Supporting Information

Understanding the Role of Parallel Pathways via In-Situ Switching of Quantum Interference in Molecular Tunneling Junctions

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1 Synthesis and Characterization

Reagents. All reagents and solvents were commercial and were used as received. 1-tert-butythio-4-ethynylbenzene, 4-iodophenylthioacetate were synthesized according to literature procedures.

NMR and Mass Spectra. $^1$HNMR and $^{13}$CNMR were performed on a Varian Unity Plus (400 MHz) instrument at 25°C, using tetramethylsilane (TMS) as an internal standard. NMR shifts are reported in ppm, relative to the residual protonated solvent signals of CDCl$_3$ ($\delta = 7.26$ ppm) or at the carbon absorption in CDCl$_3$ ($\delta = 77.23$ ppm). Multiplicities are denoted as: singlet (s), doublet (d), triplet (t) and multiplet (m). High Resolution Mass Spectroscopy (HRMS) was performed on a JEOL JMS 600 spectrometer.

Figure S1: Synthetic route for FO
1.1 Synthesis of FO

2,7-bis((4-(tert-butylthio)phenyl)ethynyl)-9H-fluoren-9-one (3). 2,7-dibromo-9H-fluoren-9-one 1 (135 mg, 0.4 mmol) and 1-tert-butylthio-4-ethynylbenzene 2 (155 mg, 0.815 mmol) were dissolved in mixture of fresh distilled Et$_3$N (5 mL) and anhydrous THF (20 mL). After degassing with dry N$_2$, the catalysts Pd(PPh$_3$)$_4$ (20 mg, 0.02 mmol) and CuI (10 mg, 0.05 mmol) were added. The reaction mixture was refluxed overnight under N$_2$. The reaction mixture was poured into water, then the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried over Na$_2$SO$_4$ and the solvents removed by rotary evaporation. The crude solid was purified by column chromatography to give product 3 (134 mg, 60%).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.80 (s, 2H), 7.65 (d, $J = 7.7$ Hz, 2H), 7.51 (m, 10H), 1.31 (s, 18H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 192.34, 143.52, 138.06, 137.47, 134.68, 134.06, 131.76, 127.67, 124.56, 123.27, 120.86, 91.17, 90.18, 46.81, 31.23.

S,S’-(((9-oxo-9H-fluorene-2,7-diyl)bis(ethyne-2,1-diyl))bis(4,1-phenylene)) diethanethioate (FO). TiCl$_4$ (0.31 mL, 0.31 mmol, 1M in DCM) was added dropwise to a solution of compound 3 (78 mg, 0.14 mmol) and CH$_3$C(O)Cl (0.03 mL, 0.31 mmol) in 20 mL CH$_2$Cl$_2$ at 0 °C. The resulting mixture was stirred at room temperature for 5 min and the conversion was monitored by TLC (hexanes/CH$_2$Cl$_2$, 1:1). Upon completion, the reaction was quenched with water (10 mL). Then the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried over Na$_2$SO$_4$ and the solvents removed by rotary evaporation. The crude solid was purified by column chromatography to give
Figure S2: $^1$HNMR spectrum of molecular wire FO

target product FO (30 mg, 51%). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.81 (d, $J = 0.7$ Hz, 2H), 7.67 (dd, $J = 7.7$, 1.4 Hz, 2H), 7.55 (dd, $J = 7.4$, 8.0 Hz, 6H), 7.42 (d, $J = 8.3$ Hz, 4H), 2.45 (s, 6H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 193.52, 192.27, 143.61, 138.14, 134.68, 134.48, 132.44, 128.80, 127.74, 124.44, 124.16, 120.89, 90.91, 90.34, 30.53. HRMS(ESI) calcd. for C$_{33}$H$_{21}$O$_3$S$_2$ [M+H]$^+$: 529.09266, found 529.09408.
Figure S3: $^{13}$CNMR spectrum of molecular wire FO
**Figure S4:** HRMS spectrum of molecular wire FO. Top is experimental data, bottom is calculation data.

**Figure S5:** Synthetic route for FH
1.2 Synthesis of FH

2,7-bis((4-(tert-butylthio)phenyl)ethynyl)-9H-fluorene (5) 2,7-dibromo-9H-fluorene (324 mg, 1 mmol) and 1-tert-Butylthio-ethynyl-benzene (418 mg, 2.2 mmol) were dissolved in mixture of fresh distilled Et$_3$N (5 mL) and anhydrous THF (20 mL). After degassing with dry N$_2$, the catalysts Pd(PPh$_3$)$_4$ (40 mg, 0.04 mmol) and CuI (20 mg, 0.1 mmol) were added. The reaction mixture was refluxed overnight under N$_2$. The reaction mixture was poured into water, then the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried over Na$_2$SO$_4$ and the solvents removed by rotary evaporation. The crude solid was purified by column chromatography to give product (120 mg, 22 %). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.76 (d, J = 7.9 Hz, 2H), 7.72 (s, 2H), 7.57 (d, J = 7.8 Hz, 2H), 7.51 (dd, J = 7.8 Hz, J = 7.8 Hz 8H), 3.93 (s, 2H), 1.31 (s, 18H).

13C NMR (101 MHz, CDCl$_3$) $\delta$ 143.79, 141.56, 137.47, 133.42, 131.67, 130.96, 128.42, 123.95, 121.81, 120.37, 91.78, 89.51, 77.55, 77.23, 76.91, 46.72, 36.79, 31.22.

S,S’-(((9H-fluorene-2,7-diyl)bis(ethyne-2,1-diyl))bis(4,1-phenylene)) diethanethioate (FH) TiCl$_4$ (0.42 mL, 0.42 mmol, 1M in DCM) was added dropwise to a solution of compound 5 (100 mg, 0.19 mmol) and CH$_3$C(O)Cl (0.04 mL, 0.42 mmol) in 20 mL CH$_2$Cl$_2$ at 0 °C. The resulting mixture was stirred at room temperature for 10 min and the conversion was monitored by TLC (hexanes/CH$_2$Cl$_2$, 2:1). Upon completion, the reaction was quenched with water (10 mL). The reaction mixture was poured into water, then the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried.
over Na$_2$SO$_4$ and the solvents removed by rotary evaporation. The crude solid was purified by column chromatography to give target product FH (18 mg, 20 %). $^1$HNMR (400 MHz, CDCl$_3$) δ 7.76 (d, J = 7.9 Hz, 2H), 7.72 (s, 2H), 7.57 (d, J = 8.2 Hz, 6H), 7.41 (d, J = 8.3 Hz, 4H), 3.93 (s, 2H), 2.44 (s, 6H). $^{13}$CNMR (101 MHz, CDCl$_3$) δ 193.71, 143.81, 141.64, 134.45, 132.36, 131.01, 128.50, 128.19, 124.86, 121.69, 120.40, 91.98, 89.30, 36.79, 30.51. HRMS(ESI) calcd. for C$_{33}$H$_{23}$O$_2$S$_2$ [M+H]$^+$: 515.11340, found 515.11293.
Figure S7: $^{13}$C NMR spectrum of molecular wire FH
**Figure S8**: HRMS spectrum of molecular wire FH. Top is experimental data, bottom is calculation data.

**Figure S9**: Synthetic route for BPh
1.3 Synthesis of BPh

4,4′-bis((trimethylsilyl)ethynyl)-1,1′-biphenyl 4,4′-dibromo-1,1′-biphenyl (3.12 g, 10 mmol) and trimethylsilylacetylene (2.16 g, 22 mmol) were dissolved in mixture of fresh distilled Et₃N (6 mL) and anhydrous THF (20 mL). After degassing with dry N₂, the catalysts Pd[PPh₃]₄ (80 mg, 0.07 mmol) and CuI (40 mg, 0.2 mmol) were added. The reaction mixture was refluxed overnight under N₂. The reaction mixture was poured into water, then the product was extracted with CH₂Cl₂, washing with saturated NaHCO₃, water and then brine. The organic phase was then collected and dried over Na₂SO₄ and the solvents removed by rotary evaporation. The crude solid was purified by column chromatography to give product (3.15 g, 91 %). ¹HNMR (400 MHz, CDCl₃) δ 7.58 – 7.48 (m, 8H), 0.29 (s, 18H). ¹³CNMR (101 MHz, CDCl₃) δ 140.37, 132.65, 126.92, 122.64, 105.07, 95.41, 0.22.

4,4′-diethynyl-1,1′-biphenyl To a solution of trimethylsilyl derivative 4,4′-bis((trimethylsilyl)ethynyl)-1,1′-biphenyl 7 (694 mg, 2 mmol) in THF (10 mL), tetrabutylammonium fluoride (1 M solution in THF, 4.4 ml, 4.4 mmol, 2.2 equiv.) was added dropwise at 0°C. After completion, then the reactant solution was stirred at room temperature under argon for 0.5 h. The reaction was quench by adding water (5 ml), then the product was extracted with CH₂Cl₂, washing with saturated NaHCO₃, water and then brine. The organic phase was then collected and dried over Na₂SO₄ and the solvents removed by rotary evaporation to provide 4,4′-diethynyl-1,1′-biphenyl (387 mg, 95%) as a yellow solid. The crude was used in next step without further purification. ¹HNMR (400 MHz, CDCl₃) δ 7.56 (q, J = 8.5 Hz, 5H), 3.15 (s, 1H). ¹³C NMR (101 MHz, CDCl₃)
S,S’-((1,1’-biphenyl)-4,4’-diylbis(ethyne-2,1-diyl))bis(4,1-phenylene) diethanethioate
diethanethioate

4,4’-diethynyl-1,1’-biphenyl (200 mg, 1 mmol) and 4-iodophenylthioacetate (612 mg, 2.2 mmol) were dissolved in mixture of fresh distilled Et₃N (5 mL) and anhydrous THF (20 mL). After degassing with dry N₂, the catalysts Pd(PPh₃)₄ (40 mg, 0.04 mmol) and CuI (20 mg, 0.1 mmol) were added. The reaction mixture was refluxed overnight under N₂. The reaction mixture was poured into water, then the product was extracted with CH₂Cl₂, washing with saturated NaHCO₃, water and then brine. The organic phase was then collected and dried over Na₂SO₄ and the solvents removed by rotary evaporation. The crude solid was purified by recrystallization from Toluene to give product (280 mg, 56%).

\[ ^1H \text{ NMR (400 MHz, CDCl}_3) \delta 7.62 (s, 8H), 7.58 (d, J = 8.3 Hz, 4H), 7.41 (d, J = 8.3 Hz, 4H), 2.44 (s, 6H). \]
\[ ^{13}C \text{ NMR (101 MHz, CDCl}_3) \delta 193.70, 140.48, 134.46, 132.43, 132.40, 128.35, 127.16, 124.71, 122.49, 91.10, 89.87, 30.52. \]

HRMS(ESI) calcd. for C₃₂H₂₃O₂S₂ [M+H]⁺: 503.11340, found 503.11293; C₃₂H₂₂O₂S₂NH₄ [M+NH₄]⁺: 520.13995, found 520.13941.

### 1.4 Synthesis of BT

5,5’-bis((trimethylsilyl)ethynyl)-2,2’-bithiophene (11) 5,5’-dibromo-2,2’-bithiophene 10 (1002 mg, 3.11 mmol) and trimethylsilylacetylene (880 mg, 9 mmol) were dissolved in mixture of fresh distilled Et₃N (10 mL) and anhydrous THF (20 mL). After degassing with dry N₂, the catalysts Pd(PPh₃)₄ (80 mg, 0.07 mmol) and CuI (15 mg, 0.08 mmol) were added. The reaction mixture was stirred at room temperature overnight under N₂. The reaction mixture was poured into water, then
Figure S10: $^1$HNMR spectrum of molecular wire BPh
Figure S11: $^{13}$CNMR spectrum of molecular wire BPh
**Figure S12:** HRMS spectrum of molecular wire BPh. Top is experimental data, bottom is calculation data.

**Figure S13:** Synthetic route for BT
the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried over Na$_2$SO$_4$ and the solvents removed by rotary evaporation. The crude solid was purified by column chromatography to give product (870 mg, 78 %). $^1$HNMR (400 MHz, CDCl$_3$) $\delta$ 7.11 (d, J = 3.8 Hz, 1H), 6.99 (d, J = 3.8 Hz, 1H), 0.25 (s, 9H). $^{13}$CNMR (101 MHz, CDCl$_3$) $\delta$ 138.17, 133.68, 123.96, 122.73, 100.72, 97.39, 0.04.

5,5’-diethynyl-2,2’-bithiophene To a solution of trimethylsilyl derivative 5,5’-bis((trimethylsilyl)ethynyl)-2,2’-bithiophene (180 mg, 0.5 mmol) in THF-methanol (10 mL : 3 mL), aqueous KOH (170 mg, 0.5 mL H$_2$O) was added to deprotect the trimethylsilyl group. The reaction solution was stirred at room temperature under N$_2$ for 1 h. The reaction was quench by adding water (5 ml), then the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried over Na$_2$SO$_4$ and the solvents removed by rotary evaporation to provide 5,5’-diethynyl-2,2’-bithiophene as a yellow solid in 95 % yield. The crude was used in next step without further purification. $^1$HNMR (400 MHz, CDCl$_3$) $\delta$ 7.16 (d, J = 3.8 Hz, 2H), 7.02 (d, J = 3.8 Hz, 2H), 3.41 (s, 2H). $^{13}$CNMR (101 MHz, CDCl$_3$) $\delta$ 138.26, 134.13, 124.08, 121.63, 82.85, 76.83, 68.14.

S,S’-((2,2’-bithiophene]-5,5’-diylbis(ethyne-2,1-diyl))bis(4,1-phenylene)) diethanethioate 5,5’-diethynyl-2,2’-bithiophene (107 mg, 0.5 mmol) and 4-iodophenylthioacetate (280 mg, 1 mmol) were dissolved in mixture of fresh distilled Et$_3$N (5 mL) and anhydrous THF (15 mL). After degassing with dry N$_2$, the catalysts Pd(PPh$_3$)$_4$ (40 mg, 0.04 mmol) and CuI (20 mg, 0.1 mmol) were added. The reaction mixture was stirred at room temperature overnight under
Figure S14: $^1$HNMR spectrum of molecular wire BT

N$_2$. The reaction mixture was poured into water, then the product was extracted with CH$_2$Cl$_2$, washing with saturated NaHCO$_3$, water and then brine. The organic phase was then collected and dried over Na$_2$SO$_4$ and the solvents removed by rotary evaporation. The crude solid was purified by recrystallization from toluene to give product (75 mg, 30%). $^1$HNMR (400 MHz, CDCl$_3$) $\delta$ 7.54 (d, J = 8.4 Hz, 4H), 7.40 (d, J = 8.4 Hz, 4H), 7.20 (d, J = 3.8 Hz, 2H), 7.10 (d, J = 3.8 Hz, 2H), 2.44 (s, 6H). $^{13}$CNMR (101 MHz, CDCl$_3$) $\delta$ 193.60, 138.62, 134.46, 133.48, 132.11, 128.63, 124.38, 124.16, 122.52, 94.10, 84.40, 30.53. HRMS (ESI) calcd. for C$_{28}$H$_{19}$O$_2$S$_4$ [M+H]$^+$: 515.02624, found: 515.02734.
**Figure S15:** $^{13}$CNMR spectrum of molecular wire BT
Figure S16: HRMS spectrum of molecular wire BT. Top is experimental data, bottom is calculation data.
Figure S17: UV-Vis spectra of BT (dark green), BPh (light green), FH (violet) and FO (blue).

1.5 UV-Vis

UV-Vis measurements were carried out on a Shimadzu UV 3600 spectrometer, in 1 cm fused quartz cuvettes with concentrations of $10^{-5}$ M in chloroform. Figure S17 shows the UV-Vis spectra of the four molecule and their calculated optical band gaps are summarized in Table 1 of the main text. UV-Vis spectra of FO and FH, with and without their treatment with trifluoroacetic acid (TFA) for QI switching of conductance in STM-BJ measurements is shown in Figure S23.

2 SAM formation and Characterization

The SAMs of were formed via in situ deprotection of the anchoring thioacetate groups to form thiols on template-stripped Au substrates (AuTS). Freshly template-stripped substrates were immersed into 3 mL of 50 µM solutions of the thioacetate precursors in freshly distilled toluene inside a nitrogen-filled glovebox and sealed under a nitrogen atmosphere. The sealed vessels were kept
inside a nitrogen flow box\(^5\) (O\(_2\) below 3\%, relative humidity below 10\%) overnight; all subsequent handling and EGaIn measurements were performed inside the flowbox. 1.5 h prior to measurement, 0.05 mL of 17 mM diazabicycloundec-7-ene (DBU) in toluene was added to the precursor/substrate solution. The substrates were then rinsed with toluene and allowed to dry for 30 min before performing the measurements. The SAMs of AQ were prepared according to the reported methods\(^6\) in dichloromethane (DCM).

The SAMs were characterized by water contact angle and X-ray photoelectron spectroscopy. SAMs of CH\(_3\)(CH\(_2\))\(_{17}\)SH on Au (on mica) were used as a reference.

### 2.1 Water Contact Angle

Water contact angles were measured under ambient conditions on a SCA20 Dataphysics instrument. Contact angles were obtained by applying 3 \(\mu\)L water droplets on SAMs modified Au\(^{TS}\) substrates using the sessile drop method. The contact angles were measured at two different samples for each molecule, three different locations on each sample. The results were averaged with the standard deviation as the error and summarized in Table S1.

**Table S1:** Water contact angles on SAMs of BT, BPh, FH, and FO.

| Compound | BT     | BPh    | FH     | FO     |
|----------|--------|--------|--------|--------|
| Water contact angle (°) | 47.1 ± 1.2 | 48.9 ± 1.5 | 47.1 ± 1.2 | 46.8 ± 4.3 |
2.2 X-ray Photoelectron Spectroscopy (XPS)

The FO, FH, BPh, and BT SAMs were characterized by synchrotron-based X-ray photoelectron spectroscopy (XPS). The measurements were performed at the HE-SGM beamline (bending magnet) of the German synchrotron radiation facility BESSY II in Berlin using a custom-designed experimental station. The acquisition of the XP spectra was carried out with a SCIENTA SES200 electron energy analyzer, in normal emission geometry. The synchrotron light served as the primary X-ray source. The photon energy (PE) was set either to 350 eV or 580 eV depending on the acquisition range. The energy resolution was \( \sim 0.3 \) eV and \( \sim 0.6 \) eV, respectively. The binding energy (BE) scale of the spectra was referenced to the Au \( 4f_{7/2} \) peak at 84.0 eV. The spectra were fitted by symmetric Voigt functions and a linear or Shirley-type background. The S \( 2p_{3/2,1/2} \) doublets were fitted by two peaks with the same full width at half-maximum (fwhm), a standard spin-orbit splitting of \( \sim 1.2 \) eV (verified by fit), and a branching ratio of 2 (\( S2p_{3/2}/S2p_{1/2} \)). The fits were performed self-consistently: the parameter settings for identical spectral regions were correlated.

The intensity values derived within the fitting procedure were used to calculate the effective thicknesses and packing densities of the monolayers. The effective thicknesses were estimated from the C1s/Au4f intensity ratio, assuming a standard exponential attenuation of the photoelectron signal and using the attenuation lengths typical of densely packed SAMs. The spectrometer specific constants were determined using a well-defined octadecanethiolate (C18) monolayer on Au(111)
as a reference; the thickness of this film was set to 20.9 Å. The packing densities of the monolayers were calculated from the $S\,2p/Au\,4f$ intensity ratio, with only thiolate stemming intensity being considered and same assumptions as in the case of the thickness evaluation. Once again, a C$_{18}$ SAM, with a well defined packing density of $4.63 \times 10^{14} \, cm^{-2}$, served as the reference; this density corresponds to a molecular footprint of 21.6 Å.

**XPS result analysis**  

The Au $4f_{7/2}$, C 1s, and S 2p XP spectra of the SAMs in questions are presented in Figure S18, along with the spectra of the reference C$_{18}$ monolayer. The Au $4f_{7/2}$ spectra of all SAMs in question in Figure S18a exhibit similar intensity of the Au $4f_{7/2}$ peak, which suggests a similar effective thickness of all these monolayers. The C 1s spectra of the SAMs in question in Figure S18b exhibit a strong peak at 284.7 eV to 285.0 eV assigned to the molecular backbone. This peak is noticeably broader than that for the reference C$_{18}$ monolayer, since it contains contributions of several different functional groups comprising the molecular backbone, such as oligophenylene, phenyl (BPh)$_{14-16}$, fluorene (BPh$_{17,18}$FO), and thiophene (BT)$_{19,20}$ In addition, there are much weaker signals at higher binding energies, which, most likely, stem from contamination that could be hardly avoided for the complex SAM-forming molecules of the present study, and, in the case of BT film, can be partly associated with the thiophene moieties.

The S 2p spectrum of the reference C$_{18}$ SAM in Figure S18c exhibits exclusively the characteristic S $2p_{3/2,1/2}$ doublet of thiolate (1) at ca. 162.0 eV (S $2p_{3/2}$), which underlines the well-defined character of this reference monolayer, with all anchoring groups bound to the substrate in the thiolate fashion. In contrast, the S 2p XP spectra of the SAMs in question exhibit complex
spectral shapes as can be expected from the chemical composition of the SAM building molecules. These spectra can be decomposed into individual contributions ($S\ 2p_{3/2,1/2}$ doublets) associated with specific sulfur-containing groups in the SAM forming molecules. These contributions include the characteristic signals of thiolate (1) at ca. 162.0 eV$^{18}$ ($S\ 2p_{3/2}$), a doublet representing the terminal, unbound SAc groups (2) at 163.8 eV to 163.9 eV$^{2,22,23}$ ($S\ 2p_{3/2}$), and, in the case of the BT film, a doublet associated with the backbone thiophene moieties (3) expected at the nearly same binding energy as for the unbound SAc groups.$^{21}$ For the BT film, the latter two doublets merge together and become hardly distinguishable; they are therefore fitted by a joint feature in the respective S 2p XP spectrum. Finally, the spectra of the SAMs in question exhibit an additional doublet (4) at ca. 161.0 eV ($S\ 2p_{3/2}$), which we assign to atomic sulfur bound to gold,$^{18}$ in view of the specific binding energy characteristic of this species$^{24}$ (see a discussion in refs 25 and 26 for alternative assignments). This feature is frequently observed in high-resolution XP spectra of thiolate SAMs,$^{18}$ while the presence of atomic sulfur at the SAM-substrate interface should not disturb the thiolate species – this interface can accommodate at least a double amount of sulfur as compared to the standard density of the thiolate groups in the densely packed monolayers.$^{27}$ In the present case, the portion of the atomic sulfur as compared to thiolate is 67%, 119%, 68%, and 71% for the FO, FH, BPh, and BT SAMs, respectively.

For all SAMs in question, except for the FO film, the intensity of the thioacetate or joint thioacetate-thiophene doublet is much higher than that of the thiolate groups, which is especially pronounced in the BT case and associated with the additional (with respect to the other films) sulfur atoms in the backbone. This behavior can only be explained by the difference in the attenuation

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Figure S18: The Au 4f\textsubscript{7/2} (a), C 1s (b), and S 2p (c) XP spectra of the BT, BPh, FH, and FO SAMs as well as reference C18 monolayer (open circles). The S 2p spectra are decomposed into individual doublets associated with specific sulfur species in the monolayers: thiolate (1, red line), unbound S (2, olive line), thiophene S (3, olive line), atomic S (4, blue line); see text for details. For the BT SAM, the doublets 2 and 3 are merged together into a joint feature.
of the respective signals, linked to the SAM-substrate (thiolate) and SAM-ambient (thioacetate) interfaces and SAM backbone (thiophene) and characteristic of an upright orientation of thiol-terminated molecules\textsuperscript{2,22} and molecules with sulfur-containing groups in the molecular backbone.\textsuperscript{23} This observation suggests that the molecules in the BT, BPh, and FH SAMs are assembled upright, in the expected SAMs fashion, with one of the terminal (deprotected) thioacetate groups bound to the substrate and the another (partially deprotected) one exposed to the SAMs-ambient interface, where it can be contacted by the top electrodes.\textsuperscript{1,2} As to the FO SAM, the signal of the thioacetate is only slightly higher than that of thiolate, which suggests larger molecular tilt as compared to other monolayers.

Based on the C 1s and Au 4f intensities and using the procedure described in the previous section, we calculated the effective thicknesses of the SAMs in question and compiled the derived values in Table S2. Also, based on the intensities of the S 2p thiolate signal and Au 4f signal and using the procedure described in the previous section, we calculated the packing density of the SAMs in question and compiled the derived values in Table S2. The derived effective thicknesses are close to each other while the derived packing densities correspond to densely packed SAMs but differ to some extent. One should, however, consider that the above values are course estimates only, in view of the difference between the kinetic energies of the Au 4f and S 2p photoelectrons at the given excitation energy (350 eV).
Table S2: The effective thickness and packing density of the SAMs in question along with the data for the reference C18 monolayer. The effective thickness of the BT SAM was corrected for the presence of the S atoms in the backbone. The accuracy of the effective thickness values is ±1 Å; the accuracy of the packing density values is ±10%.

| Sample | Effective Thickness (Å) | Packing density (molecules/cm²) |
|--------|-------------------------|--------------------------------|
| C18    | 20.9                    | $4.6 \times 10^{14}$          |
| BT     | 18.3                    | $5.5 \times 10^{14}$          |
| BPh    | 20.5                    | $3.0 \times 10^{14}$          |
| FH     | 20.4                    | $2.6 \times 10^{14}$          |
| FO     | 18.2                    | $5.1 \times 10^{14}$          |

Table S3: Summary of EGaIn junctions.

| Compound | BT   | BPh  | FH   | FO   |
|----------|------|------|------|------|
| Yield of working junctions (%) | 80.0 | 78.9 | 82.4 | 85.7 |
| Num. of working EGaIn junctions | 28   | 30   | 28   | 30   |
| Total J/V traces | 588  | 633  | 578  | 630  |
| Num. of samples | 3    | 3    | 3    | 3    |

3 Electrical Measurements

3.1 EGaIn measurements

The details of the EGaIn setup are described elsewhere.²,6 Briefly, EGaIn measurements were carried in the nitrogen flowbox. For each SAM, at least 10 junctions were measured on each of three different substrates by applying a bias from $0.00 \, \text{V} \rightarrow 1.00 \, \text{V} \rightarrow -1.00 \, \text{V} \rightarrow 0.00 \, \text{V}$ with steps of $0.05 \, \text{V}$. At least 20 trace/re-trace cycles were measured for each junction; only junctions that did not short over all 20 cycles were counted as “working junction” for computing yields. A new EGaIn tip was prepared every 4 junctions.

J-V Data Processing: Data was acquired as described above and then parsed in a “hands-off”
Figure S19: Plots of $\log |J(\text{A/cm}^2)|$ versus $V$ of Au$^{\text{TS}}$/SAM//EGaIn junctions comprising SAMs of four molecular wires in Figure 1 of the main text. Each datum is the peak position of a Gaussian fit of $\log |J|$ for that voltage. The error bars are 95% confidence intervals taking each junction as a degree of freedom.

Figure S20: $\log |J(\text{A/cm}^2)|$ Histogram of Au$^{\text{TS}}$/SAM//EGaIn junctions comprising BT (dark green), BPh (light green), FH (violet), and FO (blue) at different bias: Left panel top to bottom starting from $-1.0$ V to $-0.1$ V and right panel top to bottom starting 1.0 V to 0.1 V.
manner using Scientific Python to produce histograms of $J$ for each value of $V$ and the associated Gaussian fits (using a least-squares fitting routine). The confidence intervals for $\mu_{\log J}$ (Gaussian mean) depicted as error bars in the $J/V$ plots were calculated using $\alpha = 0.95$ from $\sigma_{\log J}$ (standard deviation) taken from Gaussian fits and a number of degree of freedom equal to the $N_{\text{junctions}} - 1$. The source code of the python GaussFit code used for the data processing is publicly available and can be downloaded from https://github.com/rchiechi/GaussFit.

Low-bias conductance were obtained by computing the slope of EGaIn data ($J$ vs. $V$) for the lowest 4 data points, i.e., from $-0.1$ V to $0.1$ V. This was done by fitting a linear equation to the linear $J - V$ data. The standard deviation of the slope from the linear fitting served as the error in the Low-bias conductance values reported in Figure 3 and Table 1 of the main text.

Differential Conductance Heatmap: The $J - V$ plots were smoothed by the polynomial model and the derivative of the current density ($J$) relative to the voltage ($dJ/dV$) were computed individually from each $J - V$ plot. Then we constructed a 2D histogram of these $dJ/dV$ values by logarithmically binning them for each bias voltage and plotting them, resulting in a heatmap with on the x-axis the bias voltage, on the y-axis the log ($dJ/dV$) and on the z-axis (in color scale) the number of counts.
**Figure S21**: Normalized differential conductance heatmap plots of Au^{TS}/SAM//EGaIn junctions comprising BT, BPh, FH, FO, BDT-2 and AQ showing histograms binned to log \( \frac{dJ}{dV} \) (normalized differential conductance, Y-axis) versus potential (\( V \), X-axis). The colors correspond to the frequencies of the histograms and lighter (more yellow) colors indicate higher frequencies.
3.2 STM-BJ measurements

We fabricated the single-molecule junction via scanning tunneling microscope break junction (STM-BJ), following the typical protocol. An oxidized silicon substrate with a diameter of 4 inches was cleaned via plasma cleaner, then an adhesion layer of 20 nm Cr and bottom electrode layer of 200 nm Au was evaporated onto it. Then the substrate was cut into 30 mm x 10 mm units. Before the STM-BJ experiments, the unit substrates were cleaned using the piranha solution. The top electrode was formed from a gold wire with a diameter of 0.25 mm (purity of 99.99 %), which cleaned via flame and formed into gold bead. Solutions with target molecules with the concentration of 0.1 mM in the mixture solvent (tetrahydrofuran and 1,3,5-trimethylbenzene \( \nu/\nu = 1 : 4 \)) were added onto the substrate. 100 mV bias voltage was added between the top and bottom electrodes for the electrical measurements using a home-built amplifier. The moving components combined by motor and piezo stack first attach the top electrode to the bottom gradually till they contact each other. With the current feedback, the distance between the top and bottom electrodes changed so that to form and break the nano junction repeatedly. During this process, the target molecules with anchoring groups which can bonded with gold electrodes can form a gold/molecule/gold junction, which exhibited a plateau in the conductance-distance plot. By statistical analysis, we can construct the conductance histogram of the target molecule. We performed multiple experiments/tests for each molecule (BT: 2, BPh: 2, FH: 5, and FO: 5), the 1-D conductance histograms of which are shown in Figure S22. By Gaussian fitting, the peak values were computed corresponding to every measurement. Then, using these peak values for every molecule, the geometric mean and standard error of mean were calculated using scientific python (scipy), same as for EGaIn data, which are
reported in Table 1 as the conductance and error values, respectively.

Figure S22 shows the conductance histograms of the four molecular wires studied using STM-BJ technique. The mean conductance values obtained by fitting the 1D histograms with gaussian curves are shown in the maintext Figure 3 and compared with the DFT and EGaIn values. The ratio of conductance of \textit{FH} and \textit{BPh} is in agreement with the reported data by Vekataraman \textit{et al.}\textsuperscript{30} \textit{FH} now becomes higher conducting than \textit{BPh} as the former is forced into a planar form because of the methylene group but still lower than the \textit{BT} molecular wire because of the lower bandgap of the latter. \textit{FO} is slightly less or almost same in conductance as \textit{FH} which is same as in the EGaIn measurements and previously reported data.\textsuperscript{31} We also studying the conductance switching of \textit{FO} upon treatment with trifluoroacetic acid (TFA). The results are shown in the Figure 4 of the main text. We recorded the UV-Vis absorption spectra of \textit{FO} and \textit{FH} before and after treatment with TFA. The results are shown in Figure S23 which were recorded in the same solvent system with the same concentration as for the STM-BJ conductance measurements (described above). The red-shift in the spectra of \textit{FO} and no effect in that of \textit{FH} can be seen in the Figure S23. We performed a bimodal fitting of the \textit{FOH} data where the first peak was assigned to the peak conductance value of \textit{FO} from the same set of measurement, \textit{i.e.}, the peak conductance before addition of TFA. The second peak was then assigned as the peak conductance of protonated \textit{FO} (\textit{FOH}). Values of one such representative peak conductance values are tabulated in Table S4. The bimodal fitting worked perfectly for this set of measurement but was not very clear in the other tests. Nevertheless the peak conductance values were reproducible over 3 tests that were performed for \textit{FOH}, which were then used to calculate the mean conductance and standard error of mean using Scientific Python,
Figure S22: (a) Single-molecule 1D Conductance histograms of Conductance counts per trace versus the Conductance in logarithmic scale in the units of the quantum of conductance ($G_0$) is shown here for the four molecular wires; BT (green), BPh (blue), FH (violet) and FO (red). Different tests (measurements) are plotted together for every molecule. The mean values of every test/measurement is used to calculate the mean conductance and standard error of mean. (b-g) Individual 2D Conductance histograms of the four molecular wires and protonated versions of FH and FO versus the displacement of the metallic tip in nanometers.
**Figure S23:** UV-Vis spectrum of FO and FH with and without addition of TFA. The spectra compared to Figure S17 (recorded in Groningen) shows similarity for FO and FH without TFA. Addition of TFA to the solution of FH doesn’t make any difference, however, addition of TFA to the solution of FO red-shifts the spectra, signifying that the functional carbonyl group has been modified in the process.

**Table S4:** Summary of STM-BJ junctions data for the switching measurements. The mean conductance values are reported of a single representative measurement for FH and FO performed only as part of the switching measurements (i.e., excluding the ones that didn’t involve addition of TFA).

| Compound   | FH    | FH-TFA | FO    | FOH-TFA |
|------------|-------|--------|-------|---------|
| STM-BJ in $\log(G/G_0)$ | $-4.06$ | $-4.01$ | $-4.28$ | $-3.96$ |

reported in Table 1 and Figure 3.

### 4 Computational Methodology

We performed the calculations using the quantum chemistry package ORCA (only for geometry optimization)\textsuperscript{32,33} ADF-BAND module of Amsterdam Density Functional (ADF) software package that implements Non-Equilibrium Green’s Function approach with Density Functional Theory.
The code uses localized basis-functions that are slater-type or numerical atomic orbital type, with frozen-core approximation. The procedure is described below step-by-step.

4.1 Theoretical methodology (NEGF)

Verzijl et al.\textsuperscript{38} in their paper described a novel implementation of NEGF formalism for molecular charge transport, in combination with the ADF/BAND periodic band-structure DFT code. Here in our study, we adapt and utilize the methodology established by the authors to compute transmission and density of states spectra for the model systems (metal-molecule-metal junctions) shown in the Figure 2. The model system comprises of an extended molecule region that consists of the geometry optimized molecule itself attached to two metal leads (pyramidal gold tips in our case). This extended molecule is then attached to a semi-infinite, periodic bulk metal electrode, creating a well-defined metal-metal interface. To perform the transport simulations, this code involves four stages. First one involves the bulk calculation of the electrode contacts. Second involves calculation of surface’s green’s function and self-energies. The third task involves self-consistent alignment of the potential levels in the electrodes with those in the extended molecule. In this step we calculate the $E_f$ level of our model system. The code uses a constrained-DIIS scheme to accelerate the convergence of alignment procedure. The final step is the calculation of the transport properties that generates the transmission and DOS spectra.
**Figure S24:** ORCA optimized geometries of molecules (attached to two metal leads) used in this study for calculation of transmission spectra shown in Figure 3: (a) **BT** (B) **BPh** (torsional angle = 40.3°) (c) **BPh** planar (d) **FH** (e) **FO** (f) **FOH** (g) **FOH-TFA** (h) **AQ**. Color code: Au (dark yellow), S (yellow), C (black), H (white), O (red), and F (green). The xyz coordinates are shown in section 4.6.
4.2 Molecular Geometry Optimization

**ORCA geometry optimization for NEGF**  We optimized geometries of all the molecules with one Au atom attached to terminal Sulfur atom (after deleting the H atoms) using $B3LYP$ basis set with $B3LYP$ functional for all atoms but Au. Specifically for the Au atoms, we used the ORCA keyword $SARC$-$ZORA$-$TZVP$ to implement $TZVP$ basis sets and ZORA relativistic effects. The two Au atoms served as the connecting point to the electrodes, replacing the atoms at the tip of the carved pyramidal leads, as shown in Figure S24, used in subsection 4.4.

**ADF optimization calculations**  We optimized all the four molecules $BT$, $BPh$, $FH$, $FO$ (and $FOH$, $FOH$-$TFA$, $BPh$ planar), along with $AQ$ as reference, with thiols as the terminal groups. For $BPh$ planar geometry, we optimized the molecule by constraining the torsional angle between the two center benzene rings to zero. We used ADF DFT package and utilized the *Triple Zeta with one Polarization function (TZP)* basis sets with $LDA$ exchange-and-correlation (XC) functional, which is known to produce good results for geometry optimization calculations in ADF.\textsuperscript{34} For sanity check, we also optimized these geometries using a higher level theory, implementing $Hybrid:B3LYP$ functional with $TZP$ basis sets and disabling any frozen core approximation with ZORA scalar relativistic effects.

We also optimized geometries of these molecular wires terminating with one Au atom attached to each terminal sulfur atom. We again used ADF DFT package and utilized the $DZ$ basis sets with $LDA$ XC-functional along with one-component scalar relativistic theory option (ZORA).
We also optimized them with *Hybrid:B3LYP* with *TZP* basis set to further use them in section 4.4 for computing the transport properties after attaching to Au leads.

Comparison between these different level of theories is discussed in subsection 4.3.

### 4.3 Single Point Energy Calculations

We performed single point energy calculations on the gas-phase geometries terminated with thiols (section 4.2) to compute the HOMO and LUMO levels and also the gas-phase $E_g$ (HOMO-LUMO gap) of the molecular wires and their analogues using ADF quantum chemistry package. As described above, the *LDA* functional and *TZP* basis set were used for geometry optimization because they are known to yield decent geometry. But they also provide bad estimation of band-gap (in comparison with the band gap values from the experimental UV-Vis absorbance spectroscopy, labeled as "UV-Vis" in Figure S26). This can be seen from Figure S26, labeled as "LDA/TZP opt". Single-point energy calculations using *GGA:PBE* functional and *TZP* basis sets on these geometries also resulted in similar values (labeled as "PBE/TZP (SPE on LDAopt)"). Furthermore, the pure functional *LDA* could not converge the FOH geometry as the erratic convergence seemed to keep switching between two different electronic states as the HOMO and LUMO level seemed to become degenerate.

Thus, for more accurate calculation of band-gaps and energies of the frontier orbitals (HOMO and LUMO), we performed single-point calculation on *LDA/TZP* optimized geometry using *Hy-
brid:B3LYP functional with TZP basis set. These values are also shown in Figure S26, labeled as "B3LYP/TZP (SPE on LDAopt)". Finally, we compare these with values optimized from the geometry optimization calculations using Hybrid:B3LYP and TZP basis set, labeled as "B3LYP/TZP (opt)" in Figure S26. The associated isoplots (with iso-value= 0.02) for HOMO and LUMO levels are shown in Figure S27.

In conclusion, Hybrid:B3LYP and TZP level of theory provides the most accurate estimation of band gap compared to UV-Vis data.

4.4 BAND/NEGF calculations

The ORCA optimized geometries were attached between two metal leads with 10 and 14 Au atoms each. This completed the "extended molecule" which was then attached to the bulk electrodes. We used single zeta (SZ) in combination with the GGA:PBE0 XC-functional for this NEGF calculation. We used scalar relativity ZORA option to account for relativistic effects. We further used "self-consistent" method for transmission calculation. This calculation provided us with the zero-bias transmission and density of states spectra as shown in Figure 2 and Figure S28. The zero-bias conductance values as shown in Figure S29 were calculated as $G = G_0 \times T(E = E_t)$, where $G_0$ is the quantum of conductance equal to $2e^2/h$ and $T(E = E_t)$ is the transmission probability value at $E_t$. We also tried with higher order basis sets, such as, DZ and TZP, and also LDA functional, for these calculations, however, none of them generated more accurate transmission spectra than SZ for these calculations.
Figure S25: HOMO and LUMO isoplots of the molecules calculated using LDA/TZP as described in subsection 4.2. The respective orbital energies are described next to the orbitals in the units of electronvolt.
**Figure S26:** Values of Band gap computed using different levels of theory for the series of molecules used in this study. For more details, please check subsection 4.3. The UV-Vis band gap for AQ was taken from the work of Valkenier et al.\textsuperscript{39}

For the simulations of protonation in STM-BJ measurements for QI switching, we added a proton to the carbonyl group in the backbone of FO in absence and presence of trifluoroacetate counter anion (TFA\textsuperscript{–}), called FOH and FOH-TFA, respectively. In the former case of FOH, the positive charge was added only in the transport calculation (fourth case of BAND/NEGF calculation) as the unit cells of the other periodic tasks have to be charge neutral. In case of the latter (FOH-TFA), TFA\textsuperscript{–} was separately optimized and added to the extended molecule region. The molecular geometries are visually presented in Figure S24 and their xyz coordinates provided in section 4.6.

Finally, we ran transmission calculations also on the Hybrid:B3LYP and TZP optimized geometries from ADF (see subsection 4.2) for sanity check. Exact calculation parameters were implemented for fair comparison as for ORCA geometries. As can be seen from Figure S30, all the prominent features are preserved in the calculation on these geometries. The inset in the figure fur-
Figure S27: HOMO and LUMO isoplots of the molecules calculated as described in subsection 4.2 calculated using the Hybrid:B3LYP functional. The respective orbital energies are described next to the orbitals in the units of electronvolt. The calculations for FOH were on a +1 charged molecule, and not in-presence of the counter anion (as the solvation model was not used), thus the energy values are non-sensical, and hence, not shown.
Figure S28: (a) Transmission probability versus electron energy, with respect to $E_f$, for BT, BPh, FH, FO, FOH, FOH-TFA, and BPh planar with AQ as a standard reference. (b) Density of States versus electron energy, referenced to $E_f$, for the same molecular wires as in the subfigure a. As a reference, we also included the DOS of just the gold leads and semi-infinite, periodic electrodes at a distance same as the length of FO. (c) For sake of clarity, we plotted Transmission and DOS together for BT, BPh, FO, FOH, BPh planar, along with DOS of only Au electrodes. (d) For the sake of clarity, we further plotted transmission and DOS of FO, FOH, FOH-TFA, AQ, along with DOS of Au electrodes for comparison with the STM-BJ data on QI switching. (e) Transmission spectra (left axis) and DOS (right axis) of BPh (twisted form with torsional angle between phenyl rings $=40.3^\circ$) and BPh planar (phenyl ring torsional angle $=0^\circ$). For the BPh planar, transmission increases compared to BPh. (f) Zoomed-in transmission spectra of all the molecular systems and their analogues to better visualize the conductance trend at $E - E_f = 0$. The discontinuities in the transmission spectra at $E - E_f \approx 0.55$eV are related to the effects of the potential in the contacts, as detailed by Verzijl et al.$^{38}$
**Figure S29:** This figure is an elaborate version of Figure 3 in the main text. (a) Comparison of low-bias EGaIn conductance trend (left axis, black) with zero-bias DFT conductance trend (right axis, red) for BT, BPh planar, FH, FO, and AQ as reference. We use the DFT conductance value for the planar form of BPh here as it has been reported that BPh adopts planar conformation in SAMs. The DFT predicts the same trend as we observe in the EGaIn experiments. (b) Comparison of low-bias STM-BJ conductance (left axis, black) with zero-bias DFT conductance trend (right axis, red) for BT, BPh, FH, and FO. Here, we use the DFT conductance value for the twisted geometry of BPh. The DFT trend again supports the experimental STM-BJ conductance values. (c) Comparison of low-bias STM-BJ conductance (left axis, black) with zero-bias DFT conductance trend (right axis, red) for FH, FO, FOH, and FOH-TFA. As it can be seen that both the geometries, FOH with +1 charge and FOH-TFA with the counter anion, predict the same increase in conductance from FO, as also seen in the STM-BJ measurements.
Figure S30: Transmission spectra of all the molecules studies in this publication using the ADF optimized Hybrid:B3LYP/TZP geometries attached to metal leads as described in the subsection 4.4, for comparison with transmission spectra from ORCA optimized geometries.

Figure S30 compares the zero-bias DFT transmission values at the Fermi level for both the ADF optimized and ORCA optimized geometries, showing the same trend in both these calculations.
Figure S31: (Left) Classical parallel circuit with two conductors in parallel. (Right) Quantum intramolecular circuit with two parallel conductance pathways connected to the electrodes via common nodes inside the molecular junction.

4.5 Superposition Model

According to Kirchoff’s law, total conductance of two conductors in parallel is calculated by summation of the conductance of individual conductors.

\[ G = G_a + G_b \]  

(S1)

This law doesn’t apply to conductance in molecules arranged parallel in molecular junctions,
bridging two metal electrodes. Further, in an earlier reported theoretical study by Magoga et al., the authors formulated a superposition model for different kind of parallel junction geometries. The authors in this work and in their follow-up discussion on the work of Vazquez et al. discussed the following points: (a) two molecules in parallel, with direct connection to electrodes follow the regular Kirchoff’s law (Equation S1), (b) parallel pathways in the molecular structure with pathways connected to the electrodes via nodes, result in a total conductance which is a sum of individual conductance plus a third quantum mechanical term which is the result of quantum interference (Equation S2).

\[
G = G_a + G_b + 2\sqrt{G_a \times G_b} 
\]  
(S2)

This was also illustrated in the work by Colin J. Lambert. Figure S32 depicts the process that we used to adapt the superposition model of Magoga et al. to explain the STM-BJ data of the QI switching in this study on FO molecule. In Figure S32, the first four molecules BPh, AC, AH, AQ were used as reference (input) variables. The single molecular conductance values for AC, AH, and AQ were taken from our previous work. Since BPh contains only one conductance pathway, conductance of BPh molecular wire equaled the conductance \( G'_0 \) of a pathway containing single bond connecting two phenyl rings. Since AC, AH, and AQ containing two equivalent parallel pathways \( G_a = G_b \) with linear-, broken-, and cross-conjugation, respectively, Equation S2 could be applied where the total conductance of the molecular wires equals to 4 times the conductance of the individual molecules (Equation S3):
| Molecular wire | Model Circuit diagram | Total Conductance |
|----------------|-----------------------|-------------------|
| BPh            | $G_{BPh}$            | $G_{BPh} = G_0'$   |
| AC             | $G_{Ac}$              | $G_{Ac} = 4 \times G_1$ |
| AH             | $G_{Ah}$              | $G_{Ah} = 4 \times G_2$ |
| AQ             | $G_{Aq}$              | $G_{Aq} = 4 \times G_3$ |
| FH             | $G_{Fh}$              | $G_{Fh} = G_2 + G_0' + 2\sqrt{G_2 \times G_0'} = ?$ |
| FO             | $G_{Fo}$              | $G_{Fo} = G_3 + G_0' + 2\sqrt{G_3 \times G_0'} = ?$ |
| FOH            | $G_{Foh}$             | $G_{Foh} = G_1 + G_0' + 2\sqrt{G_1 \times G_0'} = ?$ |

**Figure S32:** Schematic for applying superposition model on molecules under study with the corresponding intramolecular circuit model and total conductance equations. First four molecules, BPh, AC, AH, and AQ are taken as input variable for the model to calculate molecular conductance of FH, FO, and FOH.
Figure S33: (a) Zero-bias conductance data of BPh, AQ, AH, AC, FH, FO, FOH-TFA (FOH) from STM-BJ measurements in black squares and the predicted zero-bias conductance from the superposition model for FH, FO, and FOH-TFA in red circles, described in subsection 4.5. (b) Zoomed-in version of left figure for showing the STM-BJ and predicted conductance from the superposition model.

\[
G = G_a + G_b + 2 \sqrt{G_a \times G_b} = 4 \times G_a \quad (S3)
\]

This way we can determine the values of \(G_1, G_2, G_3\) corresponding to the conductance of a linear-, broken-, and a cross-conjugated pathway, respectively. We used these 4 input variables \((G_0', G_1, G_2, G_3)\) to calculate the total conductance of the molecular wires FH, FO, and protonated FOH-TFA. The equations are shown in Figure S32. FH has two parallel pathways, first one \(G_2\) and second one \(G_0'\); FO has two parallel pathways, first one \(G_3\) and second one \(G_0'\); FOH-TFA has two parallel pathways, first one \(G_1\) and second one \(G_0'\) (supporting the hypothesis that the carbocation functionally makes the pathway linearly conjugated\(^{45}\)).

The calculated values of conductance of FH, FO, and FOH-TFA are plotted in Figure S33 in
Table S5: Summary of the superposition model as graphically presented in Figure S33: (row 1 and 2) conductance values of BPh, AQ, AH, and AC used as input variables for superposition model; (row 4) experimental STM-BJ data compared with the predicted values from superposition model (row 5) for FH, FO, and FOH.

| Compound (input variable) | STMBJ/MCBJ | Compound (calculated variable) | Conductance, $G \times 10^{-5}(G_0)$ | STMBJ | Superposition Model |
|---------------------------|------------|--------------------------------|---------------------------------------|-------|---------------------|
| BPh ($G_0^*$)             | 4.47       | FH ($G_{FH}$)                  | 7.76                                  | 4.96  |                     |
| AQ ($4 \times G_1$)       | 0.00645    | FO ($G_{FO}$)                  | 5.50                                  | 4.64  |                     |
| AH ($4 \times G_2$)       | 0.0516     | FOH ($G_{FOH}$)                | 11.29                                 | 9.06  |                     |
| AC ($4 \times G_3$)       | 3.22       |                                |                                       |       |                     |

red color and compared with the conductance data from STM-BJ measurements in this study. The remarkable agreement between the two trends excellent support of the superposition model to our data. It also validates our hypothesis that upon protonation of FO to convert the molecule to FOH-TFA, the cross-conjugated carbonyl functional group converts into a linear-conjugated trivalent carbon group. This explains the increase in conductivity upon protonation to even higher value than FH or BPh.
4.6 Optimized Geometry coordinates

Below are the xyz coordinates of the DFT-optimized geometries for all the molecular wires and their analogues used in this study:

Coordinates for BT:

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | -13.85709105 | -2.04000000 | 1.44249800 |
| Au      | -15.29958905 | -4.08000000 | 0.00000000 |
| Au      | -13.85709105 | 2.04000000  | -1.44249800 |
| Au      | -13.85709105 | 2.04000000  | 1.44249800  |
| Au      | -15.29958905 | 0.00000000  | -2.88499600 |
| Au      | -15.29958905 | 0.00000000  | 2.88499600  |
| Au      | -15.29958905 | 0.00000000  | 0.00000000  |
| Au      | -15.29958905 | 4.08000000  | 0.00000000  |
| Au      | -13.85709105 | -2.04000000 | -1.44249800 |
| Au      | 12.41958905  | 0.00000000  | 0.00000000  |
| Au      | 16.74208705  | -2.04000000 | -1.44249800 |
| Au      | 13.864208705 | -2.04000000 | 1.44249800  |
| Au      | 16.74208705  | -2.04000000 | 1.44249800  |
| Au      | 15.29958905  | -4.08000000 | 0.00000000  |
| Au      | 16.74208705  | 2.04000000  | -1.44249800 |
| Au      | -12.41958905 | 0.00000000  | 0.00000000  |
| Au      | 16.74208705  | 2.04000000  | 1.44249800  |
| Au      | 15.29958905  | 0.00000000  | -2.88499600 |
| Au      | 13.864208705 | -2.04000000 | 1.44249800  |
| Au      | 15.29958905  | 0.00000000  | 2.88499600  |
| Au      | 13.864208705 | 2.04000000  | -1.44249800 |
| Au      | 13.864208705 | 2.04000000  | 1.44249800  |
| Au      | 15.29958905  | 0.00000000  | 0.00000000  |
| Au      | 15.29958905  | 4.08000000  | 0.00000000  |
| S       | -11.57138214 | 0.24007885  | -2.16635857 |
| S       | 11.56980219  | -0.23238554 | 2.16657827  |
| C       | 9.78167566   | -0.32261756 | 1.79201698  |
| H       | 9.78234607   | -2.47386269 | 1.65065353  |
| H       | 9.50581091   | 1.81285422  | 1.89943055  |
| C       | 9.17149927   | -1.56597527 | 1.61389943  |
| C       | 9.01636658   | 0.84494133  | 1.75081560  |
| C       | 7.80629381   | -1.64492422 | 1.39136121  |
| C       | 7.65099291   | 0.77386801  | 1.52629540  |
Coordinates for BPh:

Au -14.33208968 -2.04000000 1.44249800
Au -15.77458768 -4.08000000 0.00000000
Au -14.33208968 2.04000000 -1.44249800
Au -14.33208968 2.04000000 1.44249800
Au -15.77458768 0.00000000 -2.88499600
Au -15.77458768 0.00000000 2.88499600
Au -15.77458768 0.00000000 0.00000000
Au -15.77458768 4.08000000 0.00000000
Au -14.33208968 -2.04000000 -1.44249800
|   |   |   |   |
|---|---|---|---|
| C | 1.54622245 | 1.72479009 | -0.11068839 |
| C | 1.30983992 | -0.59347193 | -0.73117709 |
| C | 2.91439302 | 1.64435848 | -0.31215277 |
| C | 2.67718587 | -0.68381460 | -0.93357740 |
| H | 3.55598798 | 2.51362858 | -0.13539081 |
| H | 3.13001637 | -1.62110629 | -1.27246489 |
| C | 3.50435579 | 0.43621017 | -0.72818527 |
| C | 4.89156210 | 0.34991964 | -0.93857544 |
| C | 6.09128519 | 0.27320435 | -1.12599714 |
| C | 7.47638028 | 0.18581087 | -1.34729152 |
| H | 7.75602877 | 2.32696535 | -1.46766665 |
| H | 7.51421371 | -1.97569159 | -1.28600324 |
| C | 8.24989233 | 1.35107454 | -1.51088014 |
| C | 8.11313911 | -1.06827549 | -1.41258206 |
| C | 9.61557992 | 1.26235741 | -1.73170768 |
| C | 9.48003432 | -1.15161705 | -1.62933228 |
| H | 10.21782764 | 2.16679120 | -1.86555720 |
| H | 9.97765240 | -2.12565179 | -1.67725119 |
| C | 10.23422143 | 0.01223486 | -1.78804979 |

Coordinates for **BPh** (planar):

|   |   |   |   |
|---|---|---|---|
| Au | -14.37250200 | -2.04000000 | 1.44249800 |
| Au | -15.81500000 | -4.08000000 | 0.00000000 |
| Au | -14.37250200 | 2.04000000 | -1.44249800 |
| Au | -14.37250200 | 2.04000000 | 1.44249800 |
| Au | -15.81500000 | 0.00000000 | -2.88499600 |
| Au | -15.81500000 | 0.00000000 | 2.88499600 |
| Au | -15.81500000 | 0.00000000 | 0.00000000 |
| Au | -15.81500000 | 4.08000000 | 0.00000000 |
| Au | -14.37250200 | -2.04000000 | -1.44249800 |
| Au | 12.93500000 | 0.00000000 | 0.00000000 |
| Au | 17.25749800 | -2.04000000 | -1.44249800 |
| Au | 14.37749800 | -2.04000000 | -1.44249800 |
| Au | 17.25749800 | -2.04000000 | 1.44249800 |
| Au | 15.81500000 | -4.08000000 | 0.00000000 |
| Au | 17.25749800 | 2.04000000 | -1.44249800 |
| Au | -12.93539103 | 0.00000000 | 0.00000000 |
| Au | 17.25749800 | 2.04000000 | 1.44249800 |
| Au | 15.81500000 | 0.00000000 | -2.88499600 |
| Au | 14.37749800 | -2.04000000 | 1.44249800 |
| Au | 15.81500000 | 0.00000000 | 2.88499600 |
| Au | 14.37749800 | 2.04000000 | -1.44249800 |

S-55
|   |   |   |   |
|---|---|---|---|
| Au | 14.37749800 | 2.04000000 | 1.44249800 |
| Au | 15.81500000 | 0.00000000 | 0.00000000 |
| Au | 15.81500000 | 4.08000000 | 0.00000000 |
| S  | -12.05606632 | -0.04769304 | 2.16522570 |
| S  | 12.01998535  | -0.35807137 | -2.12651481 |
| C  | 10.23811133  | 0.87513765  | -1.73359578 |
| C  | 9.57248721   | -1.52333851 | -1.41260915 |
| C  | 8.17104292   | 0.88998739  | -1.48153893 |
| C  | 8.20922307   | -1.51389190 | -1.16014597 |
| H  | 7.61136703   | 1.83052245  | -1.50574394 |
| H  | 7.67828479   | -2.44525408 | -0.93855806 |
| C  | 7.48624732   | -0.30566727 | -1.18921461 |
| C  | 6.10443029   | -0.29311007 | -0.93740546 |
| C  | 4.90567066   | -0.28057959 | -0.72741544 |
| C  | 3.52150328   | -0.26219205 | -0.49359497 |
| H  | 3.26601112   | 1.78460522  | -1.13577860 |
| H  | 3.43277738   | -2.30395990 | 0.20677652 |
| C  | 2.76142500   | 0.89322886  | -0.74954241 |
| C  | 2.85446266   | -1.39799567 | -0.00077654 |
| C  | 1.39640342   | 0.90444808  | -0.52357143 |
| C  | 1.48903026   | -1.37308353 | 0.22264170 |
| H  | 0.84871499   | 1.82453087  | -0.74094243 |
| H  | 1.01629548   | -2.27955356 | 0.60809346 |
| C  | 0.71895100   | -0.22502396 | -0.03232494 |
| C  | -0.73247043  | -0.20678553 | 0.20204945 |
| H  | -1.02817870  | 1.84905548  | -0.43499811 |
| H  | -0.86375381  | -2.25712748 | 0.90819981 |
| C  | -1.50177432  | 0.94192270  | -0.05222939 |
| C  | -1.41090036  | -1.33667917 | 0.69093220 |
| C  | -2.86747609  | 0.96692426  | 0.16907026 |
| C  | -2.77670176  | -1.32587603 | 0.91315358 |
| H  | -3.44530963  | 1.87338816  | -0.03765780 |
| H  | -3.28239443  | -2.21789046 | 1.29630874 |
| C  | -3.53583479  | -0.17000377 | 0.65720859 |
| C  | -4.92137967  | -0.15107997 | 0.88408915 |
| C  | -6.12205549  | -0.13408543 | 1.08185297 |
| C  | -7.50751463  | -0.11394581 | 1.31399505 |
| H  | -7.64200910  | 2.04473147  | 1.30088006 |
| H  | -7.69086468  | -2.26767030 | 1.38729851 |
C -8.19986737  1.10894462  1.40687708
C -8.22655458 -1.31586853  1.45948757
C -9.56649123  1.12643099  1.63799519
C -9.59424790 -1.29302364  1.68548634
H -10.10551959  2.07600072  1.71772706
H -10.15589544 -2.22637621  1.79528368
C -10.26722469 -0.07326232  1.77445998

Coordinates for FH:
Au -14.30550200  -2.04000000  1.44249800
Au -15.74800000  -4.08000000  0.00000000
Au -14.30550200  2.04000000  -1.44249800
Au -14.30550200  2.04000000   1.44249800
Au -15.74800000  0.00000000  -2.88499600
Au -15.74800000  0.00000000   2.88499600
Au -15.74800000  0.00000000   0.00000000
Au -15.74800000   4.08000000   0.00000000
Au -14.30550200 -2.04000000  -1.44249800
Au  12.86800000  0.00000000   0.00000000
Au  17.19049800  -2.04000000  -1.44249800
Au  14.31049800  -2.04000000  -1.44249800
Au  17.19049800  -2.04000000  1.44249800
Au  15.74800000  -4.08000000  0.00000000
Au  17.19049800  2.04000000  -1.44249800
Au -12.86825733  0.00000000   0.00000000
Au  17.19049800  2.04000000   1.44249800
Au  15.74800000  0.00000000  -2.88499600
Au  14.31049800  -2.04000000  1.44249800
Au  15.74800000  0.00000000   2.88499600
Au  14.31049800  2.04000000  -1.44249800
Au  14.31049800  2.04000000   1.44249800
Au  15.74800000  0.00000000   0.00000000
Au  15.74800000   4.08000000   0.00000000
S  -11.82858245  1.97863024  0.48783135
S   11.81584399 -1.90436681 -0.70271144
H  10.36510160  -0.88117950 -3.00104269
C   9.65404125  -0.98452638 -2.18326746
C  10.11428411  -1.41500607  -0.92371157
H   7.96150060  -0.36114767 -3.36133006
C   8.30852974  -0.69216415 -2.38397845
C   9.18911336  -1.55377901  0.12909750
H   9.54005611  -1.89153415  1.10282591
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 7.37577360 | -0.82207088| -1.32834283|
| C    | 7.84308088 | -1.26169469| -0.06759977|
| H    | 7.13501732 | -1.37148153| 0.75192872 |
| C    | 5.99875979 | -0.51798607| -1.52956643|
| C    | 4.81752410 | -0.25645737| -1.70017873|
| H    | 3.69919232 | 0.62893926 | -3.96415844|
| C    | 2.97982371 | 0.50946998 | -3.15613944|
| C    | 3.43916601 | 0.04752760 | -1.89767987|
| H    | 1.30376450 | 1.16032140 | -4.34292042|
| C    | 1.63561601 | 0.80855300 | -3.36651364|
| C    | 2.51157917 | -0.11003535| -0.83844527|
| H    | 2.86463091 | -0.46369254| 0.12976760 |
| C    | 0.72531945 | 0.64819662 | -2.31240748|
| C    | 1.17290285 | 0.18783528 | -1.05052334|
| H    | -1.30342045| 1.57609020 | -4.21323767|
| C    | -0.72001249| 0.87534570 | -2.24148538|
| C    | 0.00536844 | 0.09717115 | -0.08865961|
| C    | -1.63310291| 1.32390057 | -3.20590753|
| H    | -0.13596117 | -0.92733068| 0.28881000|
| H    | 0.14873334 | 0.73971985 | 0.79362163 |
| C    | -1.16461453 | 0.55420464 | -0.93617893|
| C    | -2.97795722 | 1.44601044 | -2.86431018|
| H    | -3.70015461 | 1.79085370 | -3.60218134|
| C    | -2.50383506 | 0.67538374 | -0.59372553|
| C    | -3.43480329 | 1.12577063 | -1.56179080|
| H    | -2.85488654 | 0.42876711 | 0.40753195 |
| C    | -4.81510631 | 1.25302171 | -1.23075550|
| C    | -5.99874170 | 1.35984334 | -0.94742344|
| H    | -7.97234111 | 2.18057418 | -2.57835082|
| C    | -7.37891516 | 1.48159149 | -0.61703143|
| C    | -8.31738299 | 1.92575286 | -1.57786636|
| H    | -7.13116224 | 0.82269103 | 1.43026805 |
| C    | -7.84362880 | 1.16080476 | 0.67972091 |
| C    | -9.66560996 | 2.03981923 | -1.25417271|
| H    | -10.38098974| 2.38338046 | -1.99302383|
| C    | -9.19290908 | 1.27530967 | 0.99964661 |
| C    | -10.12311477| 1.71261078 | 0.03700059 |
| H    | -9.54202865 | 1.02670915 | 2.00030554 |

Coordinates for FO:

Au     -14.07450200  -2.04000000  1.44249800
Au     -15.51700000  -4.08000000  0.00000000
| Symbol | X       | Y       | Z       |
|--------|---------|---------|---------|
| Au     | -14.07450200 | 2.04000000 | -1.44249800 |
| Au     | -14.07450200 | 2.04000000 | 1.44249800  |
| Au     | -15.51700000 | 0.00000000 | -2.88499600 |
| Au     | -15.51700000 | 0.00000000 | 2.88499600  |
| Au     | -15.51700000 | 4.08000000 | 0.00000000  |
| Au     | -14.07450200 | -2.04000000 | -1.44249800 |
| Au     | 12.63700000  | 0.00000000 | 0.00000000  |
| Au     | 16.95949800  | -2.04000000 | -1.44249800 |
| Au     | 16.95949800  | -2.04000000 | 1.44249800  |
| Au     | 15.51700000  | -4.08000000 | 0.00000000  |
| Au     | 16.95949800  | 2.04000000  | -1.44249800 |
| Au     | 15.51700000  | 2.04000000  | 1.44249800  |
| Au     | 15.51700000  | 4.08000000  | 0.00000000  |
| Au     | 15.51700000  | 0.00000000  | 0.00000000  |
| Au     | 15.51700000  | 0.00000000  | 0.00000000  |
| H      | -10.52215892 | 2.36898993  | -2.3094883  |
| H      | -8.09877276  | 2.46898160  | -2.85221352 |
| C      | -9.77961698  | 2.28917347  | -1.51721168 |
| C      | -8.42314956  | 2.34556585  | -1.82042064 |
| H      | -3.78060867  | 2.50862595  | -3.80518688 |
| S      | -11.94735194 | 2.17033296  | 0.22040022  |
| H      | 9.69320622   | 2.19556469  | 1.66005516  |
| H      | -1.36952761  | 2.56604446  | -4.38454365 |
| C      | -10.20983044 | 2.12552840  | -0.18618512 |
| C      | -3.03429698  | 2.46669945  | -3.01378624 |
| C      | -7.45064266  | 2.24639299  | -0.79809863 |
| C      | -1.67393241  | 2.49806291  | -3.34071247 |
| C      | -6.06074582  | 2.29665050  | -1.10704448 |
| H      | 1.33661951   | 2.55981901  | -4.41465271 |
| C      | -4.86862599  | 2.33571207  | -1.36980319 |
| C      | -9.24637153  | 2.03272679  | 0.83641971  |
| C      | -3.47671215  | 2.37636626  | -1.67194465 |
| C      | -7.88848562  | 2.09312887  | 0.53752453  |
| C      | -0.73216972  | 2.43823734  | -2.31268349 |
| C      | 1.66455949   | 2.49857981  | -3.37783433 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -9.5755 | 1.9119  | 1.8669  |
| H    | 3.7605  | 2.5143  | -3.8885 |
| H    | -7.1499 | 2.0214  | -3.0875 |
| C    | 0.7457  | 2.4404  | -2.3289 |
| C    | -2.5107 | 2.3209  | -0.6345 |
| C    | 3.0319  | 2.4717  | -3.0875 |
| C    | -1.1688 | 2.3527  | -0.9709 |
| H    | -2.8179 | 2.2522  | 0.4078  |
| C    | 1.2121  | 2.3593  | -0.9967 |
| C    | 3.5042  | 2.3882  | -1.7486 |
| C    | 0.0317  | 2.3016  | -0.0667 |
| C    | 2.5613  | 2.3341  | -0.6897 |
| H    | 8.0901  | 2.2411  | -3.0502 |
| C    | 4.9027  | 2.3522  | -1.4777 |
| O    | 0.0451  | 2.2277  | 1.1416  |
| C    | 6.1007  | 2.3159  | -1.2430 |
| H    | 2.8916  | 2.2714  | 0.3456  |
| C    | 8.4419  | 2.2305  | -2.0203 |
| H    | 10.5256 | 2.1487  | -2.5646 |
| C    | 7.4978  | 2.2695  | -0.9676 |
| C    | 9.8053  | 2.1767  | -1.7488 |
| C    | 7.9717  | 2.2585  | 0.3646  |
| C    | 10.2712 | 2.1559  | -0.4200 |
| H    | 7.2557  | 2.2927  | 1.1840  |
| C    | 9.3363  | 2.2031  | 0.6319  |
| S    | 12.0212 | 2.2015  | -0.0716 |

Coordinates for AQ:

| Au   | -14.6046 | -2.0400 | 1.4424 |
|------|----------|---------|-------|
| Au   | -16.0471 | -4.0800 | 0.0000 |
| Au   | -14.6046 | 2.0400  | -1.4424 |
| Au   | -14.6046 | 2.0400  | 1.4424 |
| Au   | -16.0471 | 0.0000  | -2.8849 |
| Au   | -16.0471 | 0.0000  | 2.8849 |
| Au   | -16.0471 | 0.0000  | 0.0000 |
| Au   | -16.0471 | 0.0000  | 0.0000 |
| Au   | -16.0471 | 0.0000  | 0.0000 |
| Au   | -14.6046 | -2.0400 | -1.4424 |
| Au   | 13.1671  | 0.0000  | 0.0000 |
| Au   | 17.4896  | -2.0400 | -1.4424 |
| Au   | 14.6097  | -2.0400 | 1.4424 |
| Au   | 17.4896  | -2.0400 | -1.4424 |
| Au   | 16.0471  | -4.0800 | 0.0000 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| 0    | -1.47560307| 0.01592676 | 2.26853499 |
| C    | -3.50453931| 0.01207840 | -1.42977228|
| C    | -2.84925972| 0.01293298 | -0.18187510|
| H    | -3.42078374| 0.01325170 | 0.74753956 |
| C    | -4.92740339| 0.01141132 | -1.50593627|
| C    | -6.1466408 | 0.01145139 | -1.57463915|
| H    | -7.63875577| 0.01975718 | -3.82033732|
| C    | -8.23021015| 0.01450003 | -2.90206941|
| C    | -7.56949638| 0.00978368 | -1.65323936|
| H    | -10.10351783| 0.01679587 | -3.95771945|
| C    | -9.61823647| 0.01282249 | -2.97789984|
| H    | -7.87413120| -0.0065216 | 0.49197470 |
| C    | -8.36269873| 0.00312902 | -0.48530683|
| C    | -10.40402671| 0.00584004 | -1.80583663|
| C    | -9.75220946| 0.00932424 | -0.55960425|
| H    | -10.34164371| -0.00468699| 0.35987834 |

Coordinates for **FOH**:

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Au   | -13.90450200  | -2.04000000 | 1.44249800 |
| Au   | -15.34700000  | -4.08000000 | 0.00000000 |
| Au   | -13.90450200  | 2.04000000  | -1.44249800|
| Au   | -13.90450200  | 2.04000000  | 1.44249800 |
| Au   | -15.34700000  | 0.00000000  | -2.88499600|
| Au   | -15.34700000  | 0.00000000  | 2.88499600 |
| Au   | -15.34700000  | 0.00000000  | 0.00000000 |
| Au   | -15.34700000  | 4.08000000  | 0.00000000 |
| Au   | -13.90450200  | -2.04000000 | -1.44249800|
| Au   | 12.46742099   | 0.00000000  | -0.00000000|
| Au   | 16.78949800   | -2.04000000 | -1.44249800|
| Au   | 13.90949800   | -2.04000000 | -1.44249800|
| Au   | 16.78949800   | -2.04000000 | 1.44249800 |
| Au   | 15.34700000   | -4.08000000 | 0.00000000 |
| Au   | 16.78949800   | 2.04000000  | -1.44249800|
| S    | 11.99526246   | -1.06060946 | 1.96050680 |
| Au   | 16.78949800   | 2.04000000  | 1.44249800 |
| H    | 9.62692320    | -0.32135244 | 0.22692611 |
| Au   | 13.90949800   | -2.04000000 | 1.44249800 |
| Au   | 15.34700000   | 0.00000000  | 2.88499600 |
| Au   | 13.90949800   | 2.04000000  | -1.44249800|
| Au   | 13.90949800   | 2.04000000  | 1.44249800 |
| Au   | 15.34700000   | 0.00000000  | 0.00000000 |
| Au   | 15.34700000   | 4.08000000  | 0.00000000 |

S-62
Au  -12.46742099  0.00000000  0.00000000
S   -12.00054651 -0.55925351  2.15773002
H   -10.50630888 -1.48023065  4.78384074
C   -9.78658241  -1.17849529  3.56250159
C   -10.24509489 -0.67830016  2.32098655
H   -8.09388055  -1.67802402  4.78384074
C   -8.42862491  -1.29041175  3.82322164
C   -9.29333990  -0.30232016  1.35058508
H   -9.62803130   0.08689657  0.39081686
C   -7.46946233  -0.91455199  2.85155513
C   -7.93393952  -0.42075155  1.60959873
H   -7.21326469  -0.12783326  0.84812345
C   -6.08159038  -1.03241993  3.12047240
C   -4.88689078  -1.13822340  3.36387435
H   -3.79580212  -1.99100243  5.66547253
C   -3.05163624  -1.73148170  4.91514420
C   -3.50538970  -1.26473595  3.65413679
H   -1.39575458  -2.23274590  6.20932585
C   -1.68730637  -1.86826128  5.22558214
C   -2.53697171  -0.92414319  2.67595805
H   -2.84733860  -0.56147527  1.69865152
C   -0.73931422  -1.53606241  4.26726685
C   -1.18536297  -0.06542602  2.99640601
H   1.40203672   -2.26947279  6.18301355
C   0.73245865   -1.55914188  4.25059584
C   1.68870540  -1.91917134  5.19296754
C   -0.01292144  -0.79986639  2.19847261
O   -0.08500086  -0.35694272  0.97993640
C   1.17076647  -1.10433066  2.96908539
H   0.78393242   -0.22904792  0.56846357
C   3.04819078  -1.82778566  4.85874406
C   3.79743653  -2.11081548  5.95771163
C   2.52160203  -1.01065722  2.62940562
C   3.49814019  -1.37843321  3.58706979
H   2.85428869  -0.66476885  1.65026789
C   4.87965860  -1.29998598  3.27945970
C   6.07464987  -1.23645468  3.02460838
H   8.08387130  -1.89876946  4.68628627
C   7.46366635  -1.17101557  2.73947293
C   8.42002496  -1.55455352  3.70991867
H   7.21217971  -0.42080414  0.72169094
C   7.93055958  -0.72231062  1.48226868
| Atoms | X-Coordinates | Y-Coordinates | Z-Coordinates |
|-------|---------------|---------------|---------------|
| C     | 9.77849873    | -1.48943144   | 3.43405844    |
| H     | 10.49641958   | -1.78225630   | 4.19912399    |
| C     | 9.29020783    | -0.66351680   | 1.20340793    |
| C     | 10.23953003   | -1.04541274   | 2.17300530    |

Coordinates for **FOH-TFA**:

| Au   | X-Coordinates | Y-Coordinates | Z-Coordinates |
|------|---------------|---------------|---------------|
| Au   | -13.90450200  | -2.04000000   | 1.44249800    |
| Au   | -15.34700000  | -4.08000000   | 0.00000000    |
| Au   | -13.90450200  | 2.04000000    | -1.44249800   |
| Au   | -13.90450200  | 2.04000000    | 1.44249800    |
| Au   | -15.34700000  | 0.00000000    | -2.88499600   |
| Au   | -15.34700000  | 0.00000000    | 2.88499600    |
| Au   | -15.34700000  | 0.00000000    | 0.00000000    |
| Au   | -15.34700000  | 4.08000000    | 0.00000000    |
| Au   | -13.90450200  | -2.04000000   | -1.44249800   |
| Au   | 12.46742099   | 0.00000000    | -0.00000000   |
| Au   | 16.78949800   | -2.04000000   | -1.44249800   |
| Au   | 13.90949800   | -2.04000000   | -1.44249800   |
| Au   | 16.78949800   | -2.04000000   | 1.44249800    |
| Au   | 15.34700000   | -4.08000000   | 0.00000000    |
| Au   | 16.78949800   | 2.04000000    | 1.44249800    |
| S    | 11.99526246   | -1.06060946   | 1.96050680    |
| Au   | 16.78949800   | 2.04000000    | 1.44249800    |
| H    | 9.62692320    | -0.32135244   | 0.22692611    |
| Au   | 13.90949800   | -2.04000000   | 1.44249800    |
| Au   | 15.34700000   | 0.00000000    | 2.88499600    |
| Au   | 13.90949800   | 2.04000000    | -1.44249800   |
| Au   | 13.90949800   | 2.04000000    | 1.44249800    |
| Au   | 15.34700000   | 0.00000000    | 0.00000000    |
| Au   | 15.34700000   | 4.08000000    | 0.00000000    |
| S    | -12.00054651  | -0.55925351   | 2.15773002    |
| H    | -10.50630888  | -1.48023065   | 4.32226160    |
| C    | -9.78658241   | -1.17849529   | 3.56250159    |
| C    | -10.24509489  | -0.67830016   | 2.32098655    |
| H    | -8.09388055   | -1.67802402   | 4.78384074    |
| C    | -8.42862491   | -1.29041175   | 3.82322164    |
| C    | -9.29333990   | -0.30232016   | 1.35058508    |
| H    | -9.62803130   | 0.08689657    | 0.39081686    |
| C    | -7.46946233   | 0.91455199    | 2.85155513    |
| C    | -7.93393952   | 0.42075155    | 1.60959873    |
| H    | -7.21326469   | -0.12783326   | 0.84812345    |

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C -6.08159038 -1.03241993 3.12047240
C -4.88689078 -1.13822340 3.36387435
H -3.79580212 -1.99100243 5.66547253
C -3.05163624 -1.73148170 4.91514420
C -3.50538970 -1.26473595 3.65413679
H -1.39575458 -2.23274590 6.20932585
C -1.68730637 -1.86826128 5.22558214
C -2.53369717 -0.92414319 2.67595805
H 1.40203672 -2.26947279 6.18301355
C 0.73245865 -1.55914188 4.25059584
C 1.68870540 -1.91917134 5.19296754
C -0.01292144 -0.79986639 2.19847261
O -0.08500086 -0.35694272 0.97993640
C 1.17076647 -1.10433066 2.96908539
C -1.18536297 -1.06542602 2.99640601
H -0.73931422 -1.53606241 4.26726685
C 1.17076647 -1.10433066 2.96908539
H 0.73245865 -1.55914188 4.25059584
C -3.79436563 -2.11081548 5.59577163
C 2.52160203 -1.01065722 2.62940562
C 3.49814019 -1.37843321 3.58706979
H 2.85428869 -0.66476885 1.65026789
C 4.87965860 -1.29998598 3.27945970
C 6.07464987 -1.23645468 3.02460838
H 8.08387130 -1.89876946 4.68628627
C 7.46366635 -1.17101557 2.73947293
C 8.42002496 -1.55455352 3.70991867
H 7.21217971 -0.42080414 0.72169094
C 7.93055958 -0.72231062 1.48226868
C 9.77849873 -1.48943144 3.43405844
H 10.49641958 -1.78225630 4.19912399
C 9.29020783 -0.66351680 1.20340793
C 10.23953003 -1.04541274 2.17300530
Au 15.34700000 0.00000000 -2.88499601
C -0.07752944 -3.76926648 -0.01141092
O 0.17065042 -2.55280180 -0.00648898
O -1.13633814 -4.41763737 -0.00497514
C 1.21772078 -4.67737832 0.03732778
F 2.30647583 -4.11760932 -0.54699630
F 1.06550512 -5.88741949 -0.55746379
F 1.58700521 -4.94399875 1.32344482

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