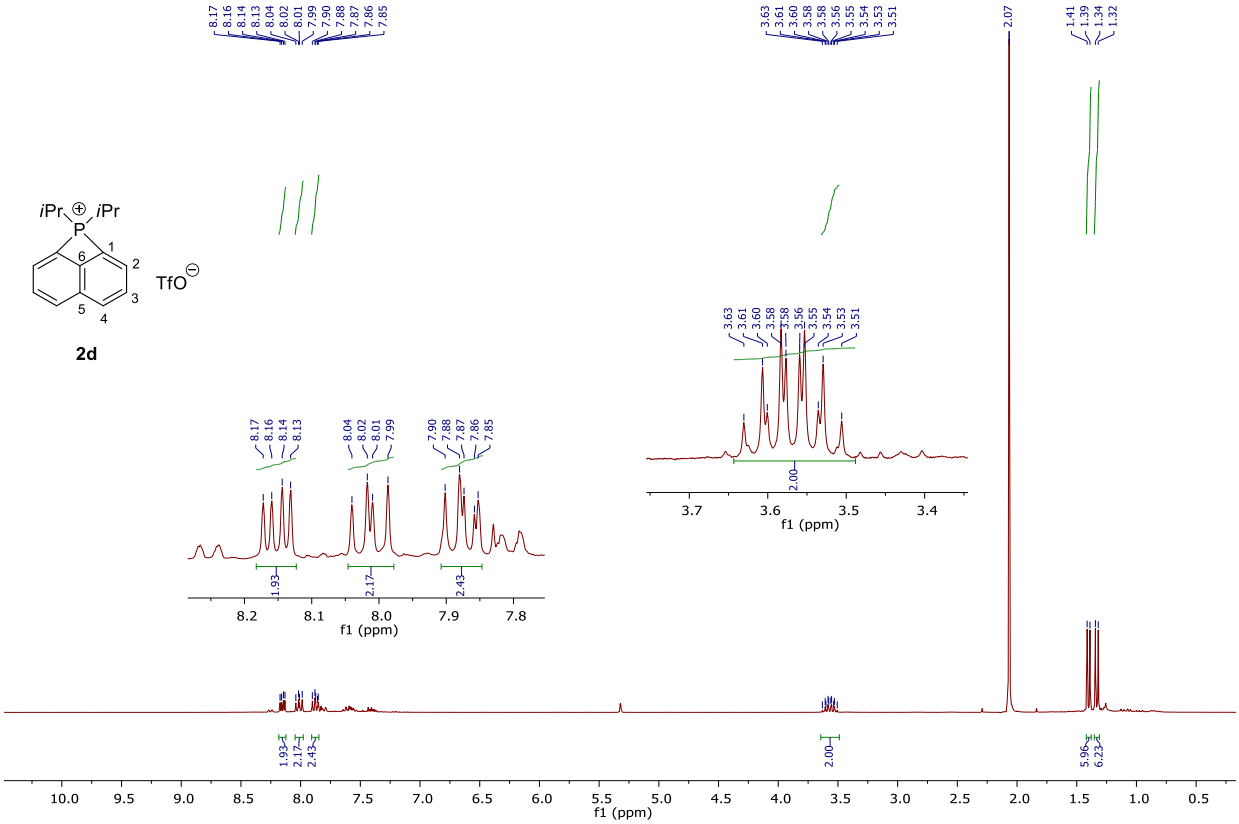


Figure S13: ^{1}H NMR spectrum of **2d** in CD_2Cl_2

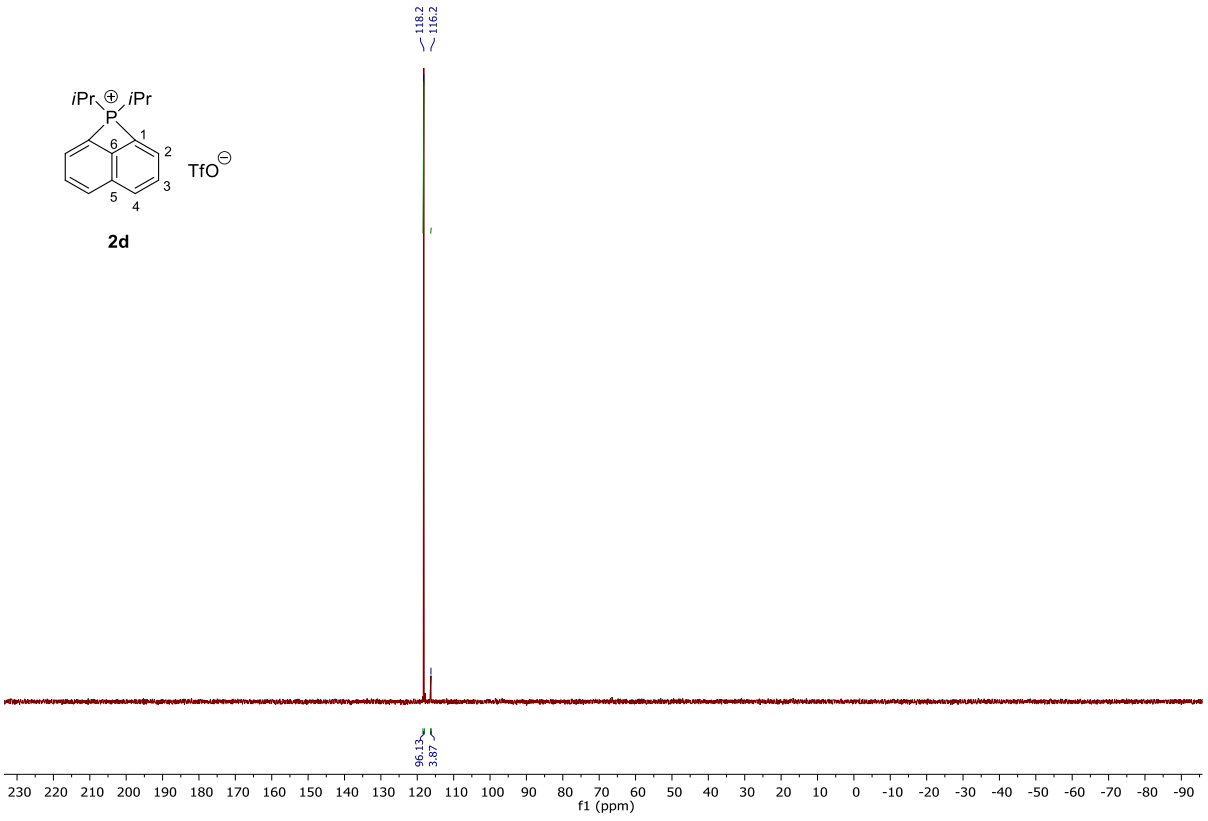


Figure S14: $^{31}P\{^{1}H\}$ NMR spectrum of **2d** in CD_2Cl_2

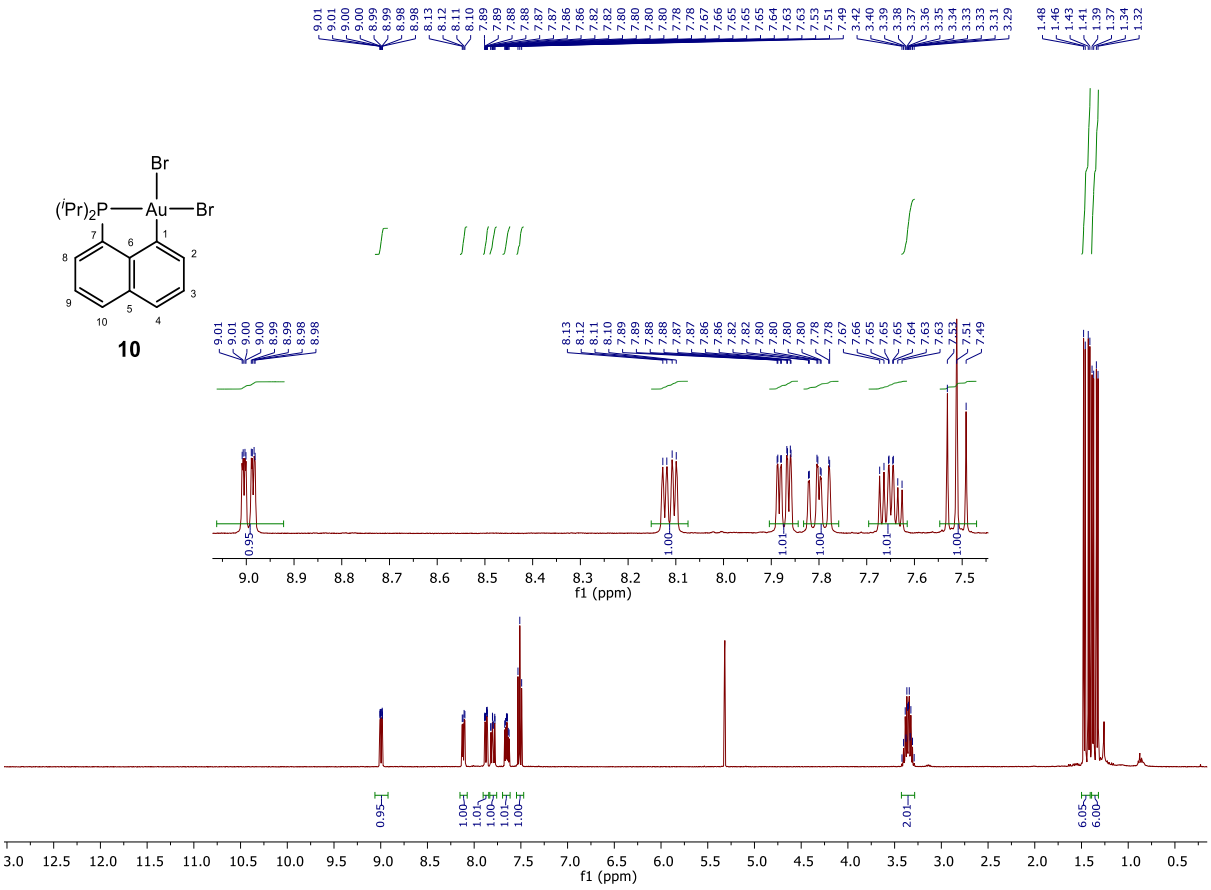


Figure S15: ^{1}H NMR spectrum of **10** in CD_2Cl_2

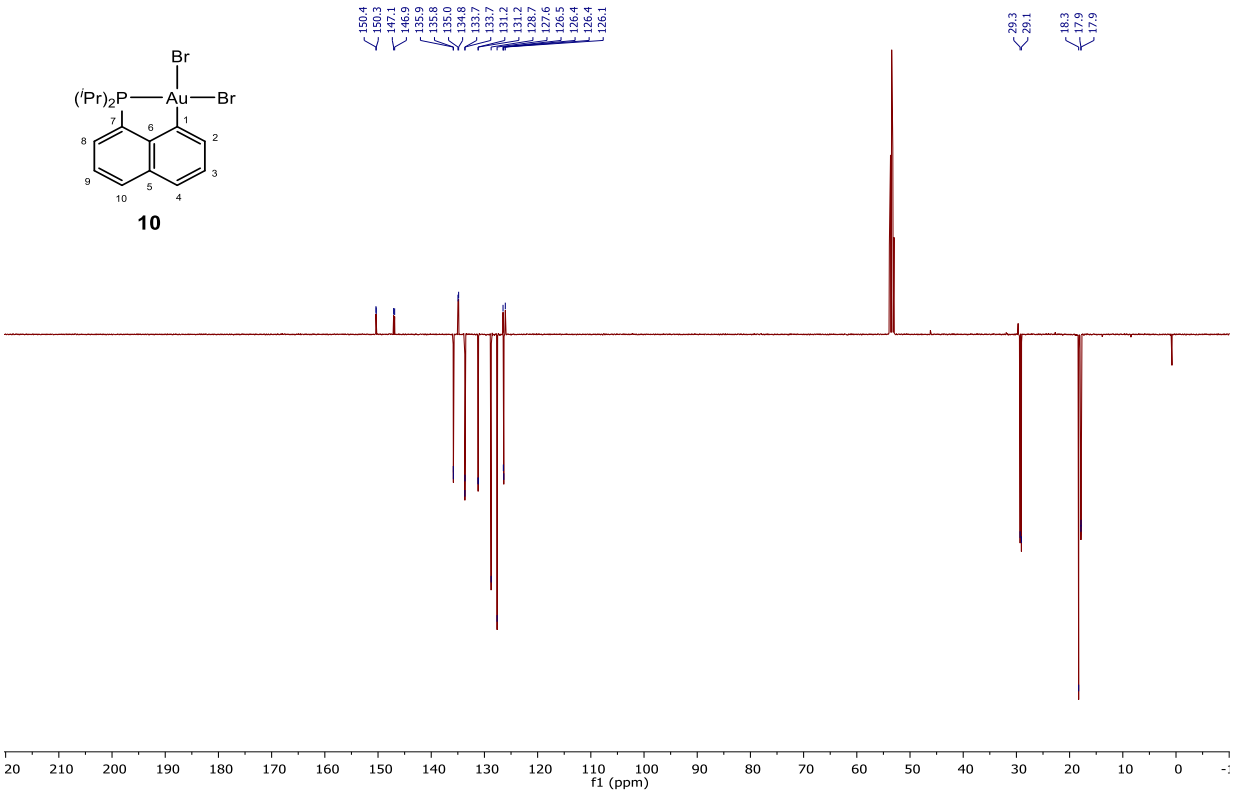


Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of **10** in CD_2Cl_2

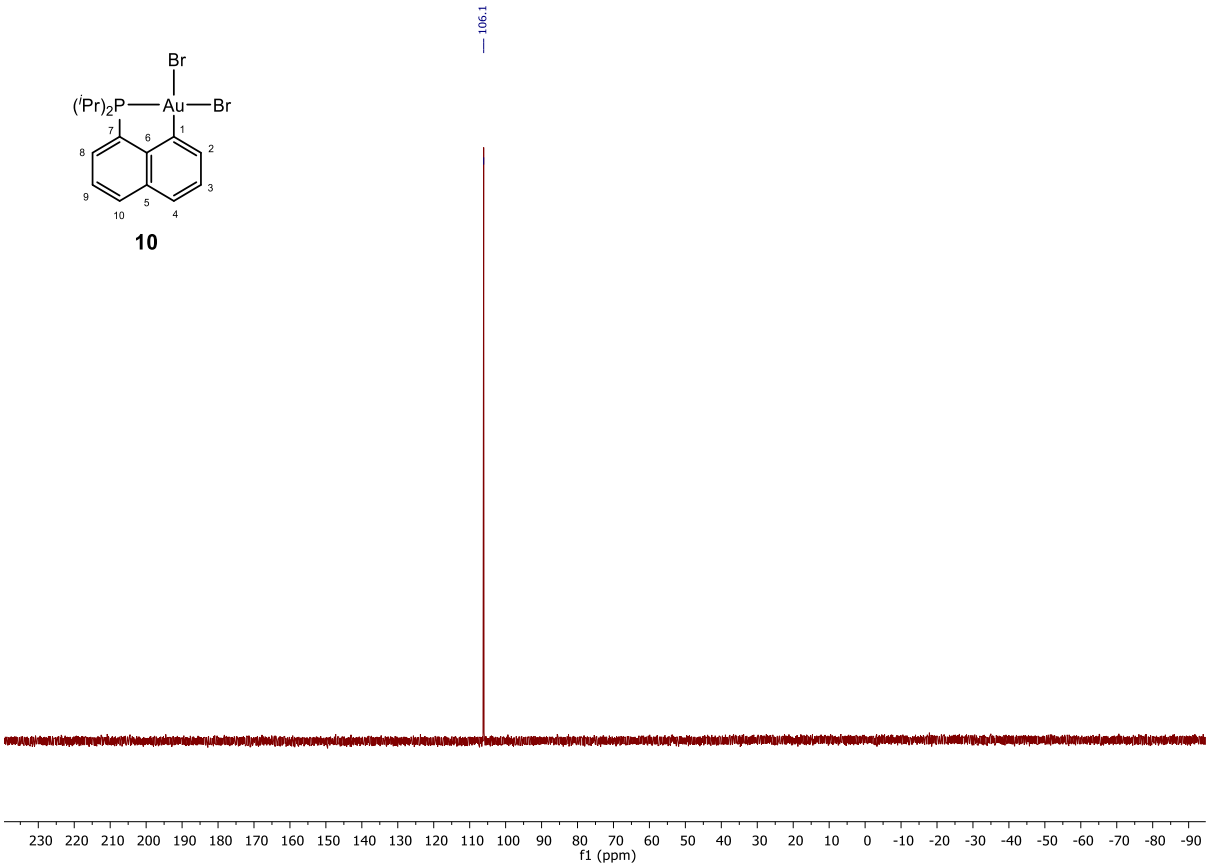


Figure S17: $^{31}P\{^{1}H\}$ NMR spectrum of **10** in CD_2Cl_2

6. Computational details

All calculations were performed on the real systems using the Gaussian 09 package and the B3PW91 hybrid[11] functional, which afforded very accurate results for the reaction of **1** with gold.[4] When dispersion effects were included [B3PW91-D3(BJ), optimization and single-point calculations], only small variations were noticed (Table S6). Solvent effects (dichloromethane, DCM and acetonitrile, CH_3CN) were taken into account by means of the universal Solvation Model based on solute electron Density (SMD).[12] The copper and gold atoms were described with the relativistic electron core potential SDD and associated basis set,[13] augmented by a set of f-orbital polarization functions.[14] The halogen atoms (I, Br, Cl) were also described with the relativistic electron core potential SDD and associated basis set.[18] The 6-31G** basis set were employed for all other atoms (C, H, P). All stationary points involved were fully optimized in gas phase or solvent. Frequency calculations were undertaken to confirm the nature of the stationary points, yielding one imaginary frequency for transition states (TS), corresponding to the expected process, and all of them positive for *minima*. The connectivity of the transition states and their adjacent *minima* was confirmed by intrinsic reaction coordinate (IRC) calculations.[15] In order to have better insight on the bonding situation in compound **6a**, Natural Bond Orbital[16] calculations (NBO, 5.9 version)[17] were carried out. All structures have been plotted with Chemcraft software.[18]

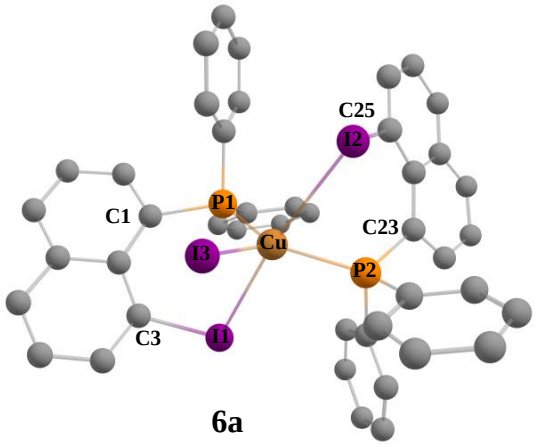
Table S6. Reaction **1-I** + **CuI** in gas phase computed with and without dispersion effects, at B3PW91 and B3PW91-D3(BJ) level of theory. Activation barriers ($\Delta G^{\#}$) and thermodynamic (ΔG) of C-I oxidative addition and P-C reductive elimination steps in kcal/mol.

	C-I Oxidative addition		**P-C Reductive elimination**	
	$\Delta G^{\#}$	**ΔG**	**$\Delta G^{\#}$**	**ΔG**
B3PW91[a]	9.3	2.7	18.5	-1.9
B3PW91-D3(BJ)[b]	8.8	1.5	15.6	3.8
B3PW91-D3(BJ)//B3PW91[c]	8.0	0.4	16.3	5.9

[a] optimization at B3PW91/SDD+f(Cu),SDD(I),6-31G**(other atoms) level; [b] optimization with dispersion effects at B3PW91-D3(BJ)/SDD+f(Cu),SDD(I),6-31G**(other atoms) level [c] dispersion effects have been taken into account by single point calculations at B3PW91-D3(BJ)/SDD+f(Cu), SDD(I), 6-31G**(other atoms) level on the geometry optimized at B3PW91.

Table S7. Main geometrical parameters for complex **6a** (distances in Å and bond/dihedral angles in °), optimized in gas phase at B3PW91/SDD+f(Cu), SDD(I), 6-31G** (other atoms) level of theory. Same numbering than in the X-ray structure.

Theory	Complex 6a
P1-Cu	2.310
P2-Cu	2.321
Cu…I3	2.619
Cu…I1	3.178
Cu…I2	3.267
C3-I1	2.138
C25-I2	2.135
P1-C1	1.871
P2-C23	1.876
P1-Cu-P2	130.45
P1-Cu-I3	108.90
P2-Cu-I3	120.53
I1…Cu…I2	172.48
I…C-C-P	-27.5 (23.6)



6a

Table S8. NBO analysis for complex **6a** at B3PW91/SDD+f(Cu), SDD(I), 6-31G** (other atoms) level of theory. Stabilizing interactions I→Cu and P→Cu, ΔE(2) in kcal/mol, found at the second order perturbation theory. Natural Localized Molecular Orbital (NLMO) associated to the iodine lone pair involved in the interaction with copper, with percentage of main atoms (%) accounting for the I→Cu interaction and hybridization of the atoms.

NBO analysis : 2nd order perturbation theory	
LP(P1) → 4s(Cu)	ΔE(2) = 85.24
LP(P2) → 4sCu)	ΔE(2) = 87.21
LP(I1) → 4s(Cu)	ΔE(2) = 12.73 // Cu-I at 3.178 Å
LP(I2) → 4s(Cu)	ΔE(2) = 10.02 // Cu-I at 3.267 Å
LP(I3) → 4s(Cu)	ΔE(2) = 77.25 // Cu-I at 2.619 Å
NLMO analysis	
LP(I1) // Cu-I at 3.178 Å	% I : 95.4 [s (4.85%), p (95.15%)] % Cu : 1.0 [s (90.58%), p (8.27%)] % P1 : 0.9 [s (10.04%), p (87.63%)] % P2 : 0.2 [s (25.71%), p (73.10%)]
LP(I2) // Cu-I at 3.267 Å	% I : 95.4 [s (3.43%), p (96.57%)] % Cu : 0.8 [s (90.33%), p (8.20%)] % P1 : 0.1 [s (24.27%), p (74.75%)] % P2 : 1.0 [s (8.25%), p (89.17%)]
LP(I3) // Cu-I at 2.619 Å	% I : 86.4 [s (15.48%), p (84.52%)] % Cu : 11.1 [s (94.14%), p (5.07%)] % P1 : 0.8 [s (4.03 %), p (93.63%)] % P2 : 0.7 [s (3.86%), p (94.26%)]

Figure S18. Energy profiles computed in gas phase and in DCM/CH_3CN solutions for the C–I oxidative addition / P–C reductive elimination sequence. Free energies (and electronic energies in brackets) in kcal/mol. Profiles computed at B3PW91/SDD+f(Cu),SDD(I),6-31G**(other atoms) level of theory in gas phase and at SMD(DCM or CH_3CN)-B3PW91/SDD+f(Cu), SDD(I),6-31G**(other atoms) level of theory in solution.

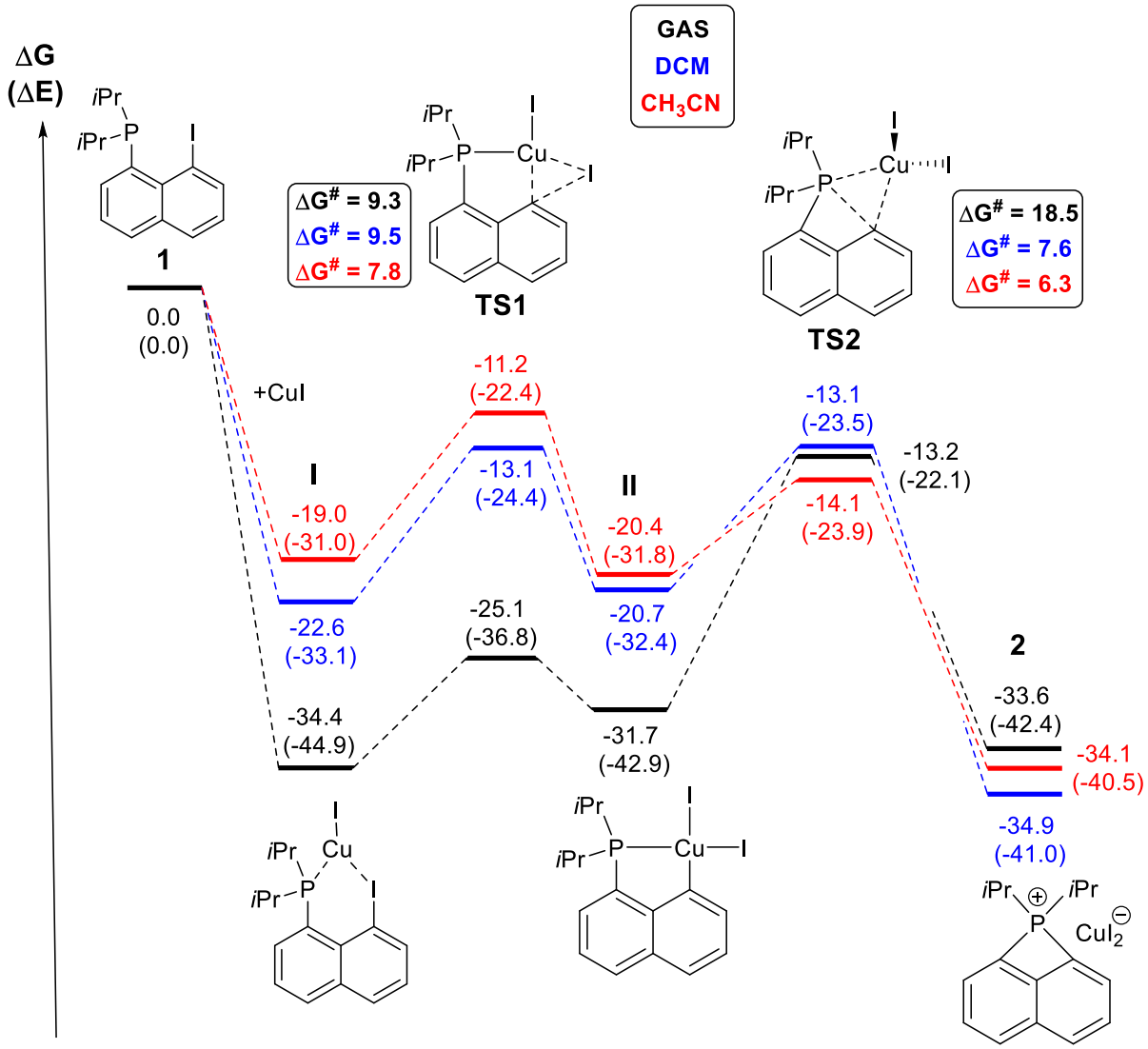


Figure S19. Reactions **1-I** + CuI in gas phase, CH_2Cl_2 (DCM) and CH_3CN. Main geometrical parameters for **TS1**, **TS2** and complexes **I**, **II**, **2** (distances in Å and bond angles in °) optimized in gas phase or in solvent at SMD(solvent)-B3PW91/SDD+f(Cu), I(SDD), 6-31G** (other atoms) level of theory.

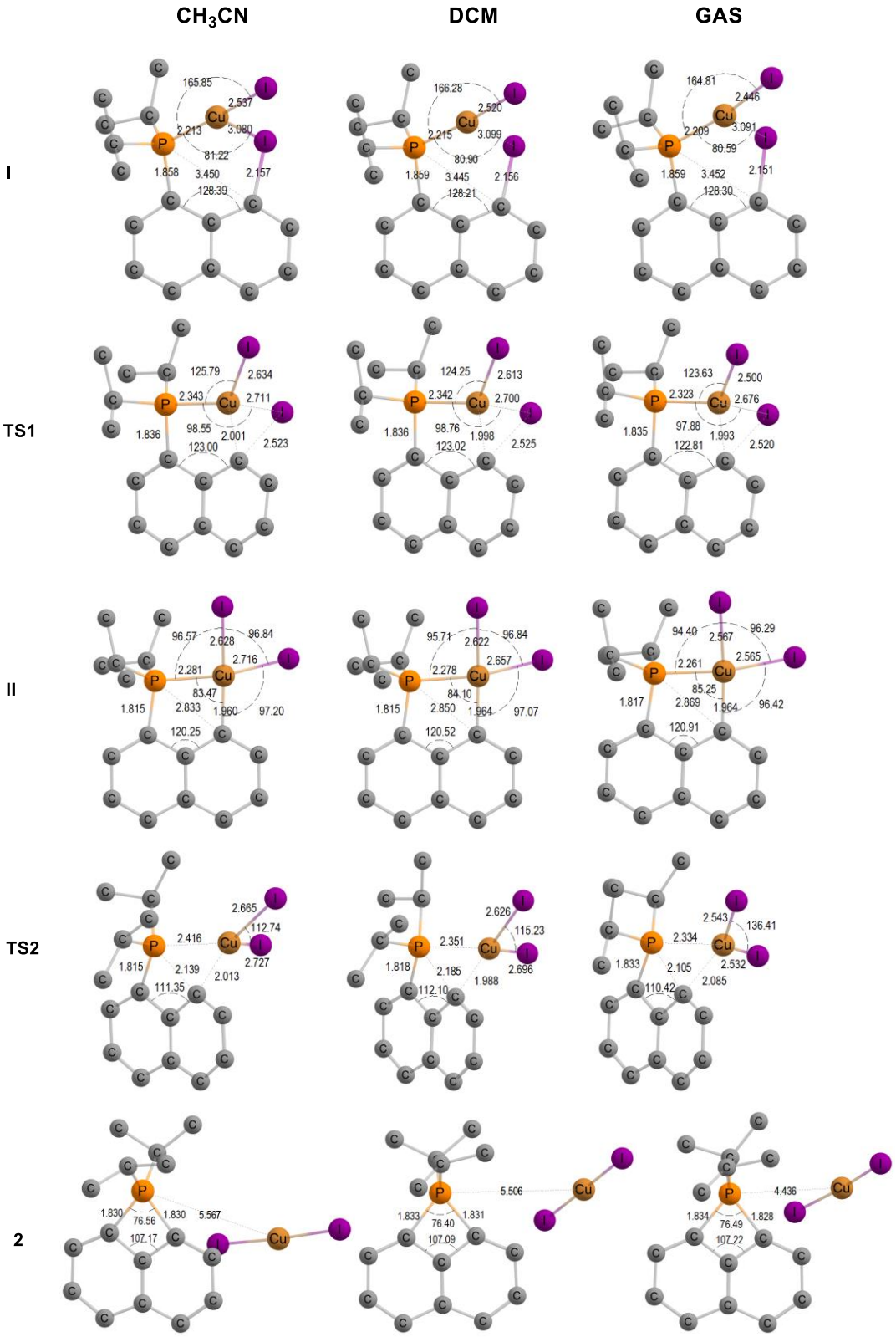


Figure S20. Energy profiles computed for the C–X oxidative addition (X : I, Br, Cl) / P–C reductive elimination sequence at the SMD(CH_3CN)-B3PW91/SDD+f(Cu), SDD(I,Br,Cl),6-31G**(other atoms) level of theory. Free energies (and electronic energies in brackets) in kcal/mol.

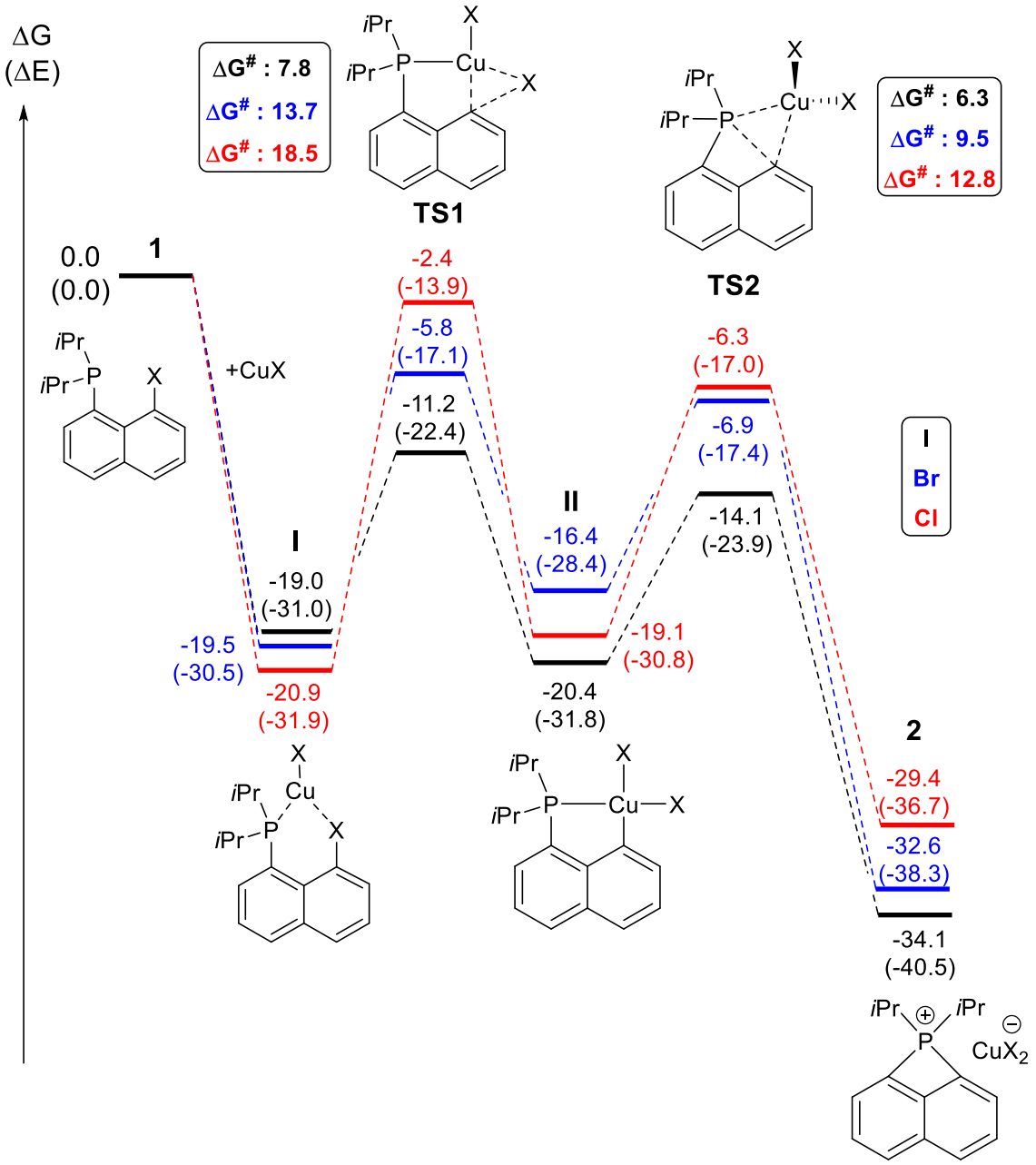


Figure S21. Reactions **1-Br** + CuBr in gas phase, DCM and CH_3CN. Main geometrical parameters for **TS1**, **TS2** and complexes **I**, **II**, **2** (distances in Å and bond angles in °) optimized in gas phase or solvent at SMD(solvent)-B3PW91/SDD+f(Cu), Br(SDD), 6-31G** (other atoms) level of theory.

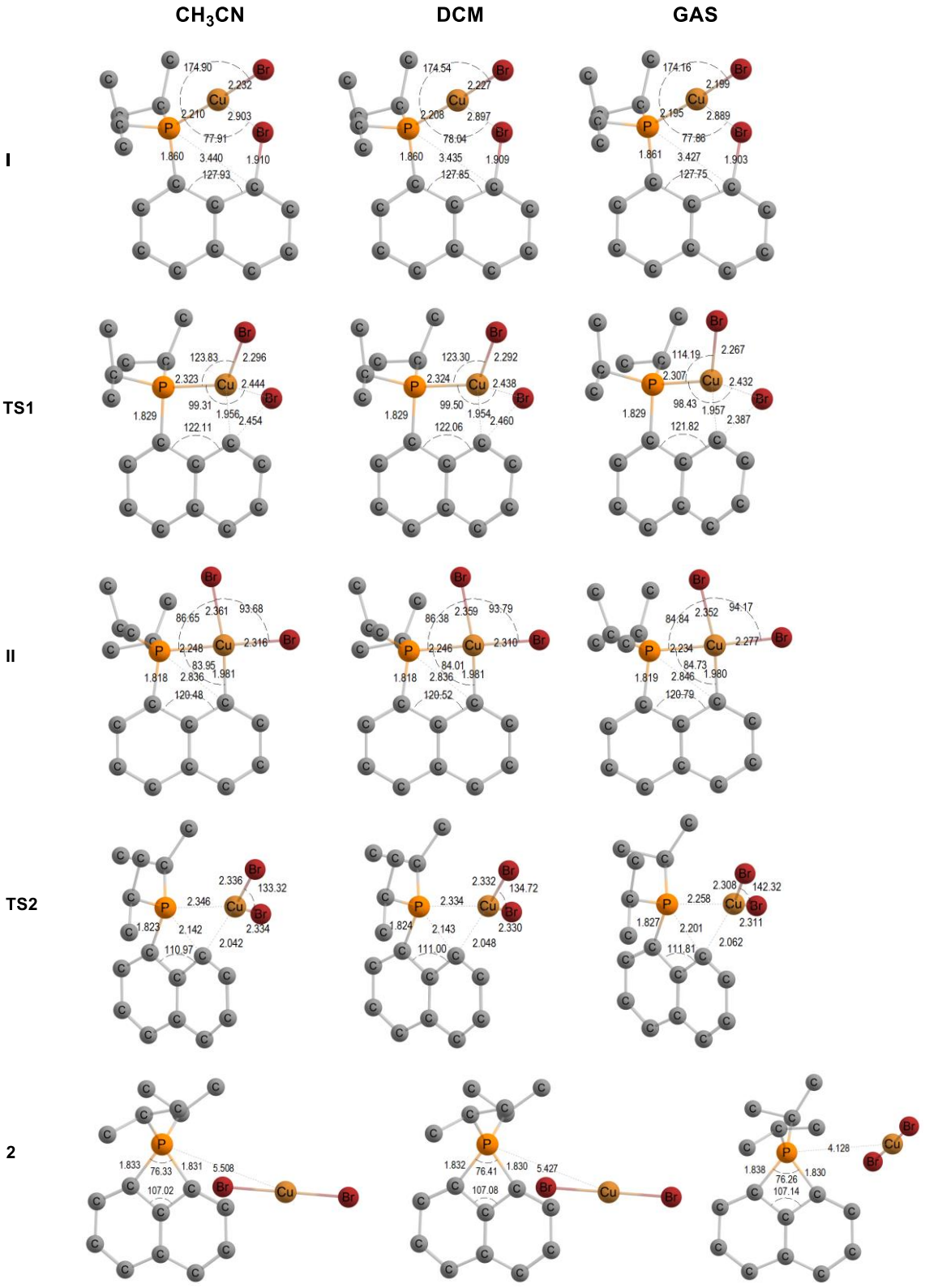


Figure S22. Reactions **1-Cl** + CuCl in gas phase, DCM and CH_3CN. Main geometrical parameters for **TS1**, **TS2** and complexes **I**, **II**, **2** (distances in Å and bond angles in °) optimized in gas phase or solvent at SMD(solvent)-B3PW91/SDD+f(Cu), Cl(SDD), 6-31G** (other atoms) level of theory.

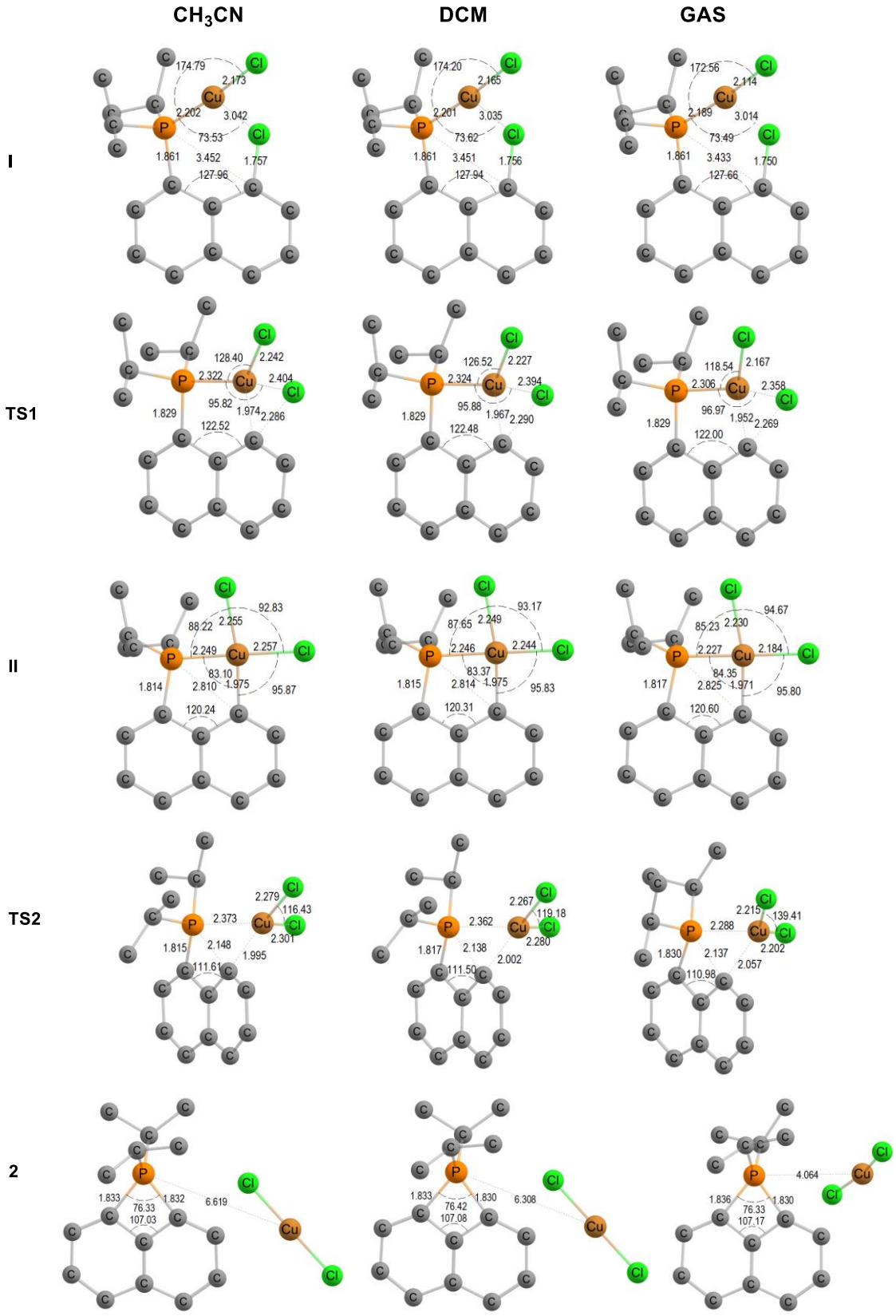


Figure S23. Energy profiles computed for the reactions of the *peri*-iodo naphthyl phosphine **1-I** with CuI and AuI at the SMD(DCM)-B3PW91/SDD+f(M),SDD(I),6-31G**(other atoms) level of theory. Free energies (and electronic energies in brackets) in kcal/mol.

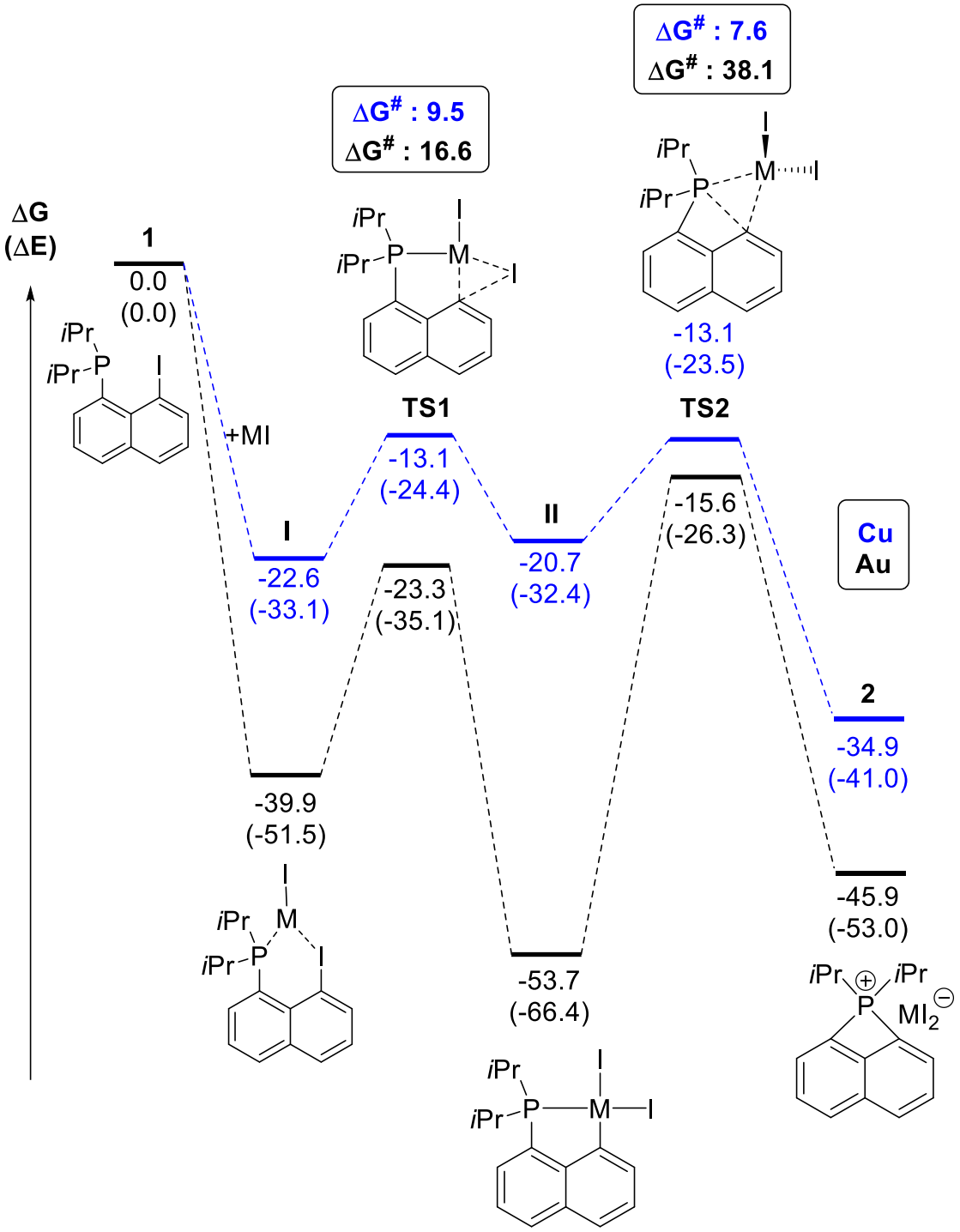


Figure S24. Energy profiles computed for the reaction of the *peri*-bromo naphthyl phosphine **1-Br** with CuBr and AuBr at the SMD(DCM)-B3PW91/SDD+f(M),SDD(Br),6-31G**(other atoms) level of theory. Free energies (and electronic energies in brackets) in kcal/mol.

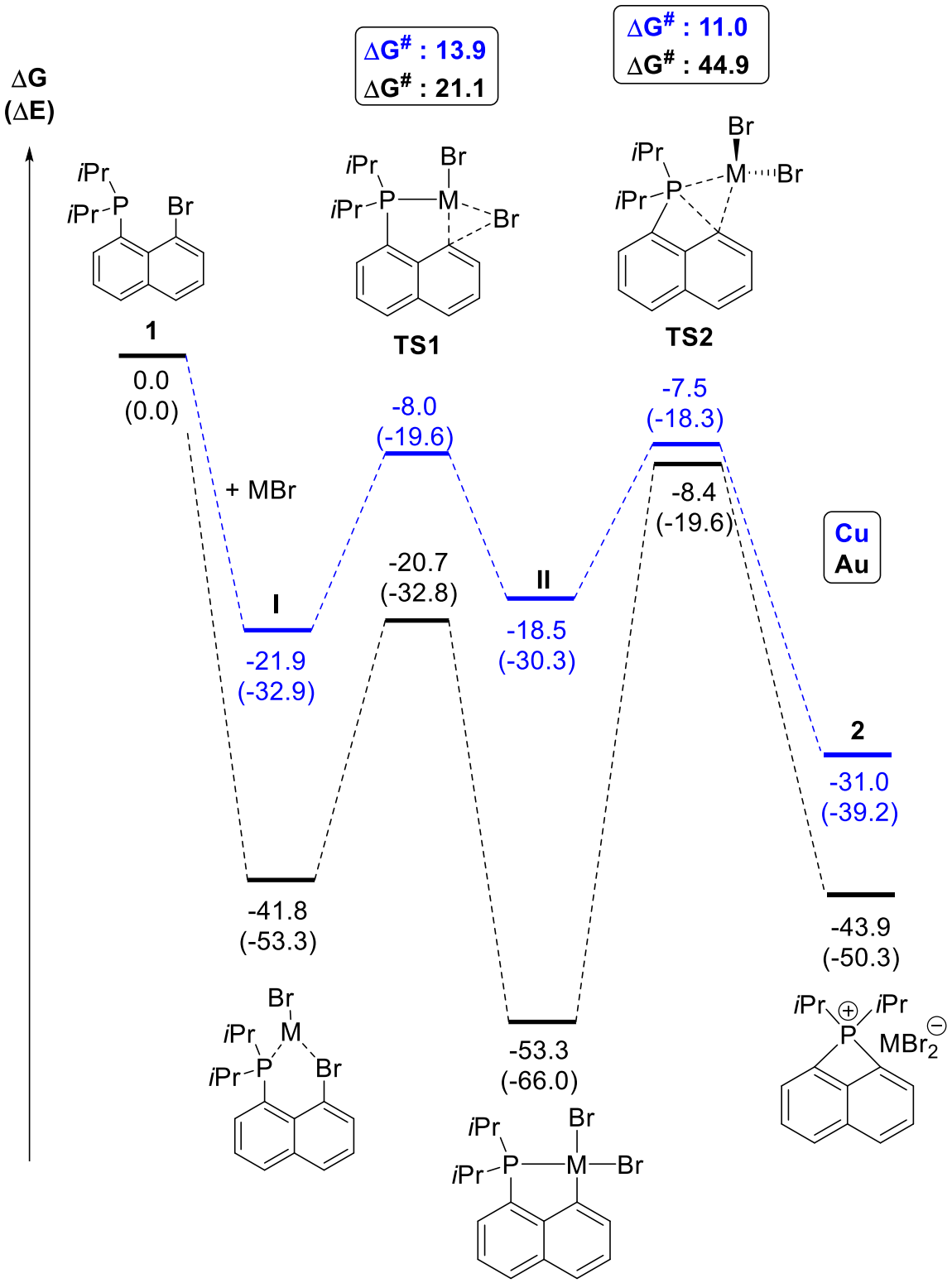
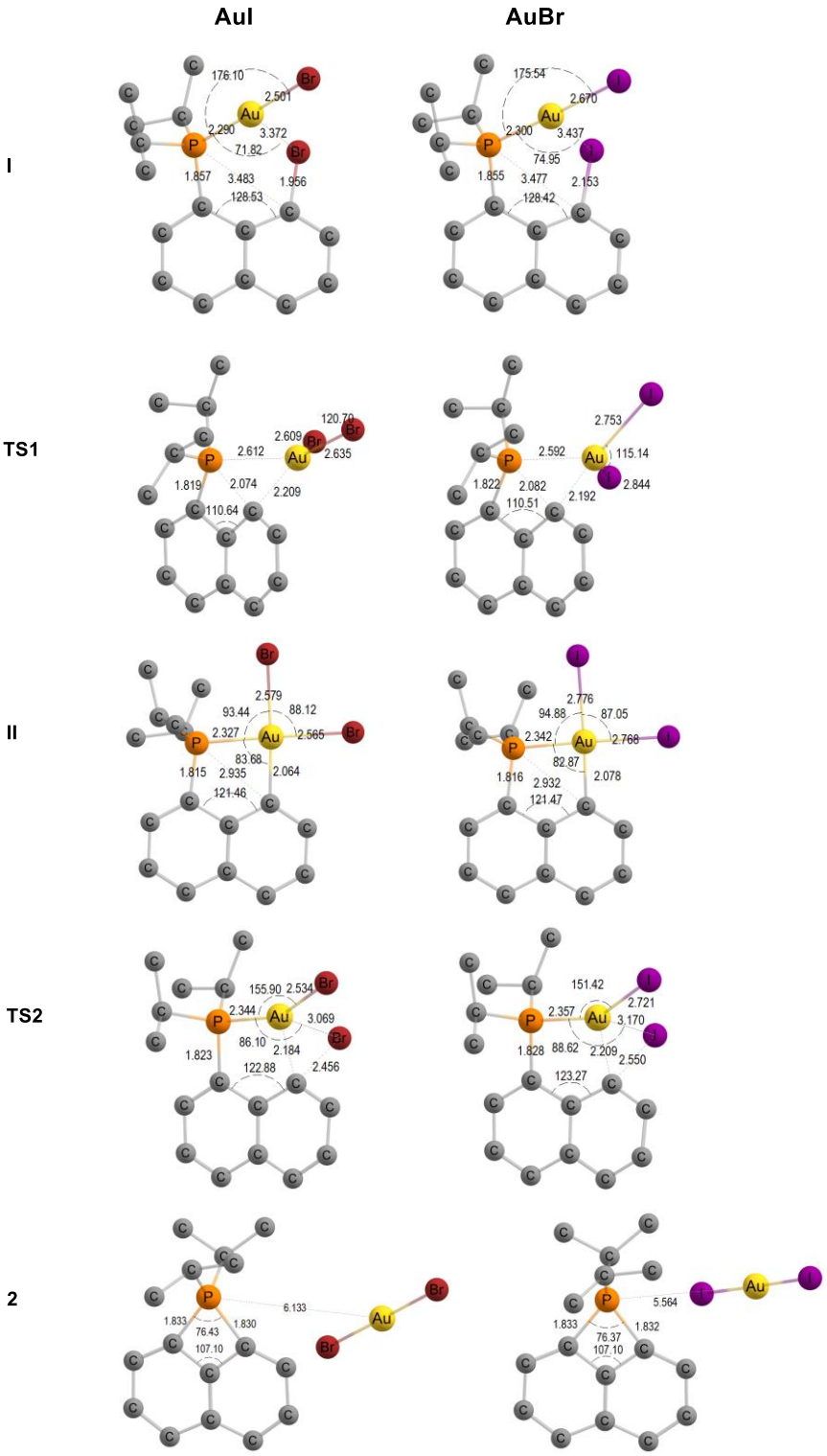


Figure S25. Reactions **1-X** (X = Br, I) + AuX in CH_2Cl_2 (DCM). Main geometrical parameters for **TS1**, **TS2** and complexes **I**, **II**, **2** (distances in Å and bond angles in °) optimized in dichloromethane at SMD(DCM)-B3PW91/SDD+f(Au), I,Br(SDD), 6-31G** (other atoms) level of theory.



7. Z-matrices and energies in au

6a in GAS Phase

Sum of electronic and zero-point Energies= -2609.149937
Sum of electronic and thermal Enthalpies = -2609.102465
Sum of electronic and thermal Free Energies = -2609.237902

C	3.38260	1.07491	0.17853
C	4.11290	-0.13935	-0.09852
C	3.71871	-1.48647	0.15422
C	4.44845	-2.57001	-0.28326
H	4.08905	-3.57348	-0.08546
C	5.66622	-2.39429	-0.96357
H	6.21756	-3.26180	-1.31263
C	6.15865	-1.12751	-1.12687
H	7.12759	-0.96233	-1.58991
C	5.42565	0.00191	-0.68843
C	6.02175	1.28028	-0.81957
H	7.01807	1.34075	-1.24979
C	5.36538	2.40520	-0.40347
H	5.82801	3.38493	-0.47361
C	4.04124	2.28934	0.05666
H	3.50413	3.20519	0.27746
C	1.20456	2.87871	-0.31230
C	0.94382	4.04113	0.42302
H	0.94112	4.01047	1.50804
C	0.69410	5.24765	-0.23165
H	0.49564	6.14291	0.35168
C	0.70923	5.30725	-1.62310
H	0.52277	6.24954	-2.13133
C	0.96583	4.15128	-2.36186
H	0.97485	4.18664	-3.44765
C	1.20411	2.94268	-1.71452
H	1.39060	2.04202	-2.29569
C	1.36641	1.57229	2.25631
C	0.07174	1.73435	2.77147
H	-0.78457	1.66342	2.10511
C	-0.12594	1.99134	4.12596
H	-1.13522	2.12206	4.50629
C	0.96732	2.07149	4.98890
H	0.81406	2.26348	6.04724
C	2.25589	1.90223	4.48746
H	3.11226	1.96081	5.15365
C	2.45625	1.65963	3.12861
H	3.46421	1.53451	2.74571
C	-3.18419	0.03561	1.01934
C	-3.38399	1.43223	0.69614
C	-2.95495	2.13873	-0.47102
C	-3.09781	3.50536	-0.60026
H	-2.73368	3.99667	-1.49528
C	-3.73179	4.26876	0.39520
H	-3.82776	5.34292	0.27015
C	-4.26371	3.63125	1.48399
H	-4.81444	4.18480	2.23969
C	-4.12383	2.23177	1.64937
C	-4.75416	1.62513	2.76467
H	-5.31984	2.25868	3.44303
C	-4.67003	0.27573	2.96542
H	-5.17977	-0.20188	3.79673
C	-3.86468	-0.49460	2.10611
H	-3.74829	-1.54733	2.33670
C	-2.93128	-2.09101	-0.98357
C	-2.24656	-2.84482	-1.94536
H	-1.16226	-2.79496	-2.00324
C	-2.95481	-3.62923	-2.85376
H	-2.41132	-4.20411	-3.59812
C	-4.34759	-3.66183	-2.81811
H	-4.89782	-4.26786	-3.53273
C	-5.03371	-2.90699	-1.86781
H	-6.11984	-2.92193	-1.83856
C	-4.33070	-2.12693	-0.95221
H	-4.87495	-1.53972	-0.21917
C	-1.67657	-2.35644	1.58699
C	-1.04213	-1.93429	2.76775
H	-0.76495	-0.89077	2.89247
C	-0.77735	-2.83689	3.79375
H	-0.29580	-2.48840	4.70323
C	-1.12279	-4.18245	3.65114
H	-0.90963	-4.88830	4.44888
C	-1.74005	-4.61191	2.48045
H	-2.01186	-5.65675	2.35844
C	-2.02075	-3.70586	1.45557
H	-2.50930	-4.05548	0.55224
P	1.53806	1.22967	0.45453
P	-1.93925	-1.12361	0.22850
Cu	0.12674	-0.33975	-0.48321
I	2.06304	-2.01756	1.39772
I	-2.18536	1.18270	-2.21861
I	1.13241	-1.12637	-2.76973

- **M-X**

CuI in GAS phase

Sum of electronic and zero-point Energies= -208.874314
Sum of electronic and thermal Enthalpies = -208.870534
Sum of electronic and thermal Free Energies = -208.899599

Cu	0.00000	0.00000	-1.54481
I	0.00000	0.00000	0.84527

CuI in DCM

Sum of electronic and zero-point Energies= -208.911403
Sum of electronic and thermal Enthalpies = -208.907564
Sum of electronic and thermal Free Energies = -208.936832

I	0.00000	0.00000	0.87160
Cu	0.00000	0.00000	-1.59293

CuI in CH_3CN

Sum of electronic and zero-point Energies= -208.917295
Sum of electronic and thermal Enthalpies = -208.913438
Sum of electronic and thermal Free Energies = -208.942765

I	0.00000	0.00000	0.87676
Cu	0.00000	0.00000	-1.60236

CuBr in GAS phase

Sum of electronic and zero-point Energies= -210.828120
Sum of electronic and thermal Enthalpies = -210.824399
Sum of electronic and thermal Free Energies = -210.852611

Br	0.00000	0.00000	1.00834
Cu	0.00000	0.00000	-1.21696

CuBr in DCM

Sum of electronic and zero-point Energies= -210.864478
Sum of electronic and thermal Enthalpies = -210.860742
Sum of electronic and thermal Free Energies = -210.889042

Br	0.00000	0.00000	1.03825
Cu	0.00000	0.00000	-1.25306

CuBr in CH_3CN

Sum of electronic and zero-point Energies= -210.869457
Sum of electronic and thermal Enthalpies = -210.865714
Sum of electronic and thermal Free Energies = -210.894036

Br	0.00000	0.00000	1.04259
Cu	0.00000	0.00000	-1.25829

CuCl in GAS phase

Sum of electronic and zero-point Energies= -657.562690
Sum of electronic and thermal Enthalpies = -657.559086
Sum of electronic and thermal Free Energies = -657.585995

Cl	0.00000	0.00000	-1.30681
Cu	0.00000	0.00000	0.76606

CuCl in DCM
Sum of electronic and zero-point Energies= -657.605170
Sum of electronic and thermal Enthalpies = -657.601464
Sum of electronic and thermal Free Energies = -657.628630

Cl	0.00000	0.00000	-1.35016
Cu	0.00000	0.00000	0.79147

CuCl in CH_3CN
Sum of electronic and zero-point Energies= -657.611043
Sum of electronic and thermal Enthalpies = -657.607318
Sum of electronic and thermal Free Energies = -657.634534

Cl	0.00000	0.00000	-1.35800
Cu	0.00000	0.00000	0.79607

AuI in DCM
Sum of electronic and zero-point Energies= -147.311516
Sum of electronic and thermal Enthalpies = -147.307607
Sum of electronic and thermal Free Energies = -147.338510

I	0.00000	0.00000	-1.56126
Au	0.00000	0.00000	1.04743

AuBr in DCM
Sum of electronic and zero-point Energies= -149.265169
Sum of electronic and thermal Enthalpies = -149.261336
Sum of electronic and thermal Free Energies -149.291386

Br	0.00000	0.00000	-1.70070
Au	0.00000	0.00000	0.75348

Profiles with Copper

- **X : I, gas phase**

CuI profile compound 1 in GAS phase
Sum of electronic and zero-point Energies= -973.963847
Sum of electronic and thermal Enthalpies = -973.943653
Sum of electronic and thermal Free Energies = -974.011950

P	1.51024	-0.06812	0.38440
C	2.10916	-0.80141	-1.26349
H	1.16155	-0.98565	-1.78541
C	-1.90981	-0.15857	0.20873
C	-1.17084	1.03213	-0.08359
C	-3.26733	-0.15207	0.45246
C	0.26172	1.18839	-0.22458
C	-1.99117	2.21363	-0.25453
C	-4.01423	1.03640	0.37450
H	-3.77640	-1.08261	0.67697
C	0.74501	2.41123	-0.66390
C	-1.41416	3.43585	-0.68210
C	-3.38524	2.18999	-0.00801
H	-5.08066	1.01576	0.57702
C	-0.07200	3.52832	-0.92141
H	1.81481	2.54164	-0.78159
H	-2.06840	4.29327	-0.81662
H	-3.94427	3.11325	-0.13415
H	0.37289	4.45689	-1.26723
C	2.92845	1.02788	0.97456
H	3.29265	1.69230	0.18053
C	2.77225	-2.16474	-1.03812
H	2.14307	-2.81823	-0.42682
H	2.94910	-2.66352	-1.99864
H	3.74061	-2.07448	-0.53659
C	2.96236	0.10333	-2.15054
H	3.92888	0.33589	-1.69052
H	3.17238	-0.39571	-3.10468
H	2.45609	1.04489	-2.38115
C	4.09699	0.13254	1.40466
H	3.77775	-0.61222	2.14224
H	4.54756	-0.39946	0.56265
H	4.88355	0.74170	1.86556
C	2.45675	1.87601	2.16030
H	2.08281	1.23852	2.96933
H	3.29024	2.46627	2.55944
H	1.65683	2.56810	1.88434
I	-1.12645	-2.16695	0.11377

CuI profile compound 2 in GAS phase
Sum of electronic and zero-point Energies= -1182.905712
Sum of electronic and thermal Enthalpies = -1182.880654
Sum of electronic and thermal Free Energies = -1182.965164

C	-5.05723	1.25518	-0.49576
C	-4.44456	1.45327	-1.72583
C	-3.17006	0.88547	-1.99678
C	-2.64924	0.14090	-0.93369
C	-4.48521	0.49501	0.56710
C	-2.31542	0.93608	-3.13135
C	-1.08742	0.28894	-3.11463
H	-2.61274	1.49081	-4.01692
H	-6.02855	1.71042	-0.32500
H	-4.94712	2.05509	-2.47804
H	-5.01811	0.39030	1.50667
H	-0.45551	0.36010	-3.99499
C	-0.58288	-0.45372	-2.00520
H	0.40237	-0.90999	-2.04242
C	-1.40310	-0.51457	-0.90674
I	3.02059	-1.62610	-0.67829
C	-3.25653	-0.06650	0.31943
C	-0.83840	-0.28382	2.20583
H	-0.48338	0.67614	1.79656
C	-2.01995	-2.84070	1.03554
H	-2.01330	-2.98876	2.12376
P	-1.77230	-1.02494	0.80983
Cu	2.24106	0.64523	-0.07416
I	1.15361	2.75437	0.60815
C	-0.84278	-3.60266	0.40740
H	0.13452	-3.26069	0.75603
H	-0.93599	-4.66479	0.65383
H	-0.85813	-3.50624	-0.68183
C	-3.36599	-3.30015	0.46776
H	-3.46596	-4.37960	0.61749
H	-4.21348	-2.81007	0.95363
H	-3.43043	-3.10725	-0.60755
C	0.37598	-1.11274	2.63075
H	0.91376	-0.55228	3.40123
H	0.08855	-2.07801	3.06152
H	1.07910	-1.27828	1.80911
C	-1.80622	-0.02138	3.36822
H	-2.62526	0.64441	3.08360
H	-2.22662	-0.94664	3.77922
H	-1.24816	0.46748	4.17227

CuI profile compound I in GAS phase
Sum of electronic and zero-point Energies= -1182.909676
Sum of electronic and thermal Enthalpies = -1182.885186
Sum of electronic and thermal Free Energies = -1182.966374

C	4.22290	1.37349	-1.28843
C	4.40966	0.06832	-1.65102
C	3.48065	-0.93284	-1.27029
C	2.33033	-0.59233	-0.46432
C	3.03080	1.73240	-0.63086
C	3.71605	-2.26614	-1.68523
C	2.88087	-3.28116	-1.30146
H	4.57989	-2.46411	-2.31359
H	4.94569	2.13860	-1.55427
H	5.27737	-0.23088	-2.23280
H	2.85016	2.78927	-0.47080
H	3.04440	-4.30103	-1.63481
C	1.83663	-3.00326	-0.40052
H	1.23940	-3.82015	-0.01127
C	1.59816	-1.71567	0.02990
I	0.23796	-1.63392	1.69436
C	2.06546	0.81253	-0.25330
C	0.60779	2.10603	1.98030
H	1.13124	1.25935	2.44061
C	0.25179	3.03994	-0.88619
H	1.09248	3.71582	-0.68958
P	0.40696	1.51935	0.20137

Cu	-1.34434	0.23302	-0.19415
I	-3.48439	-0.67104	-0.95914
C	-1.04869	3.78350	-0.55834
H	-1.92004	3.12791	-0.66595
H	-1.05458	4.19954	0.45226
H	-1.17265	4.61818	-1.25705
C	0.26674	2.62659	-2.36156
H	1.19560	2.12741	-2.64871
H	-0.56723	1.95150	-2.58371
H	0.15276	3.51538	-2.99193
C	-0.74592	2.24984	2.68373
H	-1.35042	1.34282	2.58906
H	-0.58736	2.44134	3.75097
H	-1.33391	3.08088	2.28501
C	1.48074	3.35019	2.14878
H	1.60874	3.56477	3.21564
H	2.47924	3.21358	1.72461
H	1.02744	4.23620	1.69277

CuI profile TS1 in GAS phase

Sum of electronic and zero-point Energies= -1182.896750
Sum of electronic and thermal Enthalpies = -1182.872813
Sum of electronic and thermal Free Energies = -1182.951533

C	0.73294	-2.58986	-1.03369
C	0.87209	-1.36642	-0.40254
C	2.06984	-0.59123	-0.55534
C	3.17246	-1.19690	-1.23616
C	3.00282	-2.46395	-1.85646
C	1.79020	-3.10699	-1.81759
H	-0.16419	-3.18135	-0.88920
C	2.15873	0.77454	-0.16754
C	4.38506	-0.47228	-1.34076
H	3.84464	-2.90502	-2.38324
H	1.65145	-4.05696	-2.32477
C	4.48783	0.81197	-0.85776
C	3.35564	1.45342	-0.31531
H	5.22849	-0.93948	-1.84261
H	5.42209	1.35778	-0.94982
H	3.42351	2.50643	-0.05928
I	-0.10610	-1.77766	1.88357
C	0.61092	2.09489	2.01194
H	1.03525	1.20497	2.49455
C	0.48086	3.05396	-0.88352
H	1.36102	3.67170	-0.65718
Cu	-0.79801	-0.29287	-0.23190
I	-3.15199	-0.12469	-1.05723
P	0.54154	1.55009	0.22049
C	-0.79011	3.86904	-0.62267
H	-0.85263	4.68831	-1.34730
H	-1.68625	3.25063	-0.73982
H	-0.80602	4.31315	0.37571
C	0.54695	2.60582	-2.34758
H	1.46084	2.04818	-2.56968
H	-0.31273	1.97648	-2.60161
H	0.52330	3.48492	-3.00087
C	-0.79329	2.30661	2.59105
H	-1.44335	1.44835	2.40200
H	-0.72101	2.44336	3.67563
H	-1.28106	3.19472	2.18021
C	1.53475	3.28254	2.28815
H	1.55674	3.48417	3.36514
H	2.56357	3.08846	1.97323
H	1.18804	4.19642	1.79525

CuI profile compound II in GAS phase

Sum of electronic and zero-point Energies= -1182.906529
Sum of electronic and thermal Enthalpies = -1182.882163
Sum of electronic and thermal Free Energies = -1182.962069

C	4.93611	-0.34595	0.01432
C	4.85014	0.99088	0.33065
C	3.59653	1.63720	0.46389
C	2.40502	0.87373	0.24238
C	3.76403	-1.10646	-0.18070
C	3.47638	2.99212	0.85653
C	2.23388	3.54832	1.03139
H	4.37695	3.57563	1.02886
H	5.90603	-0.82588	-0.07485
H	5.75399	1.56900	0.50628
H	3.85503	-2.16477	-0.40747
H	2.13720	4.58334	1.34754
C	1.05376	2.80301	0.78410
H	0.09760	3.29816	0.89552
C	1.12403	1.48066	0.39489
I	-2.39702	-1.19403	0.97629
C	2.52553	-0.50099	-0.08067
C	0.68368	-1.41234	-2.17118
H	0.93335	-0.38700	-2.47665
C	1.09256	-2.97082	0.47110
H	2.07303	-3.29699	0.09401
P	0.90650	-1.29079	-0.31522
Cu	-0.49866	0.38168	0.26673
I	-2.00431	2.20773	-0.72243
C	0.05677	-4.02108	0.06902
H	0.03932	-4.20296	-1.00814
H	0.31251	-4.96721	0.55879
H	-0.94700	-3.73390	0.38837
C	1.18720	-2.80841	1.99244
H	0.23403	-2.46501	2.40438
H	1.42576	-3.77651	2.44534
H	1.96853	-2.10049	2.28384
C	-0.75748	-1.69558	-2.60374
H	-0.81083	-1.65038	-3.69686
H	-1.09744	-2.68684	-2.29329
H	-1.45734	-0.95870	-2.20259
C	1.69050	-2.36752	-2.82037
H	1.50881	-3.40914	-2.53884
H	1.58931	-2.30218	-3.90897
H	2.72361	-2.11184	-2.57098

CuI profile TS2 in GAS phase

Sum of electronic and zero-point Energies= -1182.879442
Sum of electronic and thermal Enthalpies = -1182.855529
Sum of electronic and thermal Free Energies = -1182.934106

C	-4.65335	-0.41507	0.54274
C	-4.58707	-0.21090	-0.82626
C	-3.33700	-0.22589	-1.49859
C	-2.22254	-0.40342	-0.66126
C	-3.50785	-0.66692	1.34678
C	-3.04371	-0.11825	-2.88438
C	-1.74093	-0.24889	-3.33063
H	-3.84495	0.04317	-3.60009
H	-5.62575	-0.39926	1.02646
H	-5.50250	-0.04596	-1.38811
H	-3.63000	-0.85964	2.40765
H	-1.54161	-0.18975	-4.39700
C	-0.62754	-0.46057	-2.46460
H	0.37352	-0.56988	-2.86924
C	-0.89088	-0.46737	-1.11154
I	2.95434	-0.55222	-0.93103
C	-2.28537	-0.65337	0.71565
C	0.06067	-0.34750	2.56582
H	-0.43814	0.62957	2.55475
C	-0.29369	-2.86783	0.87577
H	-0.96949	-3.15622	1.69405
P	-0.49486	-1.00869	0.88342
Cu	0.74667	0.55550	-0.32551
I	-0.00140	2.83989	0.47137
C	1.12202	-3.34462	1.21368
H	1.45606	-3.00691	2.19657
H	1.12459	-4.43979	1.22341
H	1.84844	-3.00275	0.47238
C	-0.80222	-3.50497	-0.41702
H	-0.78230	-4.59365	-0.30170
H	-1.82779	-3.21313	-0.65659
H	-0.15763	-3.24326	-1.26005
C	1.55347	-0.11805	2.77911
H	1.69158	0.29162	3.78577
H	2.14269	-1.03397	2.70098
H	1.95593	0.60584	2.06798

C	-0.55846	-1.23284	3.65748
H	-1.62560	-1.42301	3.51058
H	-0.04356	-2.19277	3.75369
H	-0.45353	-0.70731	4.61285

▪ X : I, DCM

CuI profile compound 1 in DCM

Sum of electronic and zero-point Energies= -973.983712
Sum of electronic and thermal Enthalpies = -973.963550
Sum of electronic and thermal Free Energies = -974.031626

P	-1.51063	-0.04335	-0.39442
C	-2.15879	-0.84870	1.19758
H	-1.22966	-1.05971	1.74193
C	1.90722	-0.16096	-0.23875
C	1.17493	1.02312	0.09533
C	3.25246	-0.14506	-0.54298
C	-0.25400	1.17305	0.27343
C	1.99771	2.20172	0.27090
C	3.99534	1.04881	-0.47908
H	3.76009	-1.06888	-0.79901
C	-0.72773	2.37600	0.77547
C	1.43306	3.40560	0.76551
C	3.38115	2.19041	-0.03677
H	5.05138	1.03760	-0.73177
C	0.09897	3.48169	1.05784
H	-1.79430	2.50496	0.92266
H	2.08972	4.26014	0.90673
H	3.94230	3.11235	0.09135
H	-0.33590	4.39352	1.45720
C	-2.89781	1.08969	-0.98192
H	-3.26105	1.73127	-0.17020
C	-2.81848	-2.19720	0.88820
H	-2.17064	-2.83242	0.27515
H	-3.03218	-2.73516	1.82025
H	-3.76757	-2.08055	0.35543
C	-3.04142	0.01811	2.09349
H	-3.98480	0.28743	1.60665
H	-3.29597	-0.53184	3.00863
H	-2.53881	0.94023	2.39961
C	-4.07257	0.23007	-1.46200
H	-3.75811	-0.49708	-2.22020
H	-4.54945	-0.31913	-0.64565
H	-4.83922	0.86983	-1.91626
C	-2.39150	1.97028	-2.12795
H	-2.02150	1.36040	-2.96092
H	-3.20800	2.59400	-2.51213
H	-1.58198	2.63724	-1.81761
I	1.13045	-2.17158	-0.07897

CuI profile compound 2 in DCM

Sum of electronic and zero-point Energies= -1182.960416
Sum of electronic and thermal Enthalpies = -1182.935147
Sum of electronic and thermal Free Energies = -1183.024142

C	5.39650	-1.92230	-0.63433
C	4.56971	-2.25475	-1.69987
C	3.32156	-1.59514	-1.87407
C	3.05653	-0.62656	-0.90008
C	5.08401	-0.93091	0.34433
C	2.28951	-1.72916	-2.84365
C	1.14889	-0.93995	-2.76849
H	2.38563	-2.45124	-3.64998
H	6.34136	-2.44897	-0.53256
H	4.88447	-3.02575	-2.39777
H	5.77776	-0.72730	1.15341
H	0.38125	-1.07088	-3.52596
C	0.91248	0.03446	-1.75196
H	-0.00748	0.60945	-1.75134
C	1.90274	0.17655	-0.81157
I	-3.23387	2.03525	-0.73099
C	3.88459	-0.28240	0.18568
C	1.77598	0.42524	2.28341
H	1.53118	-0.63042	2.11096
C	3.02087	2.70454	0.65043
H	3.16399	2.98347	1.70216
P	2.59798	0.91135	0.71403
Cu	-2.72598	-0.30402	0.00767
I	-2.18634	-2.63065	0.75794
C	1.85076	3.50589	0.06438
H	0.91589	3.36059	0.61153
H	2.10241	4.57010	0.11174
H	1.68202	3.24599	-0.98480
C	4.32125	2.93832	-0.12149
H	4.53951	4.01106	-0.11935
H	5.16982	2.41944	0.33207
H	4.23443	2.61741	-1.16440
C	0.48379	1.20392	2.53918
H	-0.00005	0.78633	3.42770
H	0.68046	2.26259	2.73252
H	-0.22250	1.12221	1.70791
C	2.77379	0.52924	3.44235
H	3.67074	-0.07279	3.26948
H	3.07591	1.56453	3.63015
H	2.29055	0.15443	4.35020

CuI profile compound I in DCM

Sum of electronic and zero-point Energies= -1182.947903
Sum of electronic and thermal Enthalpies = -1182.923398
Sum of electronic and thermal Free Energies = -1183.004509

C	4.28413	0.87045	-1.44049
C	4.28499	-0.45835	-1.76793
C	3.25100	-1.31867	-1.31573
C	2.19166	-0.80514	-0.47774
C	3.17326	1.40539	-0.75792
C	3.29254	-2.68536	-1.68881
C	2.35364	-3.57024	-1.22612
H	4.09301	-3.01405	-2.34605
H	5.09003	1.52617	-1.75612
H	5.08104	-0.88581	-2.37173
H	3.13788	2.48163	-0.62903
H	2.36886	-4.61424	-1.52383
C	1.40380	-3.13062	-0.28390
H	0.73878	-3.85430	0.17512
C	1.35176	-1.80746	0.10073
I	0.13752	-1.48720	1.85356
C	2.11300	0.62899	-0.31694
C	0.84272	2.18628	1.88005
H	1.28648	1.31343	2.37319
C	0.54508	3.02000	-1.02396
H	1.46170	3.60220	-0.87793
P	0.55975	1.54548	0.13298
Cu	-1.29416	0.37258	-0.17001
I	-3.49577	-0.56614	-0.95889
C	-0.65095	3.91858	-0.69452
H	-1.59496	3.36249	-0.73887
H	-0.57032	4.37842	0.29369
H	-0.70852	4.72890	-1.43046
C	0.47371	2.54601	-2.47750
H	1.33262	1.93217	-2.76223
H	-0.43640	1.96057	-2.65446
H	0.44709	3.41419	-3.14606
C	-0.48014	2.49454	2.58729
H	-1.18071	1.65542	2.52239
H	-0.29084	2.69300	3.64874
H	-0.97490	3.37754	2.17216
C	1.83271	3.34623	1.98366
H	1.98885	3.59449	3.04005
H	2.81028	3.09488	1.56238
H	1.46367	4.24893	1.48647

CuI profile TS1 in DCM

Sum of electronic and zero-point Energies= -1182.933943
Sum of electronic and thermal Enthalpies = -1182.909909
Sum of electronic and thermal Free Energies = -1182.989308

C	0.73019	-2.57639	-1.10873
C	0.88373	-1.37666	-0.43866
C	2.11043	-0.63804	-0.50247

C	3.22847	-1.27246	-1.13119
C	3.04700	-2.51485	-1.79952
C	1.81008	-3.10991	-1.85331
H	-0.18742	-3.14718	-1.01742
C	2.22281	0.71538	-0.08133
C	4.47285	-0.59512	-1.14256
H	3.90291	-2.97499	-2.28585
H	1.66458	-4.04015	-2.39454
C	4.59238	0.67280	-0.61868
C	3.45291	1.34956	-0.13628
H	5.32611	-1.08348	-1.60615
H	5.55082	1.18332	-0.63628
H	3.54450	2.39364	0.14765
I	-0.19726	-1.83071	1.79717
C	0.56792	2.07266	2.00565
H	0.94718	1.17172	2.50469
C	0.72387	3.08241	-0.86980
H	1.61838	3.63202	-0.54981
Cu	-0.76545	-0.25558	-0.32077
I	-3.27883	-0.04083	-1.00327
P	0.61807	1.56034	0.20388
C	-0.50573	3.97582	-0.69040
H	-0.44346	4.82090	-1.38552
H	-1.43121	3.43265	-0.91079
H	-0.58077	4.38530	0.32001
C	0.88861	2.66829	-2.33458
H	1.78260	2.06001	-2.49863
H	0.01860	2.10207	-2.68610
H	0.97739	3.56418	-2.95943
C	-0.87020	2.29872	2.48381
H	-1.51626	1.44755	2.24819
H	-0.87388	2.43257	3.57156
H	-1.31698	3.19383	2.04119
C	1.48368	3.24504	2.36037
H	1.44458	3.41879	3.44231
H	2.52749	3.05007	2.09922
H	1.17093	4.17199	1.86935

CuI profile compound II in DCM

Sum of electronic and zero-point Energies= -1182.946728
Sum of electronic and thermal Enthalpies = -1182.922314
Sum of electronic and thermal Free Energies = -1183.001514

C	4.96469	0.31090	0.00870
C	4.86933	-1.01403	-0.35628
C	3.60796	-1.64234	-0.51214
C	2.42992	-0.87004	-0.25971
C	3.80183	1.08006	0.23315
C	3.46259	-2.98031	-0.95567
C	2.20999	-3.50835	-1.15384
H	4.35270	-3.57318	-1.14918
H	5.93883	0.77927	0.11373
H	5.76762	-1.59285	-0.55612
H	3.90404	2.12841	0.49562
H	2.09524	-4.52927	-1.50814
C	1.03950	-2.75212	-0.88047
H	0.07576	-3.22669	-1.01786
C	1.14536	-1.44918	-0.44237
I	-2.41580	1.25196	-1.03107
C	2.55901	0.48786	0.11328
C	0.68694	1.34906	2.21815
H	0.93426	0.31875	2.50646
C	1.11614	2.96034	-0.40292
H	2.09021	3.27550	0.00057
P	0.94400	1.27555	0.36907
Cu	-0.48599	-0.36560	-0.30110
I	-2.03304	-2.24171	0.76861
C	0.07913	4.00370	0.00427
H	0.03606	4.15142	1.08550
H	0.35984	4.96038	-0.45065
H	-0.91898	3.74116	-0.35245
C	1.24125	2.82855	-1.92321
H	0.29436	2.50949	-2.36894
H	1.50159	3.80519	-2.34491
H	2.02128	2.12014	-2.21778
C	-0.75754	1.62967	2.63500
H	-0.82171	1.56190	3.72657
H	-1.08796	2.63005	2.34354
H	-1.45451	0.90070	2.21420
C	1.68437	2.29542	2.89413
H	1.50045	3.34209	2.63499
H	1.56926	2.19860	3.97943
H	2.72143	2.04978	2.65164

CuI profile TS2 in DCM

Sum of electronic and zero-point Energies= -1182.932638
Sum of electronic and thermal Enthalpies = -1182.908447
Sum of electronic and thermal Free Energies = -1182.989330

C	-4.64575	0.66867	0.44756
C	-4.49817	0.88163	-0.91313
C	-3.27566	0.56886	-1.56553
C	-2.24644	0.11274	-0.71960
C	-3.62084	0.10695	1.25657
C	-2.96212	0.61747	-2.94984
C	-1.73462	0.16842	-3.40370
H	-3.70106	0.97897	-3.65952
H	-5.59446	0.91082	0.91761
H	-5.32919	1.27906	-1.48950
H	-3.81486	-0.11123	2.30104
H	-1.52490	0.18496	-4.46960
C	-0.71576	-0.32415	-2.53718
H	0.22277	-0.68024	-2.94929
C	-0.97015	-0.26704	-1.18183
I	3.12513	-0.73964	-0.80927
C	-2.41459	-0.15644	0.64836
C	-0.02313	-0.84838	2.50518
H	0.35456	0.17921	2.47309
C	-1.13324	-2.90007	0.58224
H	-1.18876	-3.27935	1.61191
P	-0.86015	-1.07900	0.84331
Cu	0.73770	0.22179	-0.28985
I	0.69802	2.73552	0.68253
C	0.06943	-3.53273	-0.12486
H	1.01769	-3.32915	0.37650
H	-0.07306	-4.61821	-0.14792
H	0.14465	-3.17878	-1.15729
C	-2.44212	-3.22046	-0.13644
H	-2.55140	-4.30938	-0.17668
H	-3.31500	-2.81506	0.38075
H	-2.43958	-2.85064	-1.16608
C	1.13433	-1.81211	2.75289
H	1.59935	-1.54076	3.70647
H	0.79559	-2.84960	2.83355
H	1.90341	-1.74758	1.97926
C	-1.11012	-0.95161	3.58458
H	-1.85147	-0.15370	3.50547
H	-1.62041	-1.92059	3.57327
H	-0.61847	-0.84792	4.55842

▪ X : I, CH_3CN

CuI profile compound 1 in CH_3CN

Sum of electronic and zero-point Energies= -973.981935
Sum of electronic and thermal Enthalpies = -973.961735
Sum of electronic and thermal Free Energies = -974.030034

P	-1.51283	-0.04287	-0.39318
C	-2.15252	-0.85391	1.19834
H	-1.22148	-1.05818	1.74197
C	1.90823	-0.15783	-0.23831
C	1.17346	1.02547	0.09406
C	3.25462	-0.14035	-0.53838
C	-0.25591	1.17418	0.27104
C	1.99452	2.20565	0.26948
C	3.99614	1.05445	-0.47287
H	3.76474	-1.06342	-0.79229
C	-0.73187	2.37715	0.77146
C	1.42775	3.41012	0.76062
C	3.37893	2.19603	-0.03422
H	5.05305	1.04398	-0.72189

C	0.09324	3.48466	1.05200
H	-1.79847	2.50496	0.91911
H	2.08326	4.26576	0.90036
H	3.93828	3.11891	0.09459
H	-0.34346	4.39650	1.44926
C	-2.90468	1.08549	-0.97634
H	-3.26808	1.72343	-0.16216
C	-2.80445	-2.20624	0.88995
H	-2.15153	-2.84062	0.28113
H	-3.01833	-2.74260	1.82284
H	-3.75255	-2.09452	0.35437
C	-3.04079	0.00869	2.09263
H	-3.98702	0.26718	1.60568
H	-3.28821	-0.54052	3.01017
H	-2.54639	0.93707	2.39335
C	-4.07714	0.22205	-1.45489
H	-3.76314	-0.50053	-2.21789
H	-4.54766	-0.33215	-0.63832
H	-4.84816	0.86070	-1.90318
C	-2.40513	1.97071	-2.12168
H	-2.03500	1.36487	-2.95779
H	-3.22595	2.59113	-2.50177
H	-1.59844	2.64149	-1.81193
I	1.13435	-2.17053	-0.08199

CuI profile compound 2 in CH_3CN

Sum of electronic and zero-point Energies= -1182.963755
Sum of electronic and thermal Enthalpies = -1182.938538
Sum of electronic and thermal Free Energies = -1183.027078

C	3.90487	2.66027	1.40358
C	2.96012	2.41173	2.38759
C	2.14129	1.24704	2.32611
C	2.40513	0.43319	1.21311
C	4.14281	1.80157	0.28646
C	1.11198	0.74287	3.16718
C	0.46418	-0.44674	2.85030
H	0.82046	1.28760	4.06417
H	4.51133	3.55737	1.48750
H	2.84160	3.11461	3.20895
H	4.90344	2.05810	-0.44498
H	-0.31519	-0.80032	3.52189
C	0.75942	-1.24109	1.70268
H	0.20835	-2.15772	1.51855
C	1.75475	-0.77296	0.88499
I	-3.68383	-1.81302	0.44406
C	3.36581	0.67330	0.21156
C	1.98942	-0.59388	-2.22198
H	1.26330	0.19737	-1.99625
C	4.00425	-2.28335	-0.65437
H	4.25795	-2.38253	-1.71416
P	2.81664	-0.87104	-0.60217
Cu	-2.59177	0.37378	-0.16064
I	-1.51845	2.53018	-0.88357
C	3.30227	-3.56837	-0.17973
H	2.37992	-3.77925	-0.72536
H	3.98354	-4.40940	-0.33600
H	3.07402	-3.51145	0.88988
C	5.26614	-1.97883	0.15508
H	5.94207	-2.83589	0.08814
H	5.79566	-1.10178	-0.23262
H	5.03914	-1.81181	1.20986
C	1.25431	-1.84159	-2.70801
H	0.68958	-1.58548	-3.61097
H	1.95007	-2.64269	-2.96400
H	0.53915	-2.22018	-1.96619
C	3.00585	-0.07019	-3.23856
H	3.51766	0.83533	-2.88675
H	3.75813	-0.82183	-3.48221
H	2.47700	0.18859	-4.16050

CuI profile compound I in CH_3CN

Sum of electronic and zero-point Energies= -1182.948621
Sum of electronic and thermal Enthalpies = -1182.925031
Sum of electronic and thermal Free Energies = -1183.003099

C	4.25793	0.81864	-1.52070
C	4.25101	-0.51769	-1.81486
C	3.22180	-1.36377	-1.32564
C	2.17485	-0.82901	-0.48394
C	3.16196	1.37144	-0.82840
C	3.25739	-2.73802	-1.67061
C	2.32281	-3.61167	-1.17894
H	4.05020	-3.08069	-2.32999
H	5.05849	1.46548	-1.86681
H	5.03521	-0.96283	-2.42152
H	3.13255	2.45013	-0.72325
H	2.33369	-4.66204	-1.45369
C	1.38187	-3.14910	-0.23891
H	0.71824	-3.86162	0.23925
C	1.33531	-1.81796	0.11975
I	0.11547	-1.46598	1.86384
C	2.10788	0.60921	-0.34924
C	0.90521	2.17418	1.87434
H	1.35102	1.29428	2.35298
C	0.56187	3.03202	-1.01351
H	1.48331	3.60767	-0.87160
P	0.57745	1.54814	0.13023
Cu	-1.28810	0.39232	-0.15249
I	-3.49387	-0.55610	-0.97072
C	-0.62450	3.93411	-0.65922
H	-1.57147	3.38195	-0.69362
H	-0.52650	4.38540	0.33126
H	-0.68840	4.75035	-1.38814
C	0.46575	2.57380	-2.47043
H	1.31726	1.95944	-2.77578
H	-0.44997	1.99367	-2.63724
H	0.43174	3.44916	-3.12921
C	-0.39814	2.49223	2.61229
H	-1.10643	1.65861	2.56019
H	-0.18263	2.68604	3.66967
H	-0.89314	3.38129	2.21029
C	1.90908	3.32373	1.95859
H	2.10082	3.55836	3.01235
H	2.86969	3.06893	1.50167
H	1.53191	4.23452	1.48285

CuI profile TS1 in CH_3CN

Sum of electronic and zero-point Energies= -1182.934934
Sum of electronic and thermal Enthalpies = -1182.910967
Sum of electronic and thermal Free Energies = -1182.990687

C	0.63688	-2.59517	-1.09423
C	0.83587	-1.39953	-0.42924
C	2.08615	-0.70409	-0.49997
C	3.17874	-1.37784	-1.13237
C	2.95148	-2.61444	-1.79767
C	1.69433	-3.16695	-1.84332
H	-0.29886	-3.13459	-0.99623
C	2.24640	0.64503	-0.08213
C	4.44635	-0.74467	-1.14770
H	3.78881	-3.10404	-2.28751
H	1.51434	-4.09278	-2.38187
C	4.61196	0.51742	-0.62212
C	3.49802	1.23515	-0.13823
H	5.28009	-1.26246	-1.61483
H	5.58782	0.99374	-0.64111
H	3.62753	2.27556	0.14380
I	-0.24315	-1.80042	1.81542
C	0.63514	2.08192	1.98722
H	0.97154	1.16996	2.49684
C	0.86133	3.05521	-0.89940
H	1.79082	3.54896	-0.58825
Cu	-0.77368	-0.21633	-0.31966
I	-3.30907	0.01421	-0.99425
P	0.67485	1.55326	0.19084
C	-0.30761	4.02845	-0.73146
H	-0.18137	4.86543	-1.42774
H	-1.26523	3.54785	-0.96096
H	-0.36505	4.44401	0.27753
C	0.99526	2.61462	-2.35972
H	1.85421	1.95704	-2.52147

H	0.09392	2.09128	-2.69929
H	1.12842	3.49735	-2.99524
C	-0.79690	2.37107	2.44878
H	-1.47294	1.54233	2.21560
H	-0.80588	2.51814	3.53482
H	-1.20158	3.27821	1.99047
C	1.59649	3.21719	2.34051
H	1.55474	3.40126	3.42074
H	2.63264	2.97486	2.08894
H	1.32840	4.15153	1.83764

CuI profile compound II in CH_3CN

Sum of electronic and zero-point Energies= -1182.949951
Sum of electronic and thermal Enthalpies = -1182.925401
Sum of electronic and thermal Free Energies = -1183.005378

C	4.97860	0.28815	0.02881
C	4.87661	-1.02926	-0.36222
C	3.61132	-1.64551	-0.53556
C	2.44116	-0.86583	-0.27476
C	3.82137	1.06403	0.26329
C	3.45153	-2.97361	-1.00419
C	2.19324	-3.48485	-1.21463
H	4.33522	-3.57300	-1.20663
H	5.95578	0.74682	0.14760
H	5.77186	-1.61042	-0.56868
H	3.92971	2.10518	0.55056
H	2.06874	-4.49791	-1.58785
C	1.02934	-2.72032	-0.93257
H	0.05934	-3.17865	-1.08291
C	1.15390	-1.42737	-0.47263
I	-2.41435	1.27613	-1.05609
C	2.57573	0.48265	0.12479
C	0.68756	1.29667	2.23679
H	0.93812	0.26201	2.50548
C	1.12486	2.96050	-0.35198
H	2.09576	3.26835	0.06475
P	0.95983	1.26418	0.39118
Cu	-0.47715	-0.34897	-0.34158
I	-2.05148	-2.24936	0.79362
C	0.08350	3.99281	0.07004
H	0.04080	4.12365	1.15334
H	0.36198	4.95662	-0.37092
H	-0.91342	3.73181	-0.29148
C	1.26095	2.85761	-1.87304
H	0.31651	2.55134	-2.33285
H	1.52910	3.84167	-2.27186
H	2.04083	2.15218	-2.17503
C	-0.76139	1.56344	2.64511
H	-0.83762	1.46174	3.73321
H	-1.08685	2.57297	2.38085
H	-1.45029	0.84626	2.19152
C	1.67517	2.23644	2.93649
H	1.48031	3.28625	2.70004
H	1.55792	2.11112	4.01870
H	2.71486	2.00735	2.68878

CuI profile TS2 in CH_3CN

Sum of electronic and zero-point Energies= -1182.937307
Sum of electronic and thermal Enthalpies = -1182.913189
Sum of electronic and thermal Free Energies = -1182.995212

C	-4.73085	0.89580	0.19887
C	-4.45641	1.10717	-1.14322
C	-3.20476	0.72373	-1.69443
C	-2.28115	0.20415	-0.76846
C	-3.81412	0.26944	1.08692
C	-2.77398	0.74618	-3.04747
C	-1.54930	0.20398	-3.39488
H	-3.42306	1.15510	-3.81679
H	-5.70134	1.19010	0.58790
H	-5.21229	1.55249	-1.78442
H	-4.10718	0.05844	2.10968
H	-1.25115	0.19455	-4.43957
C	-0.64581	-0.35830	-2.44707
H	0.29102	-0.78868	-2.78532
C	-0.99656	-0.26860	-1.11261
I	3.12748	-0.91121	-0.81681
C	-2.58067	-0.06365	0.57582
C	-0.37501	-0.67425	2.57865
H	-0.36268	0.42196	2.59058
C	-1.33906	-2.85490	0.64968
H	-1.52423	-3.21608	1.66893
P	-1.07731	-1.03354	0.88296
Cu	0.75155	0.12156	-0.19307
I	0.91805	2.70304	0.67131
C	-0.06407	-3.50666	0.10524
H	0.81498	-3.29908	0.71971
H	-0.21161	-4.59147	0.08453
H	0.13911	-3.17145	-0.91630
C	-2.55606	-3.16951	-0.21815
H	-2.67380	-4.25739	-0.25914
H	-3.47767	-2.74656	0.18929
H	-2.42720	-2.81096	-1.24386
C	1.03396	-1.20391	2.82308
H	1.35753	-0.87650	3.81692
H	1.06517	-2.29721	2.80354
H	1.74569	-0.81813	2.08820
C	-1.37585	-1.18212	3.62592
H	-2.39480	-0.82106	3.46420
H	-1.39084	-2.27423	3.68036
H	-1.04581	-0.80413	4.60027

- **X : Br, gas phase**

CuBr profile compound 1 in GAS phase

Sum of electronic and zero-point Energies= -3534.227323
Sum of electronic and thermal Enthalpies = -3534.207469
Sum of electronic and thermal Free Energies = -3534.274328

P	-1.43017	-0.09250	-0.41660
C	-1.88830	-0.83759	1.27171
H	-0.90480	-1.13061	1.65936
C	1.90344	-0.75515	-0.21887
C	1.39894	0.56092	0.02905
C	3.24821	-1.03085	-0.34907
C	0.01445	0.97817	0.10945
C	2.42237	1.56372	0.22516
C	4.21042	-0.01706	-0.21409
H	3.55751	-2.05254	-0.53911
C	-0.24593	2.28962	0.47625
C	2.06938	2.89220	0.57064
C	3.79771	1.25358	0.08779
H	5.26383	-0.25525	-0.32458
C	0.75804	3.24614	0.72063
H	-1.27463	2.61889	0.56272
H	2.86674	3.61562	0.71879
H	4.52007	2.05227	0.23284
H	0.48139	4.25758	1.00429
C	-2.78846	1.16585	-0.77117
H	-2.95655	1.84665	0.07326
C	-2.69723	-2.12724	1.10215
H	-2.18074	-2.83056	0.44213
H	-2.83827	-2.61725	2.07315
H	-3.69042	-1.94468	0.68112
C	-2.52532	0.12148	2.27458
H	-3.52574	0.43930	1.96151
H	-2.63415	-0.36884	3.24986
H	-1.91438	1.01688	2.42387
C	-4.09932	0.41018	-1.02457
H	-3.97455	-0.35630	-1.79772
H	-4.48037	-0.07869	-0.12425
H	-4.87154	1.10775	-1.36999
C	-2.41344	1.97907	-2.01528
H	-2.26426	1.31830	-2.87646
H	-3.21787	2.68002	-2.26834
H	-1.49511	2.55610	-1.87796
Br	0.79990	-2.30416	-0.32290

CuBr profile compound 2 in GAS phase

Sum of electronic and zero-point Energies= -6303.428174
Sum of electronic and thermal Enthalpies = -6303.403914
Sum of electronic and thermal Free Energies = -6303.484194

C	4.64411	-1.51264	0.30669
C	4.18309	-1.99218	-0.91204
C	2.95535	-1.52283	-1.45350
C	2.31267	-0.57724	-0.64757
C	3.95555	-0.54364	1.09594
C	2.25117	-1.82442	-2.65090
C	1.04517	-1.19658	-2.93399
H	2.65044	-2.55148	-3.35277
H	5.58551	-1.89767	0.68827
H	4.77035	-2.73375	-1.44682
H	4.37704	-0.21618	2.04086
H	0.53410	-1.45555	-3.85676
C	0.41769	-0.23585	-2.08589
H	-0.54015	0.21339	-2.33414
C	1.08532	0.05267	-0.92264
Br	-2.71636	1.35009	-1.25528
C	2.76625	-0.07999	0.58899
C	0.14768	0.57810	2.08230
H	-0.28450	-0.40499	1.82947
C	1.50115	2.77687	0.45391
H	1.19258	3.20789	1.41441
P	1.25010	0.95680	0.65932
Cu	-2.38760	-0.52127	-0.09507
Br	-1.95195	-2.33384	1.08714
C	0.57072	3.28874	-0.65825
H	-0.44605	2.88268	-0.61238
H	0.51052	4.37978	-0.60059
H	0.97812	3.02254	-1.63835
C	2.96718	3.13154	0.19043
H	3.33402	2.65898	-0.72580
H	3.05299	4.21515	0.06210
H	3.62401	2.83565	1.01297
C	-0.99534	1.58539	2.24208
H	-1.67112	1.20289	3.01306
H	-0.63787	2.56780	2.56938
H	-1.58542	1.69717	1.32760
C	1.00016	0.45666	3.35301
H	1.75451	-0.33010	3.27195
H	1.49613	1.39890	3.61498
H	0.33699	0.19575	4.18316

CuBr profile compound I in GAS phase

Sum of electronic and zero-point Energies= -6303.441459
Sum of electronic and thermal Enthalpies = -6303.417458
Sum of electronic and thermal Free Energies = -6303.495818

C	3.71909	1.77090	-1.09120
C	4.19996	0.49522	-1.19609
C	3.43978	-0.60782	-0.73186
C	2.14759	-0.39515	-0.12501
C	2.41341	1.97362	-0.60349
C	3.98436	-1.90922	-0.85969
C	3.31569	-3.00520	-0.38020
H	4.95004	-2.01673	-1.34553
H	4.30920	2.62037	-1.42119
H	5.17774	0.30113	-1.62857
H	2.02702	2.98622	-0.62341
H	3.72405	-4.00467	-0.49079
C	2.10820	-2.81996	0.31367
H	1.60553	-3.66614	0.76836
C	1.56593	-1.56176	0.45876
Br	0.06150	-1.49623	1.62167
C	1.60092	0.94173	-0.16224
C	-0.22805	1.95817	1.89929
H	0.38376	1.19641	2.39642
C	-0.51617	2.83565	-0.98982
H	0.17688	3.64842	-0.74217
P	-0.19078	1.36036	0.11477
Cu	-1.59656	-0.24801	-0.38803
Br	-3.11201	-1.71048	-1.02031
C	-1.94525	3.34073	-0.75296
H	-2.67731	2.53589	-0.88327
H	-2.08109	3.76871	0.24335
H	-2.17869	4.12458	-1.48180
C	-0.33555	2.43511	-2.45824
H	0.67401	2.07857	-2.67748
H	-1.04020	1.64193	-2.73127
H	-0.53736	3.29777	-3.10274
C	-1.63348	1.88007	2.50342
H	-2.07755	0.88979	2.36347
H	-1.58264	2.07812	3.57995
H	-2.31705	2.61258	2.06568
C	0.42995	3.32012	2.11478
H	0.46857	3.54545	3.18633
H	1.45728	3.34181	1.73949
H	-0.13067	4.12843	1.63415

CuBr profile TS1 in GAS phase

Sum of electronic and zero-point Energies= -6303.412012
Sum of electronic and thermal Enthalpies = -6303.388374
Sum of electronic and thermal Free Energies = -6303.465369

C	1.53424	-2.47246	-0.60703
C	1.13235	-1.22926	-0.15806
C	2.03995	-0.12332	-0.14694
C	3.40571	-0.36597	-0.48880
C	3.79129	-1.65687	-0.93990
C	2.86196	-2.66201	-1.05778
H	0.85429	-3.31669	-0.56891
C	1.59645	1.20613	0.07400
C	4.30979	0.72371	-0.44645
H	4.82889	-1.82986	-1.21191
H	3.15271	-3.63890	-1.43265
C	3.87772	1.99547	-0.14224
C	2.50693	2.24759	0.07379
H	5.35330	0.54485	-0.69292
H	4.58407	2.82011	-0.12149
H	2.17315	3.27312	0.20184
Br	-0.09102	-1.79727	1.81092
C	-0.71974	1.86757	1.81605
H	-0.12131	1.17386	2.42060
C	-0.62395	2.68674	-1.14316
H	-0.07542	3.59045	-0.84267
Cu	-0.78164	-0.85287	-0.32150
Br	-2.88566	-1.14893	-1.11069
P	-0.22700	1.34822	0.08815
C	-2.12725	2.98385	-1.16402
H	-2.34740	3.68617	-1.97546
H	-2.70560	2.07089	-1.34077
H	-2.47520	3.43877	-0.23329
C	-0.13914	2.24009	-2.52746
H	0.93373	2.02923	-2.54531
H	-0.67343	1.34059	-2.85094
H	-0.33897	3.03088	-3.25866
C	-2.19591	1.57278	2.10734
H	-2.45985	0.54141	1.86036
H	-2.38695	1.72468	3.17533
H	-2.86843	2.23344	1.55402
C	-0.32840	3.30252	2.17098
H	-0.57975	3.50220	3.21866
H	0.74473	3.47691	2.05333
H	-0.86833	4.03504	1.56226

CuBr profile compound II in GAS phase

Sum of electronic and zero-point Energies= -6303.431159
Sum of electronic and thermal Enthalpies = -6303.407539
Sum of electronic and thermal Free Energies = -6303.483704

C	4.28976	1.33022	-0.64318
C	4.57316	0.00078	-0.43016
C	3.54891	-0.93378	-0.13375
C	2.19438	-0.47084	-0.08716
C	2.96214	1.79918	-0.54003
C	3.80833	-2.30456	0.10122
C	2.76835	-3.16070	0.36728
H	4.83355	-2.66405	0.06892
H	5.08698	2.02878	-0.87894
H	5.59818	-0.35587	-0.49562

H	2.76574	2.85839	-0.67939
H	2.96272	-4.21303	0.55664
C	1.42590	-2.70908	0.37887
H	0.62958	-3.42423	0.54739
C	1.12284	-1.38704	0.13249
Br	-2.76331	0.45045	-0.23629
C	1.94224	0.91285	-0.25531
C	0.18310	1.90008	1.84295
H	0.71856	1.07502	2.33323
C	-0.21088	2.64374	-1.15971
H	0.72568	3.21832	-1.18429
P	0.19588	1.30290	0.07000
Cu	-0.73708	-0.72470	-0.02100
Br	-1.73340	-2.77259	-0.01307
C	-1.34670	3.59671	-0.78780
H	-1.15474	4.13475	0.14388
H	-1.45269	4.34231	-1.58360
H	-2.28721	3.05366	-0.68982
C	-0.42153	2.00392	-2.53685
H	-1.34654	1.42111	-2.54035
H	-0.50063	2.78925	-3.29569
H	0.40883	1.34817	-2.81728
C	-1.20499	2.01159	2.47782
H	-1.08090	2.22134	3.54590
H	-1.78853	2.82600	2.04144
H	-1.78675	1.09553	2.36695
C	1.00691	3.17891	2.03095
H	0.54591	4.03922	1.53690
H	1.06227	3.40943	3.10022
H	2.03068	3.07161	1.66443

CuBr profile compound TS2 in GAS phase

Sum of electronic and zero-point Energies= -6303.396435
Sum of electronic and thermal Enthalpies = -6303.372805
Sum of electronic and thermal Free Energies = -6303.449669

C	4.19637	1.22206	0.51512
C	4.40149	-0.01522	-0.07197
C	3.30708	-0.77546	-0.56069
C	2.03998	-0.19809	-0.35043
C	2.90871	1.80776	0.64841
C	3.31038	-2.02135	-1.24200
C	2.12505	-2.56515	-1.69963
H	4.24815	-2.53954	-1.42219
H	5.05553	1.77922	0.87747
H	5.41215	-0.40431	-0.16365
H	2.81245	2.79693	1.08394
H	2.15043	-3.50827	-2.23878
C	0.85319	-1.95014	-1.50373
H	-0.04898	-2.40978	-1.89431
C	0.83448	-0.78792	-0.76808
Br	-2.74421	-1.00748	-1.11963
C	1.83335	1.07315	0.20425
C	-0.77082	2.08366	1.31058
H	-0.24907	1.61326	2.15361
C	-0.21880	2.12173	-1.69129
H	0.30064	3.06402	-1.46214
P	0.03611	1.15630	-0.11440
Cu	-0.92959	-0.84309	0.29739
Br	-0.27453	-1.21952	2.48167
C	-1.69243	2.41808	-1.99063
H	-2.16048	3.03504	-1.22055
H	-1.75186	2.96906	-2.93521
H	-2.26591	1.49200	-2.08607
C	0.46827	1.46544	-2.88933
H	0.37787	2.13165	-3.75373
H	1.53162	1.28098	-2.71788
H	-0.01417	0.51701	-3.13999
C	-2.26976	1.86762	1.51336
H	-2.57794	2.44093	2.39479
H	-2.86941	2.20225	0.66447
H	-2.49950	0.81774	1.70614
C	-0.39874	3.57027	1.22486
H	0.67213	3.74070	1.08038
H	-0.94152	4.08774	0.42876
H	-0.67672	4.04488	2.17230

▪ X : Br, DCM

CuBr profile compound 1 in DCM

Sum of electronic and zero-point Energies= -3534.247868
Sum of electronic and thermal Enthalpies = -3534.228083
Sum of electronic and thermal Free Energies = -3534.294368

P	-1.42986	-0.08335	-0.42038
C	-1.95024	-0.85989	1.23349
H	-0.98400	-1.16674	1.65265
C	1.91484	-0.75558	-0.22541
C	1.40379	0.55418	0.04204
C	3.25742	-1.01921	-0.39758
C	0.01793	0.96168	0.15081
C	2.42435	1.56251	0.22979
C	4.21407	0.00393	-0.28225
H	3.57810	-2.03531	-0.60075
C	-0.24430	2.25977	0.56329
C	2.06993	2.87980	0.61866
C	3.79912	1.26737	0.04933
H	5.26572	-0.22473	-0.42633
C	0.75916	3.21647	0.81569
H	-1.27280	2.58174	0.67589
H	2.86597	3.60556	0.76288
H	4.51732	2.07126	0.18677
H	0.48053	4.21651	1.13600
C	-2.76028	1.19618	-0.79791
H	-2.93963	1.86106	0.05549
C	-2.76411	-2.13763	1.01111
H	-2.23572	-2.83772	0.35568
H	-2.94044	-2.64516	1.96778
H	-3.74183	-1.93718	0.56205
C	-2.61911	0.08466	2.22872
H	-3.60798	0.40939	1.88759
H	-2.75919	-0.42320	3.19156
H	-2.01327	0.97692	2.41516
C	-4.07423	0.46573	-1.10091
H	-3.94917	-0.28169	-1.89359
H	-4.48391	-0.03921	-0.22211
H	-4.82681	1.18623	-1.44422
C	-2.34139	2.03071	-2.01279
H	-2.18488	1.39204	-2.89040
H	-3.12897	2.75155	-2.26473
H	-1.41843	2.59242	-1.84211
Br	0.81673	-2.31621	-0.27760

CuBr profile compound 2 in DCM

Sum of electronic and zero-point Energies= -6303.475416
Sum of electronic and thermal Enthalpies = -6303.451014
Sum of electronic and thermal Free Energies = -6303.533264

C	3.21072	-2.98846	1.15524
C	2.43818	-3.48925	0.11528
C	1.78446	-2.60368	-0.78539
C	2.01250	-1.25157	-0.50997
C	3.41179	-1.59761	1.40672
C	0.93995	-2.82455	-1.90813
C	0.42002	-1.74932	-2.61767
H	0.69138	-3.83643	-2.21637
H	3.69174	-3.69564	1.82535
H	2.33406	-4.56453	-0.00171
H	4.02510	-1.27954	2.24348
H	-0.22418	-1.95684	-3.46746
C	0.67221	-0.38074	-2.29881
H	0.22316	0.40808	-2.89304
C	1.48882	-0.15349	-1.21919
Br	-4.45505	0.45110	-1.15306
C	2.79155	-0.73137	0.54135
C	1.28089	1.88163	1.11931
H	0.51798	1.14000	1.40091
C	3.71132	1.97635	-0.74507
H	3.87863	2.75682	0.00773
P	2.35041	0.94933	-0.04018
Cu	-2.96972	-0.02891	0.40085
Br	-1.49297	-0.51835	1.97487

C	3.25318	2.62534	-2.05764
H	2.33181	3.20347	-1.94782
H	4.03653	3.30833	-2.40126
H	3.09758	1.87128	-2.83506
C	4.99399	1.16107	-0.92197
H	4.85334	0.33426	-1.62519
H	5.77093	1.81658	-1.32870
H	5.35784	0.75414	0.02516
C	0.59193	3.06901	0.44210
H	-0.12225	3.50173	1.15018
H	1.30429	3.85225	0.16512
H	0.03056	2.76922	-0.44773
C	2.07631	2.28618	2.36492
H	2.54264	1.42667	2.85609
H	2.85241	3.02339	2.13571
H	1.38592	2.74160	3.08228

CuBr profile compound I in DCM

Sum of electronic and zero-point Energies= -6303.475221
Sum of electronic and thermal Enthalpies = -6303.451034
Sum of electronic and thermal Free Energies = -6303.530371

C	3.77034	1.69534	-1.04391
C	4.21077	0.40601	-1.17076
C	3.41375	-0.67865	-0.72258
C	2.12911	-0.43094	-0.11204
C	2.46759	1.93397	-0.56226
C	3.91732	-1.99631	-0.86340
C	3.21854	-3.07531	-0.38604
H	4.87751	-2.12852	-1.35422
H	4.38881	2.53139	-1.35624
H	5.18216	0.18605	-1.60539
H	2.11635	2.95943	-0.56947
H	3.59595	-4.08649	-0.50216
C	2.02312	-2.85769	0.32185
H	1.51034	-3.69416	0.78426
C	1.52097	-1.58371	0.47186
Br	0.03979	-1.46238	1.67001
C	1.62040	0.92078	-0.14139
C	-0.23598	2.03284	1.86813
H	0.35793	1.28411	2.40549
C	-0.44346	2.82403	-1.06069
H	0.27344	3.62091	-0.83579
P	-0.16374	1.38721	0.10325
Cu	-1.59316	-0.22482	-0.37836
Br	-3.11583	-1.72184	-1.01169
C	-1.85559	3.38357	-0.85744
H	-2.61701	2.60218	-0.96676
H	-1.98428	3.85228	0.12153
H	-2.05363	4.14850	-1.61699
C	-0.25790	2.36381	-2.50942
H	0.74204	1.96613	-2.70340
H	-0.98656	1.58614	-2.76721
H	-0.42069	3.21006	-3.18650
C	-1.65644	1.98950	2.43741
H	-2.11158	0.99984	2.32286
H	-1.62828	2.22158	3.50837
H	-2.31887	2.71659	1.95893
C	0.42593	3.39616	2.05882
H	0.43683	3.64851	3.12551
H	1.46331	3.40091	1.71140
H	-0.11560	4.19343	1.53937

CuBr profile TS1 in DCM

Sum of electronic and zero-point Energies= -6303.444566
Sum of electronic and thermal Enthalpies = -6303.420888
Sum of electronic and thermal Free Energies = -6303.497857

C	1.05198	-2.68248	-0.51504
C	0.89277	-1.36564	-0.13868
C	1.98006	-0.44458	-0.14348
C	3.28011	-0.95019	-0.45887
C	3.42242	-2.30766	-0.85539
C	2.32571	-3.13163	-0.94286
H	0.22875	-3.38622	-0.45670
C	1.78708	0.94854	0.03550
C	4.37054	-0.04541	-0.44420
H	4.41242	-2.67882	-1.10586
H	2.43186	-4.16132	-1.27172
C	4.17680	1.29365	-0.18318
C	2.87557	1.80278	0.01455
H	5.36317	-0.42176	-0.67810
H	5.02191	1.97583	-0.18141
H	2.73769	2.87506	0.11659
Br	-0.46744	-1.65648	1.89018
C	-0.35248	2.09353	1.75485
H	0.13402	1.34485	2.39276
C	-0.09300	2.80664	-1.21243
H	0.64717	3.56141	-0.91524
Cu	-0.92258	-0.65949	-0.28788
Br	-3.02955	-0.96892	-1.13648
P	0.02424	1.43687	0.04425
C	-1.48142	3.44956	-1.23267
H	-1.51691	4.20144	-2.02913
H	-2.26489	2.71271	-1.43800
H	-1.72173	3.95420	-0.29370
C	0.28055	2.25553	-2.59169
H	1.28907	1.83240	-2.61205
H	-0.42340	1.47863	-2.91060
H	0.24405	3.06405	-3.33046
C	-1.85259	2.06562	2.06422
H	-2.27876	1.06822	1.92476
H	-2.00756	2.35009	3.11128
H	-2.41795	2.76613	1.44342
C	0.27328	3.46007	2.04029
H	0.08072	3.73223	3.08467
H	1.35731	3.45508	1.89734
H	-0.15548	4.24692	1.41181

CuBr profile compound II in DCM

Sum of electronic and zero-point Energies= -6303.464523
Sum of electronic and thermal Enthalpies = -6303.440934
Sum of electronic and thermal Free Energies = -6303.516803

C	-4.29418	-1.22769	-0.79452
C	-4.56278	0.09230	-0.51174
C	-3.52824	0.98797	-0.13497
C	-2.18459	0.49597	-0.09505
C	-2.97897	-1.73276	-0.67944
C	-3.76604	2.34537	0.19050
C	-2.71468	3.15928	0.53814
H	-4.78373	2.72625	0.16670
H	-5.09654	-1.89708	-1.09064
H	-5.57962	0.47122	-0.57893
H	-2.80123	-2.78767	-0.86387
H	-2.89261	4.19836	0.80334
C	-1.37983	2.68168	0.53205
H	-0.57704	3.37360	0.75671
C	-1.09987	1.37548	0.18933
Br	2.79549	-0.47179	-0.16133
C	-1.95237	-0.88183	-0.32203
C	-0.29363	-1.91438	1.83954
H	-0.86604	-1.10184	2.30699
C	0.21108	-2.65677	-1.14690
H	-0.72038	-3.23977	-1.16598
P	-0.23218	-1.32191	0.07065
Cu	0.75180	0.69617	0.00097
Br	1.75309	2.77425	-0.12469
C	1.34626	-3.60026	-0.75495
H	1.16652	-4.09821	0.20094
H	1.42926	-4.37679	-1.52390
H	2.29487	-3.06547	-0.69602
C	0.42466	-2.03635	-2.53046
H	1.35423	-1.45983	-2.54970
H	0.49836	-2.83475	-3.27653
H	-0.40042	-1.37954	-2.82447
C	1.06493	-2.00319	2.53465
H	0.89363	-2.23935	3.59084
H	1.69165	-2.79196	2.11105
H	1.62012	-1.06470	2.47958
C	-1.09904	-3.21069	1.97534
H	-0.59293	-4.05948	1.50670

H	-1.21084	-3.43955	3.04096
H	-2.10327	-3.12473	1.55229

CuBr profile TS2 in DCM

Sum of electronic and zero-point Energies= -6303.434903
Sum of electronic and thermal Enthalpies = -6303.411269
Sum of electronic and thermal Free Energies = -6303.488329

C	4.31872	0.69910	0.84957
C	4.41260	-0.39723	0.00620
C	3.26069	-0.90304	-0.65318
C	2.05857	-0.24780	-0.32855
C	3.09932	1.38987	1.09158
C	3.15017	-1.94190	-1.61629
C	1.93216	-2.20215	-2.21852
H	4.02908	-2.51187	-1.90477
H	5.22000	1.06612	1.33252
H	5.37891	-0.86568	-0.16129
H	3.09257	2.27544	1.71855
H	1.87325	-2.97700	-2.97832
C	0.73214	-1.49792	-1.90350
H	-0.18870	-1.73080	-2.42783
C	0.80773	-0.56380	-0.89183
Br	-2.83151	-0.55183	-1.31914
C	1.96935	0.88840	0.48746
C	-0.61378	1.79846	1.72155
H	-0.16926	1.09308	2.43388
C	0.08815	2.54734	-1.17354
H	0.62463	3.37955	-0.69617
P	0.21292	1.22491	0.12852
Cu	-0.98124	-0.77991	0.08236
Br	-0.58148	-1.86189	2.10668
C	-1.35837	2.97079	-1.44597
H	-1.82325	3.43704	-0.57438
H	-1.35496	3.71085	-2.25340
H	-1.97315	2.12030	-1.75407
C	0.81749	2.16916	-2.46176
H	0.82513	3.04330	-3.12153
H	1.85609	1.87429	-2.29052
H	0.30283	1.35771	-2.98432
C	-2.13243	1.69058	1.82059
H	-2.42435	2.01069	2.82721
H	-2.64878	2.32970	1.10147
H	-2.48236	0.66462	1.68642
C	-0.11301	3.21831	2.01763
H	0.97427	3.31557	1.95281
H	-0.57284	3.95934	1.35807
H	-0.39936	3.46261	3.04708

▪ X : Br, CH_3CN

CuBr profile compound 1 in CH_3CN

Sum of electronic and zero-point Energies= -3534.245497
Sum of electronic and thermal Enthalpies = -3534.225714
Sum of electronic and thermal Free Energies = -3534.291966

P	-1.43056	-0.08209	-0.42163
C	-1.95180	-0.86481	1.22858
H	-0.98583	-1.17005	1.64955
C	1.91605	-0.75442	-0.22703
C	1.40368	0.55453	0.04202
C	3.25851	-1.01651	-0.40256
C	0.01753	0.96066	0.15228
C	2.42355	1.56352	0.23073
C	4.21411	0.00813	-0.28892
H	3.58124	-2.03181	-0.60680
C	-0.24589	2.25730	0.56909
C	2.06840	2.87963	0.62345
C	3.79847	1.27047	0.04672
H	5.26563	-0.21904	-0.43619
C	0.75730	3.21390	0.82396
H	-1.27441	2.57812	0.68459
H	2.86397	3.60591	0.76789
H	4.51590	2.07489	0.18488
H	0.47786	4.21252	1.14787
C	-2.76017	1.19814	-0.79666
H	-2.93989	1.85877	0.05964
C	-2.76245	-2.14369	1.00180
H	-2.22990	-2.84324	0.34892
H	-2.94209	-2.65151	1.95768
H	-3.73860	-1.94384	0.54897
C	-2.62606	0.07663	2.22309
H	-3.61618	0.39568	1.88057
H	-2.76361	-0.43242	3.18567
H	-2.02580	0.97276	2.40928
C	-4.07349	0.46845	-1.10420
H	-3.94892	-0.27258	-1.90318
H	-4.48181	-0.04342	-0.22885
H	-4.82650	1.19140	-1.44127
C	-2.34068	2.03872	-2.00703
H	-2.18251	1.40494	-2.88811
H	-3.12949	2.75913	-2.25596
H	-1.41941	2.60206	-1.83215
Br	0.81933	-2.31659	-0.27430

CuBr profile compound 2 in CH_3CN

Sum of electronic and zero-point Energies= -6303.476945
Sum of electronic and thermal Enthalpies = -6303.452548
Sum of electronic and thermal Free Energies = -6303.534752

C	3.18126	-3.00061	1.18666
C	2.40723	-3.49781	0.14569
C	1.77383	-2.60872	-0.76639
C	2.02018	-1.25810	-0.49872
C	3.40389	-1.61090	1.42802
C	0.93844	-2.82488	-1.89722
C	0.44691	-1.74629	-2.62256
H	0.67907	-3.83518	-2.20203
H	3.64850	-3.70997	1.86427
H	2.28875	-4.57231	0.03494
H	4.01978	-1.29475	2.26352
H	-0.18651	-1.95019	-3.48151
C	0.71995	-0.37910	-2.31243
H	0.29848	0.41289	-2.92255
C	1.52505	-0.15679	-1.22309
Br	-4.51475	0.45272	-1.14212
C	2.80160	-0.74217	0.55269
C	1.32513	1.88835	1.10231
H	0.54616	1.15937	1.37064
C	3.77598	1.94537	-0.74147
H	3.94481	2.72770	0.00870
P	2.39582	0.94201	-0.04488
Cu	-3.01016	-0.01529	0.39595
Br	-1.51558	-0.49252	1.95367
C	3.34033	2.59050	-2.06320
H	2.42728	3.18349	-1.96443
H	4.13835	3.25816	-2.40324
H	3.17946	1.83248	-2.83577
C	5.04695	1.10864	-0.89792
H	4.89961	0.27794	-1.59534
H	5.83762	1.74896	-1.30236
H	5.39313	0.70567	0.05749
C	0.66993	3.09192	0.42088
H	-0.04114	3.53980	1.12295
H	1.40533	3.85679	0.15397
H	0.11472	2.80639	-0.47763
C	2.11301	2.27176	2.35924
H	2.54747	1.39878	2.85573
H	2.91402	2.98424	2.13842
H	1.42570	2.74892	3.06549

CuBr profile compound I in CH_3CN

Sum of electronic and zero-point Energies= -6303.473667
Sum of electronic and thermal Enthalpies = -6303.449488
Sum of electronic and thermal Free Energies = -6303.528640

C	3.76298	1.70363	-1.05926
C	4.21078	0.41639	-1.18127
C	3.42021	-0.67074	-0.72749
C	2.13319	-0.42874	-0.11879
C	2.46016	1.93708	-0.57518

C	3.93419	-1.98514	-0.86176
C	3.24291	-3.06748	-0.38074
H	4.89673	-2.11125	-1.34958
H	4.37603	2.54228	-1.37526
H	5.18300	0.19921	-1.61546
H	2.10512	2.96108	-0.58269
H	3.62879	-4.07621	-0.49045
C	2.04347	-2.85571	0.32236
H	1.53647	-3.69480	0.78656
C	1.53131	-1.58474	0.46582
Br	0.04309	-1.47251	1.65707
C	1.61853	0.92094	-0.14987
C	-0.22264	2.01900	1.87763
H	0.38222	1.27156	2.40444
C	-0.45346	2.83072	-1.04422
H	0.25848	3.63031	-0.81438
P	-0.16349	1.38724	0.10775
Cu	-1.60190	-0.21807	-0.37901
Br	-3.12562	-1.72073	-1.01301
C	-1.86887	3.37871	-0.83234
H	-2.62476	2.59201	-0.94428
H	-1.99699	3.83956	0.15036
H	-2.07396	4.14738	-1.58627
C	-0.26939	2.38406	-2.49716
H	0.73480	2.00129	-2.69926
H	-0.98990	1.59942	-2.75766
H	-0.44606	3.23412	-3.16589
C	-1.63682	1.96276	2.46063
H	-2.08443	0.96922	2.34826
H	-1.59949	2.19247	3.53182
H	-2.30864	2.68633	1.98990
C	0.43110	3.38613	2.06824
H	0.45427	3.63059	3.13660
H	1.46303	3.40174	1.70538
H	-0.12478	4.18111	1.56096

CuBr profile TS1 in CH_3CN

Sum of electronic and zero-point Energies= -6303.442958
Sum of electronic and thermal Enthalpies = -6303.419291
Sum of electronic and thermal Free Energies = -6303.496207

C	1.03517	-2.68855	-0.50713
C	0.88493	-1.37015	-0.13195
C	1.97703	-0.45458	-0.14131
C	3.27332	-0.96865	-0.45899
C	3.40697	-2.32760	-0.85405
C	2.30516	-3.14530	-0.93856
H	0.20883	-3.38839	-0.44512
C	1.79266	0.94013	0.03397
C	4.36915	-0.07025	-0.44993
H	4.39442	-2.70435	-1.10623
H	2.40441	-4.17580	-1.26715
C	4.18365	1.27058	-0.19097
C	2.88593	1.78832	0.00830
H	5.35852	-0.45326	-0.68668
H	5.03264	1.94792	-0.19322
H	2.75432	2.86160	0.10750
Br	-0.47128	-1.64643	1.89424
C	-0.33623	2.10156	1.75428
H	0.15540	1.35699	2.39305
C	-0.08163	2.80487	-1.21660
H	0.65632	3.56134	-0.91928
Cu	-0.92612	-0.64849	-0.28977
Br	-3.03787	-0.96463	-1.13384
P	0.03369	1.44039	0.04449
C	-1.47146	3.44438	-1.24234
H	-1.50462	4.19553	-2.03959
H	-2.25222	2.70505	-1.45039
H	-1.71603	3.94857	-0.30426
C	0.29633	2.25018	-2.59300
H	1.30657	1.83092	-2.60983
H	-0.40445	1.46973	-2.91093
H	0.25839	3.05668	-3.33384
C	-1.83472	2.07183	2.06995
H	-2.25782	1.07181	1.93832
H	-1.98584	2.36300	3.11577
H	-2.40305	2.76766	1.44651
C	0.28761	3.47088	2.03036
H	0.10069	3.74516	3.07525
H	1.37045	3.46818	1.87873
H	-0.14798	4.25331	1.40123

CuBr profile compound II in CH_3CN

Sum of electronic and zero-point Energies= -6303.463738
Sum of electronic and thermal Enthalpies = -6303.440121
Sum of electronic and thermal Free Energies = -6303.515894

C	-4.29867	-1.20858	-0.80316
C	-4.56262	0.11125	-0.51482
C	-3.52417	1.00089	-0.13356
C	-2.18300	0.50248	-0.09488
C	-2.98558	-1.72043	-0.68954
C	-3.75610	2.35773	0.19927
C	-2.70140	3.16475	0.55371
H	-4.77211	2.74314	0.17625
H	-5.10353	-1.87386	-1.10179
H	-5.57786	0.49471	-0.58044
H	-2.81191	-2.77551	-0.87643
H	-2.87509	4.20301	0.82514
C	-1.36861	2.68045	0.54729
H	-0.56341	3.36761	0.77804
C	-1.09482	1.37503	0.19604
Br	2.80047	-0.47797	-0.14742
C	-1.95603	-0.87489	-0.32829
C	-0.30922	-1.92052	1.83523
H	-0.88174	-1.10790	2.30220
C	0.20538	-2.65408	-1.15379
H	-0.72655	-3.23633	-1.17449
P	-0.23998	-1.32562	0.06849
Cu	0.75430	0.69005	0.00614
Br	1.76022	2.77177	-0.13693
C	1.33931	-3.59973	-0.76451
H	1.15703	-4.10116	0.18896
H	1.42096	-4.37270	-1.53723
H	2.28865	-3.06631	-0.70274
C	0.41957	-2.02814	-2.53448
H	1.35045	-1.45326	-2.55213
H	0.49093	-2.82422	-3.28317
H	-0.40477	-1.36877	-2.82495
C	1.04656	-2.01433	2.53450
H	0.87024	-2.25584	3.58865
H	1.67284	-2.80221	2.10848
H	1.60222	-1.07559	2.48637
C	-1.11651	-3.21634	1.96288
H	-0.60517	-4.06424	1.49875
H	-1.23905	-3.44351	3.02770
H	-2.11577	-3.13052	1.52816

CuBr profile TS2 in CH_3CN

Sum of electronic and zero-point Energies= -6303.435143
Sum of electronic and thermal Enthalpies = -6303.411346
Sum of electronic and thermal Free Energies = -6303.489303

C	4.32889	0.62566	0.87588
C	4.40710	-0.45619	0.01209
C	3.24893	-0.92764	-0.66199
C	2.05681	-0.25998	-0.32634
C	3.12115	1.33422	1.12602
C	3.12431	-1.94270	-1.64860
C	1.90386	-2.16887	-2.26030
H	3.99510	-2.51931	-1.94834
H	5.23467	0.96801	1.36846
H	5.36585	-0.93738	-0.16244
H	3.12720	2.20997	1.76649
H	1.83528	-2.92402	-3.03890
C	0.71449	-1.45268	-1.93200
H	-0.20773	-1.65776	-2.46552
C	0.80166	-0.54367	-0.89783
Br	-2.84707	-0.51099	-1.31762
C	1.98499	0.86276	0.50977
C	-0.59317	1.78675	1.74596
H	-0.16572	1.06137	2.44854
C	0.13119	2.57553	-1.13754

H	0.66790	3.39986	-0.64789
P	0.23844	1.23795	0.14846
Cu	-0.98368	-0.76253	0.06912
Br	-0.61795	-1.91252	2.06696
C	-1.31206	3.00798	-1.41344
H	-1.77462	3.47577	-0.54152
H	-1.29972	3.74989	-2.21910
H	-1.93216	2.16279	-1.72624
C	0.86753	2.20744	-2.42451
H	0.88432	3.08985	-3.07287
H	1.90349	1.90586	-2.24856
H	0.35265	1.40465	-2.96029
C	-2.11429	1.70392	1.82858
H	-2.40861	2.00060	2.84163
H	-2.60964	2.37504	1.12402
H	-2.48360	0.68984	1.65926
C	-0.07121	3.19230	2.07379
H	1.01821	3.27075	2.02333
H	-0.51080	3.95113	1.42065
H	-0.36750	3.42109	3.10399

- **X : Cl, gas phase**

CuCl profile compound 1 in GAS phase

Sum of electronic and zero-point Energies= -1422.676616
Sum of electronic and thermal Enthalpies = -1422.657027
Sum of electronic and thermal Free Energies = -1422.722702

P	1.36975	0.26705	-0.45410
C	1.86904	1.04943	1.20385
H	0.90633	1.42549	1.57199
C	-1.90653	1.17745	-0.34861
C	-1.50491	-0.15563	-0.01170
C	-3.22682	1.54686	-0.49759
C	-0.15521	-0.66783	0.10243
C	-2.60201	-1.06174	0.24386
C	-4.26372	0.62192	-0.29578
H	-3.45432	2.57499	-0.75699
C	0.00450	-1.97283	0.54302
C	-2.35035	-2.39087	0.66625
C	-3.95004	-0.65537	0.08638
H	-5.29607	0.93338	-0.42155
C	-1.06920	-2.83519	0.83664
H	1.00506	-2.37323	0.65599
H	-3.19989	-3.04176	0.85516
H	-4.73164	-1.38476	0.28057
H	-0.86971	-3.84731	1.17695
C	2.63385	-1.10066	-0.74738
H	2.75330	-1.75449	0.12648
C	2.77424	2.26706	0.99089
H	2.33830	2.96614	0.27132
H	2.91941	2.80175	1.93737
H	3.76534	1.98689	0.62093
C	2.42712	0.09198	2.25490
H	3.40278	-0.31223	1.96447
H	2.56676	0.61642	3.20823
H	1.75062	-0.74818	2.43838
C	3.99548	-0.45213	-1.02867
H	3.92884	0.27439	-1.84623
H	4.40250	0.06179	-0.15400
H	4.72061	-1.21954	-1.32452
C	2.20495	-1.94099	-1.95572
H	2.09522	-1.30968	-2.84450
H	2.96397	-2.70051	-2.17812
H	1.25332	-2.45428	-1.79456
Cl	-0.76761	2.49236	-0.54309

CuCl profile compound 2 in GAS phase

Sum of electronic and zero-point Energies= -2080.292192
Sum of electronic and thermal Enthalpies = -2080.267931
Sum of electronic and thermal Free Energies = -2080.347386

C	4.25515	-0.93147	1.13619
C	3.86853	-2.00684	0.34774
C	2.64509	-1.96803	-0.37491
C	1.92770	-0.77988	-0.20092
C	3.48999	0.26338	1.28685
C	2.00358	-2.90107	-1.23385
C	0.77855	-2.59597	-1.81220
H	2.46435	-3.86342	-1.43936
H	5.19491	-1.00092	1.67659
H	4.50944	-2.88263	0.29311
H	3.85349	1.06275	1.92453
H	0.31534	-3.33766	-2.45649
C	0.07089	-1.37371	-1.60596
H	-0.90009	-1.19484	-2.05964
C	0.68228	-0.46695	-0.77721
Cl	-3.14767	0.11391	-1.68672
C	2.30550	0.31860	0.59406
C	-0.39282	1.50743	1.49125
H	-0.73610	0.51248	1.82124
C	0.93176	2.59554	-1.03129
H	0.69691	3.46380	-0.40167
P	0.74207	1.14155	0.09318
Cu	-2.80720	-0.83510	0.21123
Cl	-2.14668	-1.54980	2.11197
C	-0.09563	2.49541	-2.16975
H	-1.11427	2.29364	-1.82820
H	-0.10048	3.43682	-2.72787
H	0.17909	1.69318	-2.86032
C	2.36291	2.72449	-1.55957
H	2.65310	1.84438	-2.14167
H	2.42107	3.59365	-2.22218
H	3.09353	2.85936	-0.75785
C	-1.61550	2.33138	1.07757
H	-2.27297	2.41215	1.94833
H	-1.34597	3.34765	0.76922
H	-2.19215	1.84974	0.28249
C	0.41163	2.18013	2.61313
H	1.23277	1.55243	2.96889
H	0.81407	3.15520	2.31351
H	-0.26193	2.35235	3.45791

CuCl profile compound I in GAS phase

Sum of electronic and zero-point Energies= -2080.314469
Sum of electronic and thermal Enthalpies = -2080.290972
Sum of electronic and thermal Free Energies = -2080.367129

C	-2.61621	-2.68241	-0.91232
C	-3.58499	-1.71807	-0.93614
C	-3.31670	-0.40808	-0.46550
C	-2.01252	-0.07589	0.05606
C	-1.31478	-2.33721	-0.49960
C	-4.35830	0.55108	-0.50363
C	-4.17081	1.81687	-0.01342
H	-5.31404	0.25547	-0.92696
H	-2.82469	-3.69401	-1.24678
H	-4.58264	-1.93794	-1.30627
H	-0.55067	-3.10185	-0.57478
H	-4.96387	2.55671	-0.05259
C	-2.94688	2.14065	0.59490
H	-2.80447	3.11174	1.05603
C	-1.92158	1.22139	0.65034
Cl	-0.54564	1.71689	1.61079
C	-0.96922	-1.06968	-0.05900
C	1.17067	-1.23154	1.94164
H	0.30405	-0.79567	2.45187
C	1.70630	-2.00710	-0.93565
H	1.39934	-3.01744	-0.63920
P	0.85055	-0.74167	0.15040
Cu	1.56133	1.22806	-0.48823
Cl	2.43304	2.99473	-1.25520
C	3.22409	-1.89784	-0.73967
H	3.58027	-0.88350	-0.95130
H	3.54026	-2.16692	0.27104
H	3.72821	-2.57884	-1.43416
C	1.35011	-1.77124	-2.40763
H	0.27864	-1.85883	-2.60327
H	1.67062	-0.77390	-2.72843
H	1.86961	-2.50540	-3.03329
C	2.42449	-0.56179	2.51126

H	2.40413	0.52214	2.36498
H	2.48947	-0.75702	3.58759
H	3.34255	-0.93986	2.05319
C	1.14911	-2.74111	2.18248
H	1.20646	-2.94192	3.25800
H	0.22770	-3.20167	1.81356
H	1.99994	-3.24564	1.71353

CuCl profile TS1 in GAS phase

Sum of electronic and zero-point Energies= -2080.275974
Sum of electronic and thermal Enthalpies = -2080.252679
Sum of electronic and thermal Free Energies = -2080.327606

C	2.27726	-2.03172	-0.08633
C	1.37018	-1.02457	0.17066
C	1.74806	0.35229	0.10723
C	3.12654	0.65957	-0.11152
C	4.04192	-0.39515	-0.37191
C	3.61122	-1.69910	-0.42193
H	1.98931	-3.07110	0.02750
C	0.78881	1.39675	0.12960
C	3.50875	2.02308	-0.14639
H	5.08568	-0.15230	-0.55073
H	4.30801	-2.50061	-0.64827
C	2.57399	3.02779	-0.02976
C	1.20171	2.71531	0.06351
H	4.55670	2.26631	-0.30181
H	2.88547	4.06756	-0.06462
H	0.47430	3.52161	0.04463
Cl	0.27348	-1.84330	1.97987
C	-1.75378	1.17827	1.64858
H	-0.97986	0.85900	2.35816
C	-1.71567	1.75997	-1.36015
H	-1.62588	2.82437	-1.10117
Cu	-0.49041	-1.46864	-0.21950
Cl	-1.97023	-2.71602	-1.19499
P	-0.92997	0.78240	0.01665
C	-3.19652	1.39590	-1.51152
H	-3.60742	1.90264	-2.39145
H	-3.32411	0.31768	-1.65395
H	-3.79219	1.70258	-0.64811
C	-0.95195	1.49247	-2.66177
H	0.10571	1.75923	-2.58555
H	-1.02256	0.43646	-2.94261
H	-1.39055	2.08510	-3.47190
C	-2.98992	0.30527	1.89287
H	-2.76599	-0.75608	1.75992
H	-3.33570	0.45139	2.92200
H	-3.81837	0.56287	1.22749
C	-2.03655	2.66722	1.85750
H	-2.43784	2.82496	2.86481
H	-1.13222	3.27583	1.76775
H	-2.78073	3.04530	1.14897

CuCl profile compound II in GAS phase

Sum of electronic and zero-point Energies= -2080.297432
Sum of electronic and thermal Enthalpies = -2080.274259
Sum of electronic and thermal Free Energies = -2080.348369

C	-2.85954	-2.85341	-0.56412
C	-3.74254	-1.81934	-0.35172
C	-3.28764	-0.50345	-0.08312
C	-1.87685	-0.26336	-0.06468
C	-1.46723	-2.62882	-0.48979
C	-4.16376	0.58245	0.15222
C	-3.65286	1.83392	0.39598
H	-5.23697	0.41113	0.14021
H	-3.22881	-3.85189	-0.77801
H	-4.81377	-1.99986	-0.39590
H	-0.78872	-3.46513	-0.63183
H	-4.32269	2.66796	0.58717
C	-2.25690	2.07801	0.38288
H	-1.89172	3.08485	0.54525
C	-1.36999	1.05491	0.12992
Cl	2.77895	1.33551	-0.33182
C	-0.99388	-1.35751	-0.23291
C	1.06903	-1.33578	1.82357
H	0.18592	-0.91709	2.32584
C	1.72187	-1.81209	-1.18069
H	1.22959	-2.79476	-1.13387
P	0.72362	-0.83997	0.05366
Cu	0.56399	1.37720	-0.07363
Cl	0.42128	3.55609	-0.11528
C	3.20611	-2.00728	-0.87226
H	3.37592	-2.47017	0.10277
H	3.63254	-2.67283	-1.63105
H	3.74051	-1.05740	-0.90278
C	1.49876	-1.22592	-2.57961
H	1.97108	-0.24321	-2.66060
H	1.95183	-1.88761	-3.32524
H	0.43637	-1.12692	-2.82236
C	2.31570	-0.69175	2.43447
H	2.35210	-0.94667	3.49925
H	3.23612	-1.05303	1.96994
H	2.30718	0.39540	2.33898
C	1.04623	-2.85679	2.01050
H	1.89142	-3.34434	1.51589
H	1.12015	-3.08279	3.07950
H	0.11923	-3.30506	1.64411

CuCl profile TS2 in GAS phase

Sum of electronic and zero-point Energies= -2080.265499
Sum of electronic and thermal Enthalpies = -2080.242187
Sum of electronic and thermal Free Energies = -2080.317182

C	3.53527	1.94401	0.80629
C	4.04761	0.70146	0.47031
C	3.18952	-0.33954	0.02800
C	1.82111	-0.01362	0.02274
C	2.15256	2.26206	0.71503
C	3.50776	-1.64496	-0.43179
C	2.50845	-2.48046	-0.89736
H	4.54046	-1.98244	-0.43942
H	4.21977	2.71919	1.13861
H	5.11806	0.52698	0.53946
H	1.81602	3.26653	0.95064
H	2.77659	-3.46625	-1.26740
C	1.12929	-2.11872	-0.92332
H	0.38162	-2.80232	-1.31315
C	0.80164	-0.88949	-0.39415
Cl	-2.45806	-1.99397	-0.95108
C	1.30274	1.25520	0.31925
C	-1.60302	1.75603	0.95169
H	-1.13589	1.53099	1.91849
C	-0.64604	1.49571	-1.93372
H	-0.45762	2.57181	-1.80623
P	-0.40805	0.86131	-0.19568
Cu	-1.00469	-1.22431	0.53216
Cl	-0.76359	-1.07633	2.71633
C	-2.07320	1.29214	-2.45434
H	-2.81122	1.85167	-1.87596
H	-2.12209	1.65445	-3.48669
H	-2.35578	0.23611	-2.43752
C	0.38981	0.93580	-2.90860
H	0.27786	1.44904	-3.86935
H	1.41653	1.08702	-2.56611
H	0.23145	-0.13252	-3.07627
C	-3.04013	1.24039	0.99650
H	-3.57978	1.81391	1.75807
H	-3.56600	1.36137	0.04739
H	-3.08274	0.18789	1.28226
C	-1.53163	3.26158	0.66198
H	-0.50892	3.64804	0.61777
H	-2.04294	3.52496	-0.26870
H	-2.04116	3.78821	1.47625

- **X : Cl, DCM**

CuCl profile compound 1 in DCM

Sum of electronic and zero-point Energies= -1422.697293
Sum of electronic and thermal Enthalpies = -1422.677777
Sum of electronic and thermal Free Energies = -1422.743021

P	1.36771	0.26188	-0.44600
C	1.93129	1.04478	1.18906
H	0.98713	1.43120	1.59290
C	-1.91722	1.18575	-0.33746
C	-1.51043	-0.14386	0.00675
C	-3.23541	1.54625	-0.52211
C	-0.16000	-0.65020	0.13968
C	-2.60691	-1.05528	0.24946
C	-4.26927	0.61056	-0.34640
H	-3.47111	2.57223	-0.78492
C	0.00132	-1.94599	0.60782
C	-2.35481	-2.37609	0.70033
C	-3.95498	-0.66148	0.05540
H	-5.30041	0.91321	-0.50162
C	-1.07327	-2.80735	0.90594
H	1.00201	-2.34197	0.73603
H	-3.20463	-3.02837	0.88350
H	-4.73466	-1.39605	0.23780
H	-0.87294	-3.81111	1.27002
C	2.59818	-1.12143	-0.78892
H	2.72719	-1.77835	0.07992
C	2.84643	2.24881	0.94574
H	2.40340	2.95851	0.23950
H	3.02553	2.78219	1.88770
H	3.82281	1.95291	0.54889
C	2.51796	0.08103	2.21819
H	3.48242	-0.32533	1.89535
H	2.68802	0.60463	3.16761
H	1.84570	-0.75775	2.42400
C	3.96188	-0.49595	-1.10597
H	3.89164	0.23535	-1.92009
H	4.40324	0.00495	-0.24010
H	4.66339	-1.27685	-1.42435
C	2.11917	-1.95159	-1.98443
H	2.00264	-1.32328	-2.87557
H	2.85569	-2.72913	-2.22161
H	1.16154	-2.44696	-1.79992
Cl	-0.77987	2.51672	-0.47667

CuCl profile compound 2 in DCM

Sum of electronic and zero-point Energies= -2080.350909
Sum of electronic and thermal Enthalpies = -2080.326516
Sum of electronic and thermal Free Energies = -2080.408437

C	2.82557	2.80333	-2.03043
C	1.78720	3.42172	-1.34581
C	1.06954	2.71712	-0.33983
C	1.52313	1.40943	-0.13695
C	3.25109	1.46032	-1.79951
C	-0.02226	3.08017	0.49654
C	-0.54425	2.16809	1.40526
H	-0.45967	4.07247	0.42817
H	3.34860	3.37206	-2.79426
H	1.52527	4.44790	-1.58901
H	4.06747	1.04109	-2.37839
H	-1.38213	2.47852	2.02280
C	-0.05597	0.83746	1.57690
H	-0.52079	0.17677	2.30093
C	1.00169	0.47597	0.78010
Cl	-5.09923	0.87247	1.18842
C	2.57204	0.77064	-0.82612
C	1.54677	-2.12737	-0.82229
H	0.75422	-1.64912	-1.41109
C	3.51741	-1.28106	1.35922
H	3.91391	-2.20858	0.92764
P	2.22651	-0.73451	0.16108
Cu	-4.06110	-0.39143	-0.21242
Cl	-3.02082	-1.66201	-1.60834
C	2.87276	-1.58880	2.71707
H	2.06367	-2.32095	2.64625
H	3.63861	-2.00235	3.38099
H	2.47865	-0.67961	3.18074
C	4.64527	-0.25297	1.47271
H	5.38826	-0.62741	2.18418
H	5.14773	-0.08653	0.51615
H	4.27935	0.70856	1.84616
C	0.92966	-3.20891	0.06810
H	0.45527	-3.95631	-0.57558
H	1.68722	-3.71995	0.67002
H	0.15890	-2.80848	0.73232
C	2.61973	-2.67733	-1.76806
H	3.01367	-1.90714	-2.43752
H	3.45373	-3.12907	-1.22140
H	2.16679	-3.45745	-2.38797

CuCl profile compound I in DCM

Sum of electronic and zero-point Energies= -2080.354790
Sum of electronic and thermal Enthalpies = -2080.331382
Sum of electronic and thermal Free Energies = -2080.406554

C	-2.66526	-2.67030	-0.85435
C	-3.62066	-1.69236	-0.89793
C	-3.33029	-0.37706	-0.45351
C	-2.01882	-0.05352	0.05787
C	-1.35581	-2.33571	-0.45618
C	-4.36011	0.59552	-0.50730
C	-4.15760	1.86671	-0.03576
H	-5.31961	0.30256	-0.92416
H	-2.88919	-3.68690	-1.16328
H	-4.62356	-1.90363	-1.25916
H	-0.60672	-3.11663	-0.51430
H	-4.94168	2.61606	-0.08291
C	-2.92985	2.18302	0.57125
H	-2.78366	3.15708	1.02619
C	-1.91660	1.25112	0.63497
Cl	-0.53340	1.73897	1.60090
C	-0.98897	-1.06326	-0.04524
C	1.17929	-1.24531	1.93592
H	0.31877	-0.81004	2.45696
C	1.66111	-2.04200	-0.95337
H	1.34349	-3.04617	-0.65157
P	0.83904	-0.76881	0.14624
Cu	1.58533	1.19699	-0.50371
Cl	2.50078	3.02756	-1.21046
C	3.18113	-1.95522	-0.77719
H	3.55285	-0.94752	-0.99785
H	3.50323	-2.22492	0.23153
H	3.66478	-2.64856	-1.47477
C	1.28469	-1.80366	-2.41844
H	0.20921	-1.88077	-2.59908
H	1.61162	-0.81079	-2.74994
H	1.78498	-2.54620	-3.05055
C	2.44044	-0.57553	2.48690
H	2.41759	0.50999	2.34542
H	2.51814	-0.77169	3.56267
H	3.35245	-0.95555	2.01678
C	1.16387	-2.75344	2.18170
H	1.22679	-2.94617	3.25899
H	0.24200	-3.21915	1.82036
H	2.01352	-3.25646	1.70919

CuCl profile TS1 in DCM

Sum of electronic and zero-point Energies= -2080.315834
Sum of electronic and thermal Enthalpies = -2080.292588
Sum of electronic and thermal Free Energies = -2080.366991

C	2.35339	-1.93988	-0.01441
C	1.40962	-0.95939	0.19917
C	1.71778	0.42965	0.11893
C	3.08621	0.78642	-0.09844
C	4.04767	-0.23533	-0.32653
C	3.67563	-1.55828	-0.35090
H	2.11196	-2.98857	0.12036
C	0.71617	1.43257	0.11643
C	3.41386	2.16322	-0.16547
H	5.08178	0.04927	-0.49999

H	4.40641	-2.33610	-0.55161
C	2.43711	3.13044	-0.06894
C	1.07761	2.76547	0.02770
H	4.45140	2.44295	-0.32892
H	2.70461	4.18154	-0.12518
H	0.31750	3.54029	-0.00547
Cl	0.29052	-1.80559	2.00962
C	-1.81529	1.14381	1.63834
H	-1.03182	0.85698	2.35083
C	-1.78551	1.74235	-1.36634
H	-1.68132	2.80153	-1.09481
Cu	-0.43543	-1.47597	-0.24759
Cl	-1.69448	-3.05029	-1.19507
P	-0.98416	0.76801	0.00403
C	-3.27149	1.40407	-1.50613
H	-3.68415	1.94429	-2.36564
H	-3.42498	0.33391	-1.68274
H	-3.85062	1.69362	-0.62591
C	-1.03776	1.48577	-2.67763
H	0.02160	1.75091	-2.61467
H	-1.11091	0.43333	-2.97401
H	-1.48517	2.08862	-3.47576
C	-3.02878	0.24534	1.89248
H	-2.78281	-0.81361	1.77281
H	-3.37547	0.39360	2.92150
H	-3.86454	0.47913	1.22672
C	-2.13911	2.62562	1.83465
H	-2.52740	2.77669	2.84864
H	-1.25603	3.26122	1.72444
H	-2.90555	2.97218	1.13441

CuCl profile compound II in DCM

Sum of electronic and zero-point Energies= -2080.339922
Sum of electronic and thermal Enthalpies = -2080.316663
Sum of electronic and thermal Free Energies = -2080.390286

C	-2.94485	-2.76972	-0.63551
C	-3.79833	-1.71406	-0.40566
C	-3.30080	-0.41914	-0.10631
C	-1.88347	-0.22773	-0.08435
C	-1.54493	-2.59467	-0.55020
C	-4.13971	0.68889	0.16596
C	-3.58568	1.91215	0.45765
H	-5.21807	0.55451	0.14960
H	-3.34315	-3.75270	-0.86893
H	-4.87450	-1.85990	-0.45510
H	-0.89457	-3.45160	-0.69572
H	-4.22458	2.76187	0.68367
C	-2.18046	2.10702	0.45100
H	-1.79017	3.09580	0.65793
C	-1.33251	1.06454	0.14638
Cl	2.84023	1.32199	-0.35772
C	-1.03396	-1.34310	-0.26998
C	0.98144	-1.35797	1.85071
H	0.08723	-0.93303	2.32582
C	1.70985	-1.88275	-1.12954
H	1.22248	-2.86500	-1.03809
P	0.69112	-0.88972	0.06657
Cu	0.60790	1.34985	-0.08469
Cl	0.49922	3.58887	-0.17949
C	3.18944	-2.06504	-0.79757
H	3.34917	-2.45776	0.20915
H	3.60970	-2.78862	-1.50530
H	3.73850	-1.12801	-0.89649
C	1.49515	-1.36520	-2.55417
H	1.96379	-0.38586	-2.68743
H	1.95817	-2.06266	-3.26032
H	0.43524	-1.28353	-2.81365
C	2.21209	-0.70653	2.48216
H	2.22810	-0.96339	3.54713
H	3.14500	-1.06028	2.03649
H	2.18835	0.38239	2.39702
C	0.95657	-2.87673	2.05023
H	1.82164	-3.36892	1.59747
H	0.98595	-3.08214	3.12607
H	0.04600	-3.33548	1.65577

CuCl profile TS2 in DCM

Sum of electronic and zero-point Energies= -2080.316578
Sum of electronic and thermal Enthalpies = -2080.293195
Sum of electronic and thermal Free Energies = -2080.368158

C	3.74241	1.10584	1.22842
C	4.01181	-0.16670	0.75161
C	2.99286	-0.93685	0.12967
C	1.71953	-0.33825	0.11587
C	2.46810	1.72473	1.10517
C	3.08385	-2.20315	-0.50677
C	1.98122	-2.74169	-1.14657
H	4.02927	-2.73832	-0.51697
H	4.54466	1.67226	1.69240
H	5.01524	-0.57407	0.84066
H	2.33084	2.75089	1.42917
H	2.07791	-3.69839	-1.65238
C	0.70774	-2.10309	-1.18199
H	-0.11849	-2.56733	-1.70952
C	0.57760	-0.92525	-0.47143
Cl	-2.96806	-1.86979	-0.75503
C	1.46001	0.97277	0.54727
C	-1.44302	2.03139	0.80693
H	-1.49160	1.49947	1.76291
C	-0.18039	1.74270	-1.90938
H	-0.61470	2.74185	-1.77944
P	-0.20189	1.04494	-0.18417
Cu	-1.22171	-1.00315	0.40199
Cl	-1.25275	-1.07506	2.68032
C	-1.09166	0.92316	-2.82865
H	-2.09638	0.78447	-2.42250
H	-1.18326	1.44681	-3.78597
H	-0.66361	-0.06480	-3.02099
C	1.22892	1.88439	-2.48151
H	1.15285	2.33256	-3.47785
H	1.86381	2.52974	-1.86918
H	1.72125	0.91361	-2.59282
C	-2.82678	2.06374	0.16296
H	-3.50653	2.59710	0.83575
H	-2.82031	2.59691	-0.79303
H	-3.23021	1.05969	0.00399
C	-0.86204	3.43365	1.03107
H	0.07916	3.41350	1.58528
H	-0.71387	3.98352	0.09637
H	-1.58518	3.99574	1.63307

- **X : Cl, CH_3CN**

CuCl profile compound 1 in CH_3CN

Sum of electronic and zero-point Energies= -1422.695152
Sum of electronic and thermal Enthalpies = -1422.675638
Sum of electronic and thermal Free Energies = -1422.740932

P	1.37021	0.26084	-0.44547
C	1.91954	1.04961	1.19071
H	0.97103	1.43147	1.58881
C	-1.91911	1.18281	-0.34082
C	-1.50979	-0.14659	0.00181
C	-3.23831	1.54417	-0.51669
C	-0.15899	-0.65324	0.13130
C	-2.60565	-1.05830	0.24844
C	-4.27162	0.60900	-0.33426
H	-3.47603	2.57008	-0.77821
C	0.00375	-1.95057	0.59532
C	-2.35243	-2.38080	0.69411
C	-3.95498	-0.66397	0.06320
H	-5.30354	0.91254	-0.48214
C	-1.07004	-2.81319	0.89300
H	1.00460	-2.34656	0.72174
H	-3.20198	-3.03304	0.87856
H	-4.73346	-1.39889	0.24926
H	-0.86823	-3.81809	1.25301
C	2.60730	-1.11751	-0.77985
H	2.73278	-1.77125	0.09162
C	2.83057	2.25754	0.95221
H	2.38776	2.96655	0.24485

H	3.00262	2.79064	1.89560
H	3.81001	1.96522	0.56031
C	2.50524	0.08830	2.22255
H	3.47416	-0.31125	1.90493
H	2.66523	0.61249	3.17340
H	1.83737	-0.75547	2.42233
C	3.97032	-0.48713	-1.08994
H	3.90296	0.24121	-1.90719
H	4.40370	0.01786	-0.22252
H	4.67623	-1.26683	-1.40127
C	2.13935	-1.95248	-1.97637
H	2.02643	-1.32752	-2.87055
H	2.88115	-2.72711	-2.20610
H	1.18312	-2.45244	-1.79665
Cl	-0.78235	2.51422	-0.49211

CuCl profile compound 2 in CH_3CN

Sum of electronic and zero-point Energies= -2080.354926

Sum of electronic and thermal Enthalpies = -2080.330454

Sum of electronic and thermal Free Energies = -2080.413254

C	2.78708	2.84272	-2.04394
C	1.72706	3.41699	-1.35368
C	1.04771	2.68349	-0.34164
C	1.55758	1.39629	-0.14134
C	3.27289	1.51993	-1.81303
C	-0.04904	3.00271	0.50617
C	-0.52156	2.07140	1.42301
H	-0.52561	3.97724	0.44328
H	3.28070	3.43267	-2.81130
H	1.42046	4.43124	-1.59490
H	4.10461	1.13550	-2.39409
H	-1.36025	2.35129	2.05444
C	0.02341	0.76187	1.59041
H	-0.40084	0.08441	2.32400
C	1.08521	0.44247	0.78105
Cl	-5.28797	0.85864	1.20218
C	2.62969	0.80316	-0.83518
C	1.72541	-2.12584	-0.83643
H	0.91934	-1.66866	-1.42405
C	3.67580	-1.21101	1.34269
H	4.10451	-2.12186	0.90715
P	2.35786	-0.71586	0.15383
Cu	-4.24433	-0.40904	-0.19489
Cl	-3.20459	-1.68147	-1.59129
C	3.05331	-1.54280	2.70477
H	2.27308	-2.30596	2.63829
H	3.84069	-1.92610	3.36168
H	2.62750	-0.64924	3.17098
C	4.76178	-0.13801	1.44543
H	5.52670	-0.48424	2.14790
H	5.24550	0.04875	0.48297
H	4.36056	0.80696	1.82509
C	1.14496	-3.23223	0.04718
H	0.70014	-3.99446	-0.60066
H	1.92040	-3.71548	0.64885
H	0.36129	-2.85997	0.71327
C	2.81910	-2.63066	-1.78298
H	3.19554	-1.83790	-2.43609
H	3.66148	-3.06450	-1.23507
H	2.39309	-3.41440	-2.41751

CuCl profile compound I in CH_3CN

Sum of electronic and zero-point Energies= -2080.354879

Sum of electronic and thermal Enthalpies = -2080.331446

Sum of electronic and thermal Free Energies = -2080.406612

C	-2.67051	-2.66962	-0.84493
C	-3.62381	-1.68952	-0.89219
C	-3.33012	-0.37351	-0.45155
C	-2.01783	-0.05179	0.05914
C	-1.36001	-2.33716	-0.44776
C	-4.35801	0.60118	-0.50773
C	-4.15279	1.87322	-0.03908
H	-5.31821	0.30899	-0.92354
H	-2.89665	-3.68685	-1.15016
H	-4.62716	-1.89880	-1.25330
H	-0.61289	-3.12025	-0.50266
H	-4.93545	2.62399	-0.08748
C	-2.92443	2.18831	0.56799
H	-2.77787	3.16266	1.02246
C	-1.91347	1.25388	0.63374
Cl	-0.53079	1.73810	1.60380
C	-0.99027	-1.06401	-0.04136
C	1.18094	-1.24657	1.93513
H	0.31938	-0.81452	2.45720
C	1.65586	-2.04773	-0.95422
H	1.34237	-3.05122	-0.64680
P	0.83834	-0.77299	0.14568
Cu	1.58927	1.19141	-0.50844
Cl	2.49795	3.03872	-1.20537
C	3.17660	-1.95501	-0.78766
H	3.54222	-0.94597	-1.01345
H	3.50566	-2.22072	0.21987
H	3.65756	-2.64895	-1.48659
C	1.27051	-1.81551	-2.41766
H	0.19471	-1.90074	-2.59271
H	1.58980	-0.82121	-2.75296
H	1.77234	-2.55722	-3.04956
C	2.44094	-0.57205	2.48232
H	2.41331	0.51336	2.33959
H	2.52269	-0.76760	3.55793
H	3.35190	-0.95024	2.00863
C	1.17251	-2.75462	2.18137
H	1.23396	-2.94569	3.25910
H	0.25440	-3.22529	1.81687
H	2.02590	-3.25251	1.71036

CuCl profile TS1 in CH_3CN

Sum of electronic and zero-point Energies= -2080.316209

Sum of electronic and thermal Enthalpies = -2080.292977

Sum of electronic and thermal Free Energies = -2080.367057

C	2.33783	-1.94946	-0.02241
C	1.40244	-0.96331	0.19949
C	1.71788	0.42378	0.12561
C	3.08907	0.77204	-0.08942
C	4.04327	-0.25460	-0.32664
C	3.66192	-1.57481	-0.36063
H	2.09043	-2.99737	0.10748
C	0.72240	1.43252	0.12438
C	3.42613	2.14695	-0.14800
H	5.07891	0.02459	-0.49953
H	4.38636	-2.35653	-0.56912
C	2.45498	3.11976	-0.04894
C	1.09259	2.76364	0.04155
H	4.46573	2.42024	-0.30898
H	2.72916	4.16938	-0.09970
H	0.33783	3.54354	0.00800
Cl	0.28331	-1.80350	2.00749
C	-1.81996	1.15728	1.63011
H	-1.04153	0.86812	2.34719
C	-1.76704	1.76117	-1.37323
H	-1.66302	2.81780	-1.09328
Cu	-0.45133	-1.46644	-0.25643
Cl	-1.69530	-3.09647	-1.16272
P	-0.98180	0.77973	0.00020
C	-3.25225	1.42789	-1.52975
H	-3.65460	1.97809	-2.38781
H	-3.40712	0.35970	-1.71858
H	-3.83804	1.71075	-0.65180
C	-1.00638	1.51100	-2.67810
H	0.05231	1.77560	-2.60270
H	-1.07648	0.46007	-2.98127
H	-1.44579	2.11898	-3.47675
C	-3.03851	0.26364	1.87596
H	-2.79483	-0.79645	1.75932
H	-3.39308	0.41478	2.90190
H	-3.86742	0.50049	1.20275
C	-2.13974	2.64021	1.82399
H	-2.53268	2.79221	2.83611
H	-1.25383	3.27213	1.71661

H	-2.90080	2.98802	1.11873

CuCl profile compound II in CH_3CN

Sum of electronic and zero-point Energies= -2080.341444
Sum of electronic and thermal Enthalpies = -2080.318134
Sum of electronic and thermal Free Energies = -2080.391892

C	-2.97680	-2.74062	-0.64184
C	-3.81830	-1.67513	-0.41204
C	-3.30534	-0.38649	-0.11076
C	-1.88602	-0.21264	-0.08890
C	-1.57449	-2.58331	-0.55534
C	-4.13050	0.73127	0.16427
C	-3.56092	1.94662	0.45999
H	-5.21045	0.61032	0.14797
H	-3.38668	-3.71882	-0.87534
H	-4.89618	-1.80751	-0.46197
H	-0.93363	-3.44763	-0.69812
H	-4.18906	2.80358	0.68918
C	-2.15299	2.12356	0.45441
H	-1.75140	3.10659	0.66713
C	-1.31849	1.07145	0.14461
Cl	2.86174	1.30198	-0.36691
C	-1.04994	-1.33745	-0.27505
C	0.95380	-1.36357	1.85645
H	0.05656	-0.93568	2.32279
C	1.69413	-1.90462	-1.12088
H	1.19973	-2.88289	-1.02720
P	0.67772	-0.90419	0.06944
Cu	0.62453	1.33890	-0.08968
Cl	0.53819	3.59246	-0.17987
C	3.17105	-2.09682	-0.78396
H	3.32385	-2.48821	0.22426
H	3.58650	-2.82615	-1.48864
H	3.72815	-1.16457	-0.88475
C	1.48491	-1.39129	-2.54757
H	1.95889	-0.41492	-2.68476
H	1.94480	-2.09520	-3.24931
H	0.42568	-1.30532	-2.80833
C	2.18064	-0.70914	2.49096
H	2.19126	-0.96136	3.55707
H	3.11479	-1.06670	2.05065
H	2.15432	0.37950	2.40024
C	0.92870	-2.88160	2.05980
H	1.80204	-3.37095	1.62028
H	0.94235	-3.08250	3.13684
H	0.02589	-3.34347	1.65140

CuCl profile TS2 in CH_3CN

Sum of electronic and zero-point Energies= -2080.320376
Sum of electronic and thermal Enthalpies = -2080.296675
Sum of electronic and thermal Free Energies = -2080.373315

C	3.75787	1.04023	1.25428
C	4.00389	-0.23603	0.77407
C	2.97284	-0.98303	0.14354
C	1.71047	-0.36100	0.12765
C	2.49721	1.68521	1.12525
C	3.04633	-2.24427	-0.50517
C	1.94064	-2.75323	-1.16370
H	3.98245	-2.79559	-0.51384
H	4.56960	1.59004	1.72178
H	4.99902	-0.66313	0.86383
H	2.37860	2.71486	1.44529
H	2.02485	-3.70396	-1.68283
C	0.68042	-2.08882	-1.20447
H	-0.14520	-2.52836	-1.75365
C	0.56300	-0.92117	-0.47518
Cl	-3.03177	-1.89092	-0.71362
C	1.47670	0.95374	0.56247
C	-1.39798	2.06428	0.81850
H	-1.42844	1.52690	1.77254
C	-0.10888	1.77313	-1.90930
H	-0.44224	2.80964	-1.77344
P	-0.17147	1.07633	-0.18738
Cu	-1.24785	-0.96615	0.36189
Cl	-1.25633	-1.09721	2.65919
C	-1.10327	1.04342	-2.81852
H	-2.11769	1.02302	-2.41364
H	-1.13835	1.56512	-3.78061
H	-0.78166	0.01371	-3.00149
C	1.29946	1.77922	-2.50100
H	1.25224	2.24775	-3.48962
H	2.00439	2.34925	-1.89087
H	1.68791	0.76496	-2.63396
C	-2.79352	2.09947	0.20163
H	-3.45978	2.63075	0.88948
H	-2.80128	2.63636	-0.75183
H	-3.19856	1.09555	0.04505
C	-0.81815	3.46657	1.04280
H	0.14543	3.44655	1.55718
H	-0.71395	4.03122	0.11170
H	-1.52220	4.01064	1.68296

Profiles with Gold

- **X : I, DCM**

AuI profile compound 1 in DCM

Sum of electronic and zero-point Energies= -973.983712
Sum of electronic and thermal Enthalpies = -973.963549
Sum of electronic and thermal Free Energies = -974.031624

P	-1.51063	-0.04332	-0.39444
C	-2.15884	-0.84876	1.19749
H	-1.22973	-1.05984	1.74184
C	1.90721	-0.16097	-0.23878
C	1.17494	1.02310	0.09533
C	3.25244	-0.14507	-0.54307
C	-0.25399	1.17303	0.27348
C	1.99772	2.20170	0.27090
C	3.99532	1.04880	-0.47919
H	3.76006	-1.06889	-0.79912
C	-0.72769	2.37595	0.77560
C	1.43309	3.40555	0.76558
C	3.38114	2.19040	-0.03682
H	5.05134	1.03760	-0.73193
C	0.09902	3.48163	1.05798
H	-1.79426	2.50492	0.92284
H	2.08976	4.26009	0.90681
H	3.94230	3.11233	0.09128
H	-0.33584	4.39344	1.45741
C	-2.89777	1.08978	-0.98190
H	-3.26099	1.73136	-0.17017
C	-2.81855	-2.19722	0.88797
H	-2.17066	-2.83243	0.27497
H	-3.03236	-2.73522	1.81997
H	-3.76757	-2.08052	0.35510
C	-3.04147	0.01801	2.09344
H	-3.98482	0.28742	1.60658
H	-3.29609	-0.53200	3.00852
H	-2.53883	0.94008	2.39965
C	-4.07257	0.23024	-1.46201
H	-3.75814	-0.49697	-2.22017
H	-4.54955	-0.31888	-0.64566
H	-4.83914	0.87005	-1.91634
C	-2.39139	1.97037	-2.12790
H	-2.02145	1.36050	-2.96090
H	-3.20784	2.59418	-2.51205
H	-1.58182	2.63725	-1.81754
I	1.13044	-2.17158	-0.07893

AuI profile compound 2 in DCM

Sum of electronic and zero-point Energies= -1121.379672
Sum of electronic and thermal Enthalpies = -1121.354310
Sum of electronic and thermal Free Energies = -1121.443237

C	5.50665	2.18537	1.15089
C	4.77402	1.97850	2.31273
C	3.68881	1.05940	2.32403
C	3.47675	0.42335	1.09631
C	5.25105	1.52109	-0.08667
C	2.77849	0.65853	3.34092
C	1.78988	-0.27858	3.06816
H	2.84817	1.08463	4.33804
H	6.32604	2.89834	1.17939
H	5.03440	2.52949	3.21237
H	5.86347	1.73631	-0.95616
H	1.11102	-0.55876	3.86865
C	1.60230	-0.90097	1.79653
H	0.80250	-1.61961	1.65400
C	2.47814	-0.52696	0.80772
I	-2.61933	-2.42773	0.54904
C	4.21098	0.62511	-0.08811
C	2.02451	0.17728	-2.19075
H	1.56782	1.02412	-1.66307
C	3.84141	-2.17072	-1.47760
H	3.84910	-2.08893	-2.57216
P	3.10263	-0.57918	-0.91332
I	-2.03828	2.73113	-0.49933
C	2.94597	-3.34461	-1.05936
H	1.91232	-3.23530	-1.39763
H	3.34628	-4.26223	-1.50177
H	2.94314	-3.46736	0.02780
C	5.27578	-2.33159	-0.96914
H	5.31537	-2.35200	0.12453
H	5.67187	-3.28426	-1.33511
H	5.93152	-1.53317	-1.32640
C	0.92625	-0.77771	-2.66367
H	0.28917	-0.24343	-3.37534
H	1.34065	-1.64991	-3.17819
H	0.28909	-1.11706	-1.84259
C	2.89054	0.70274	-3.34149
H	3.63795	1.42429	-2.99900
H	3.40122	-0.10842	-3.87099
H	2.24073	1.21089	-4.06088
Au	-2.33136	0.15466	0.03312

AuI profile compound I in DCM

Sum of electronic and zero-point Energies= -1121.377263
Sum of electronic and thermal Enthalpies = -1121.352808
Sum of electronic and thermal Free Energies = -1121.433642

C	4.40999	0.86678	-1.63840
C	4.37114	-0.44673	-2.01983
C	3.36942	-1.31958	-1.52052
C	2.38800	-0.83752	-0.57655
C	3.35399	1.38126	-0.85988
C	3.37290	-2.67133	-1.94613
C	2.47616	-3.57227	-1.43314
H	4.11176	-2.97616	-2.68209
H	5.19585	1.53011	-1.98637
H	5.11260	-0.85360	-2.70216
H	3.33117	2.45288	-0.69789
H	2.46057	-4.60466	-1.76869
C	1.62473	-3.16904	-0.38644
H	1.01168	-3.91154	0.11314
C	1.61137	-1.86084	0.05145
I	0.62195	-1.61575	1.94818
C	2.32383	0.59232	-0.37196
C	1.13049	2.05525	1.95440
H	1.59141	1.15962	2.38503
C	0.77347	3.05503	-0.89186
H	1.69901	3.61779	-0.72344
P	0.81775	1.52183	0.18227
I	-3.48889	-0.75757	-0.77926
C	-0.40624	3.94416	-0.48633
H	-1.35710	3.40464	-0.56528
H	-0.31326	4.33161	0.53105
H	-0.45287	4.80460	-1.16353
C	0.66845	2.67464	-2.37026
H	1.51056	2.06805	-2.71345
H	-0.25489	2.11596	-2.56195
H	0.64201	3.58651	-2.97755
C	-0.16729	2.32479	2.71906
H	-0.85825	1.47850	2.65228
H	0.06502	2.48996	3.77751
H	-0.68733	3.21481	2.35339
C	2.12803	3.20808	2.07623
H	2.34875	3.37632	3.13645
H	3.07677	2.99090	1.57684
H	1.72932	4.14400	1.67310
Au	-1.15003	0.39479	-0.20433

AuI profile TS1 in DCM

Sum of electronic and zero-point Energies= -1121.351087
Sum of electronic and thermal Enthalpies = -1121.326910
Sum of electronic and thermal Free Energies = -1121.407316

C	0.03333	-2.61239	-0.92298
C	0.59221	-1.47023	-0.38098
C	1.92459	-1.06258	-0.71436
C	2.72117	-1.97238	-1.48007
C	2.13132	-3.15306	-2.00674
C	0.80162	-3.42413	-1.79014
H	-0.96171	-2.92952	-0.63283
C	2.44595	0.22451	-0.40869
C	4.06802	-1.62501	-1.75507
H	2.74507	-3.82567	-2.59936
H	0.34038	-4.31055	-2.21593
C	4.58909	-0.41817	-1.34749
C	3.76048	0.53182	-0.71532
H	4.67670	-2.32313	-2.32387
H	5.62212	-0.16537	-1.56694
H	4.15577	1.52309	-0.51512
I	0.08155	-1.70571	2.10652
C	1.56056	1.90248	1.91158
H	1.78018	0.91787	2.34191
C	1.48770	2.93819	-0.96857
H	2.53306	3.23569	-0.80980
I	-3.44861	0.15069	-0.73155
P	1.21584	1.46468	0.13068
C	0.57008	4.10151	-0.58504
H	0.71940	4.92362	-1.29369
H	-0.48567	3.81165	-0.63040
H	0.77952	4.48633	0.41594
C	1.29133	2.54244	-2.43390
H	1.94950	1.72481	-2.74088
H	0.25531	2.23920	-2.62343
H	1.50989	3.40524	-3.07272
C	0.32438	2.45755	2.62389
H	-0.53542	1.78949	2.51681
H	0.54281	2.55524	3.69315
H	0.03848	3.44583	2.25290
C	2.78931	2.79765	2.08472
H	2.98294	2.93107	3.15516
H	3.68766	2.35828	1.64198
H	2.63923	3.79155	1.65165
Au	-0.77602	0.25712	-0.22966

AuI profile compound II in DCM

Sum of electronic and zero-point Energies= -1121.400977
Sum of electronic and thermal Enthalpies = -1121.376812
Sum of electronic and thermal Free Energies = -1121.455682

C	-5.06417	0.22891	-0.78790
C	-4.84891	1.56960	-0.56912
C	-3.56536	2.05940	-0.21537
C	-2.47556	1.13501	-0.12240
C	-4.00826	-0.69537	-0.63236
C	-3.32992	3.43062	0.04968
C	-2.07250	3.85258	0.40322
H	-4.15658	4.13258	-0.02123
H	-6.05113	-0.13066	-1.06312
H	-5.66600	2.28026	-0.66501
H	-4.21253	-1.75320	-0.76634
H	-1.88749	4.89949	0.62827
C	-0.98625	2.94511	0.45775
H	-0.00831	3.33409	0.71260

C	-1.15829	1.60837	0.16425
I	2.42301	-1.64759	-0.19049
C	-2.74362	-0.24778	-0.30136
C	-1.61320	-1.86504	1.85994
H	-1.86911	-0.90787	2.33387
C	-1.38280	-2.70282	-1.13747
H	-2.45636	-2.93817	-1.14897
P	-1.33248	-1.31778	0.10018
I	2.40313	2.16647	-0.01445
C	-0.63098	-3.97913	-0.76348
H	-0.94082	-4.37952	0.20444
H	-0.85207	-4.73837	-1.52196
H	0.44915	-3.82304	-0.74655
C	-0.98943	-2.17516	-2.51957
H	0.07764	-1.93630	-2.55954
H	-1.19202	-2.94923	-3.26732
H	-1.55683	-1.28255	-2.80074
C	-0.35873	-2.41218	2.54044
H	-0.58971	-2.60155	3.59443
H	-0.02404	-3.35330	2.09697
H	0.46875	-1.69968	2.49847
C	-2.81134	-2.80824	1.99394
H	-2.61798	-3.78440	1.54020
H	-3.00543	-2.97184	3.05964
H	-3.72221	-2.39161	1.55571
Au	0.40824	0.24807	0.04018

AuI profile TS2 in DCM

Sum of electronic and zero-point Energies= -1121.337080
Sum of electronic and thermal Enthalpies = -1121.312716
Sum of electronic and thermal Free Energies = -1121.394974

C	-4.76793	0.99069	0.48850
C	-4.57552	1.23837	-0.86132
C	-3.39198	0.79993	-1.51367
C	-2.43708	0.20585	-0.67098
C	-3.83595	0.26950	1.28452
C	-3.06613	0.81032	-2.89627
C	-1.91982	0.17537	-3.34537
H	-3.74044	1.27553	-3.60984
H	-5.68865	1.32676	0.95648
H	-5.34719	1.74974	-1.43021
H	-4.08015	0.02214	2.31189
H	-1.71206	0.15411	-4.41147
C	-0.98928	-0.46411	-2.47978
H	-0.12226	-0.96678	-2.89515
C	-1.21238	-0.35057	-1.11478
I	3.27064	-0.84579	-0.61019
C	-2.65872	-0.10721	0.67862
C	-0.36192	-1.17852	2.44879
H	0.06278	-0.17133	2.51693
C	-1.65388	-2.98443	0.41751
H	-1.71143	-3.43858	1.41480
P	-1.21570	-1.21477	0.77951
I	0.61781	2.81024	0.77685
C	-0.52259	-3.64897	-0.37493
H	0.45851	-3.52481	0.08964
H	-0.72679	-4.72256	-0.44225
H	-0.47347	-3.25017	-1.39239
C	-3.00409	-3.13829	-0.27893
H	-3.19791	-4.20652	-0.42280
H	-3.82596	-2.72318	0.30946
H	-3.00689	-2.66672	-1.26603
C	0.74705	-2.21591	2.59784
H	1.22667	-2.06369	3.57050
H	0.35717	-3.23829	2.57885
H	1.51722	-2.11348	1.82919
C	-1.45241	-1.33447	3.51839
H	-2.16171	-0.50428	3.51515
H	-2.00012	-2.27817	3.42733
H	-0.95485	-1.33630	4.49465
Au	0.73279	0.15668	-0.24125

▪ X : Br, DCM

AuBr profile compound 1 in DCM

Sum of electronic and zero-point Energies= -975.947529
Sum of electronic and thermal Enthalpies = -975.927432
Sum of electronic and thermal Free Energies = -975.994886

P	-1.43653	-0.10359	-0.40428
C	-2.01161	-0.82429	1.25634
H	-1.06247	-1.12723	1.71559
C	1.94175	-0.72593	-0.22339
C	1.39583	0.56641	0.05153
C	3.28556	-0.96509	-0.40528
C	0.00397	0.95274	0.16666
C	2.40038	1.59392	0.23934
C	4.22108	0.07863	-0.29122
H	3.63055	-1.97192	-0.61366
C	-0.27707	2.24613	0.58173
C	2.02472	2.90373	0.63341
C	3.78000	1.32963	0.05054
H	5.27635	-0.12712	-0.44261
C	0.70975	3.21915	0.83512
H	-1.31084	2.55169	0.69249
H	2.80966	3.64199	0.77515
H	4.48088	2.14813	0.19030
H	0.41530	4.21402	1.15710
C	-2.74474	1.17226	-0.86449
H	-2.94675	1.86352	-0.03803
C	-2.84127	-2.09485	1.04902
H	-2.32613	-2.81339	0.40336
H	-3.02841	-2.58475	2.01281
H	-3.81535	-1.88360	0.59668
C	-2.69839	0.15270	2.20876
H	-3.67100	0.48272	1.82838
H	-2.87751	-0.33258	3.17676
H	-2.08700	1.04030	2.39824
C	-4.05292	0.44122	-1.18918
H	-3.90602	-0.33238	-1.95240
H	-4.49592	-0.03254	-0.30909
H	-4.78820	1.15484	-1.58096
C	-2.27619	1.96657	-2.08771
H	-2.09110	1.30043	-2.93901
H	-3.04902	2.68353	-2.39098
H	-1.35671	2.52842	-1.89920
Br	0.87379	-2.36937	-0.25097

AuBr profile compound 2 in DCM

Sum of electronic and zero-point Energies= -1125.292922
Sum of electronic and thermal Enthalpies = -1125.267769
Sum of electronic and thermal Free Energies = -1125.356273

C	-4.70344	2.98327	-0.00069
C	-3.93222	3.14589	-1.14440
C	-3.09451	2.09130	-1.60197
C	-3.15142	0.94180	-0.80702
C	-4.72620	1.79393	0.78886
C	-2.20486	1.98051	-2.70609
C	-1.48801	0.80891	-2.91513
H	-2.07772	2.81197	-3.39389
H	-5.32856	3.81200	0.31999
H	-3.97156	4.08800	-1.68443
H	-5.35033	1.74117	1.67484
H	-0.81584	0.76177	-3.76739
C	-1.57060	-0.34269	-2.07511
H	-0.97419	-1.22151	-2.29602
C	-2.42917	-0.25074	-1.00778
Br	3.47021	-1.99253	-0.98895
C	-3.92809	0.76509	0.35451
C	-2.09175	-1.09716	1.95833
H	-1.48295	-0.18535	1.90838
C	-4.33954	-2.34936	0.28733
H	-4.46802	-2.75590	1.29837
P	-3.20679	-0.91250	0.51110
Br	2.16861	2.28299	1.17278
C	-3.67571	-3.40250	-0.60996
H	-2.69575	-3.71931	-0.24289

H	-4.32008	-4.28657	-0.64551
H	-3.55839	-3.02882	-1.63163
C	-5.69998	-1.90548	-0.25557
H	-6.33489	-2.78987	-0.37035
H	-6.20614	-1.21134	0.42033
H	-5.60828	-1.43047	-1.23743
C	-1.17657	-2.31827	1.83729
H	-0.47102	-2.30454	2.67419
H	-1.74022	-3.25454	1.89123
H	-0.59161	-2.30857	0.91324
C	-2.90384	-1.09109	3.25763
H	-3.54302	-0.20724	3.34416
H	-3.52596	-1.98652	3.35349
H	-2.20583	-1.07986	4.10065
Au	2.81910	0.14628	0.08998

AuBr profile compound I in DCM

Sum of electronic and zero-point Energies= -1125.297709
Sum of electronic and thermal Enthalpies = -1125.273590
Sum of electronic and thermal Free Energies = -1125.352855

C	4.05767	1.41398	-1.40708
C	4.35963	0.09292	-1.59484
C	3.54959	-0.92378	-1.02607
C	2.40084	-0.57335	-0.22316
C	2.85230	1.75512	-0.76155
C	3.90981	-2.27788	-1.23840
C	3.21105	-3.29635	-0.64334
H	4.76381	-2.48734	-1.87625
H	4.69397	2.19789	-1.80601
H	5.23194	-0.20673	-2.16962
H	2.57686	2.80322	-0.74785
H	3.47487	-4.33541	-0.81389
C	2.18777	-2.98096	0.27011
H	1.71158	-3.77374	0.83668
C	1.83001	-1.67001	0.48824
Br	0.67186	-1.41791	2.04394
C	1.99172	0.81281	-0.21986
C	0.38305	2.12681	1.91774
H	1.00519	1.38318	2.42682
C	0.00786	2.86711	-0.99944
H	0.78651	3.61434	-0.81171
P	0.28758	1.43687	0.17391
Br	-3.28726	-1.58603	-0.83094
C	-1.35146	3.51773	-0.72043
H	-2.16965	2.79683	-0.83068
H	-1.41421	3.95889	0.27714
H	-1.51435	4.32204	-1.44679
C	0.08271	2.40499	-2.45674
H	1.05157	1.97242	-2.71865
H	-0.69178	1.65910	-2.66979
H	-0.08985	3.26379	-3.11521
C	-0.97637	2.15645	2.61911
H	-1.47333	1.18198	2.58276
H	-0.83268	2.42309	3.67247
H	-1.65425	2.89467	2.18136
C	1.11012	3.47138	1.99262
H	1.23139	3.75004	3.04552
H	2.11070	3.42516	1.55218
H	0.55078	4.27433	1.50281
Au	-1.38939	-0.06221	-0.25464

AuBr profile TS1 in DCM

Sum of electronic and zero-point Energies= -1125.265009
Sum of electronic and thermal Enthalpies = -1125.241145
Sum of electronic and thermal Free Energies = -1125.319241

C	-0.24633	-2.79427	-0.23238
C	0.31294	-1.56263	0.02879
C	1.67839	-1.27360	-0.26495
C	2.49991	-2.35316	-0.72059
C	1.91073	-3.61882	-0.98116
C	0.56180	-3.81054	-0.79645
H	-1.26971	-3.01336	0.04824
C	2.21911	0.03692	-0.20260
C	3.87329	-2.09343	-0.95951
H	2.54060	-4.42751	-1.34079
H	0.10468	-4.77177	-1.01313
C	4.39964	-0.83107	-0.80062
C	3.56119	0.25114	-0.46021
H	4.50302	-2.91180	-1.29886
H	5.45373	-0.65129	-0.98944
H	3.97092	1.25648	-0.43983
Br	-0.26341	-1.21558	2.39041
C	1.22016	2.14591	1.67815
H	1.39611	1.26665	2.30983
C	1.33628	2.58514	-1.35593
H	2.37538	2.90409	-1.19441
Br	-3.45555	-0.17335	-0.80407
P	0.98802	1.36527	0.00113
C	0.41455	3.80389	-1.27498
H	0.62841	4.46871	-2.11894
H	-0.63985	3.51301	-1.34043
H	0.55804	4.37800	-0.35649
C	1.22870	1.89792	-2.71919
H	1.90135	1.04081	-2.81158
H	0.20553	1.55381	-2.90816
H	1.49073	2.61504	-3.50479
C	-0.04917	2.83795	2.18011
H	-0.90593	2.15792	2.17449
H	0.11031	3.16638	3.21313
H	-0.30597	3.72074	1.58781
C	2.45212	3.05232	1.73897
H	2.58884	3.39281	2.77146
H	3.36559	2.52833	1.44306
H	2.33869	3.94051	1.11031
Au	-1.00388	0.15650	-0.25348

AuBr profile compound II in DCM

Sum of electronic and zero-point Energies= -1125.317841
Sum of electronic and thermal Enthalpies = -1125.293948
Sum of electronic and thermal Free Energies = -1125.371279

C	4.74203	0.37911	-0.60461
C	4.69942	-0.98141	-0.40499
C	3.47715	-1.64519	-0.12543
C	2.27114	-0.87524	-0.07382
C	3.56359	1.15025	-0.50498
C	3.41071	-3.04307	0.09401
C	2.20192	-3.63965	0.35484
H	4.32647	-3.62701	0.05617
H	5.68376	0.87226	-0.82636
H	5.60927	-1.57359	-0.46327
H	3.62518	2.22596	-0.63784
H	2.14613	-4.70980	0.53536
C	1.00372	-2.88415	0.37478
H	0.06759	-3.39893	0.55463
C	1.01765	-1.52511	0.14265
Br	-2.76076	1.14590	-0.21054
C	2.35794	0.53263	-0.23361
C	0.92558	2.07125	1.80942
H	1.31877	1.19251	2.33869
C	0.66215	2.70480	-1.23748
H	1.68172	3.11575	-1.23951
P	0.79430	1.40068	0.07493
Br	-2.29011	-2.39429	-0.00577
C	-0.31385	3.84504	-0.95339
H	-0.09412	4.35898	-0.01472
H	-0.22676	4.57928	-1.76210
H	-1.34637	3.49076	-0.92476
C	0.40240	2.04342	-2.59347
H	-0.60776	1.62515	-2.63915
H	0.49003	2.79980	-3.38061
H	1.11941	1.24677	-2.81418
C	-0.41452	2.44879	2.44049
H	-0.23505	2.73104	3.48375
H	-0.88421	3.29849	1.93903
H	-1.12194	1.61638	2.43278
C	1.95330	3.20179	1.91424
H	1.62064	4.10814	1.40075
H	2.08393	3.45047	2.97296
H	2.93316	2.91604	1.52386

Au	-0.69729	-0.38398	0.01923

AuBr profile TS2 in DCM

Sum of electronic and zero-point Energies= -1125.243970

Sum of electronic and thermal Enthalpies = -1125.219963

Sum of electronic and thermal Free Energies = -1125.299675

C	-4.37502	-0.50769	1.58933
C	-4.10295	0.80661	1.93178
C	-2.94951	1.46329	1.42192
C	-2.09830	0.65325	0.64969
C	-3.56114	-1.25929	0.69645
C	-2.57350	2.82825	1.52202
C	-1.48122	3.30101	0.81278
H	-3.16653	3.51315	2.12176
H	-5.27002	-0.97807	1.98619
H	-4.78950	1.34851	2.57662
H	-3.86795	-2.25358	0.38986
H	-1.23140	4.35679	0.87070
C	-0.65580	2.47360	0.00393
H	0.18200	2.90495	-0.53308
C	-0.92133	1.11055	0.00031
Br	3.00812	1.52591	-0.67281
C	-2.41320	-0.65337	0.24159
C	-0.32409	-2.38409	-1.24521
H	0.07033	-2.62921	-0.25284
C	-1.66111	-0.12688	-2.69190
H	-1.76427	-1.06271	-3.25485
P	-1.09450	-0.69222	-1.01059
Br	1.46487	-1.78940	2.04649
C	-0.57077	0.72971	-3.34539
H	0.41048	0.24866	-3.34594
H	-0.85147	0.91824	-4.38688
H	-0.47652	1.69514	-2.84053
C	-3.00819	0.59069	-2.66164
H	-3.27779	0.86092	-3.68820
H	-3.80571	-0.03806	-2.25805
H	-2.96149	1.51601	-2.07925
C	0.80970	-2.40516	-2.26670
H	1.21802	-3.42060	-2.30587
H	0.46159	-2.14855	-3.27183
H	1.62477	-1.72940	-1.99263
C	-1.44820	-3.36735	-1.59792
H	-2.22871	-3.40745	-0.83424
H	-1.91011	-3.15532	-2.56700
H	-1.00058	-4.36589	-1.65923
Au	1.01905	0.10017	0.30430

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