# Supporting Information

# 9,10-Dihydro-*as*-indacenodithiophenes: Isomers with an *as*-Indacene Core

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## 1. Chemical Structures of Dihydroindacenodithiophenes

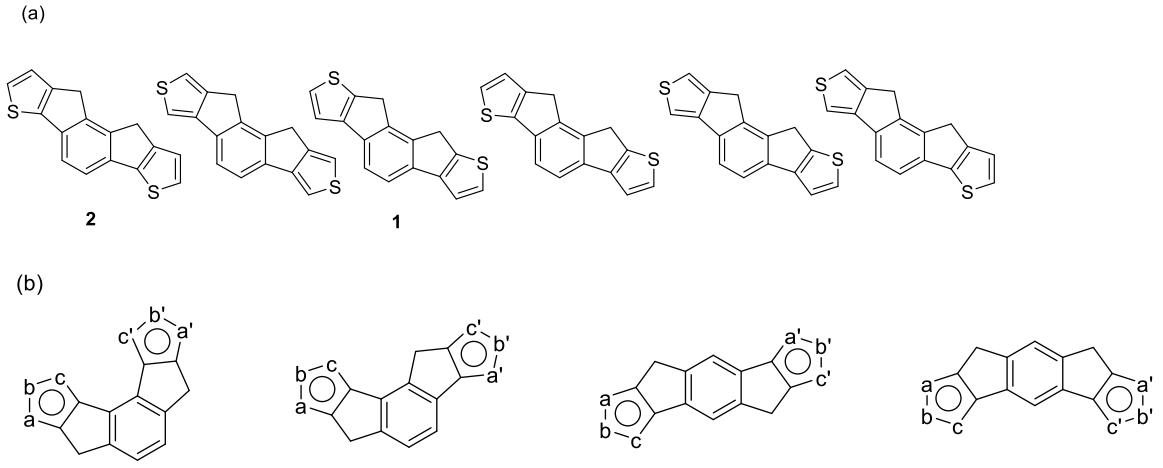


Figure S1. (a) Chemical structures of dihydro-*as*-indacenodithiophene isomers of **1** and **2**. (b) All Isomers where sulfur atoms locate at one of positions a, b, c and one of a', b', c'. In total 31 isomers are possible.

## 2. [1]HNMR Spectrum of a Mixture of Diketones

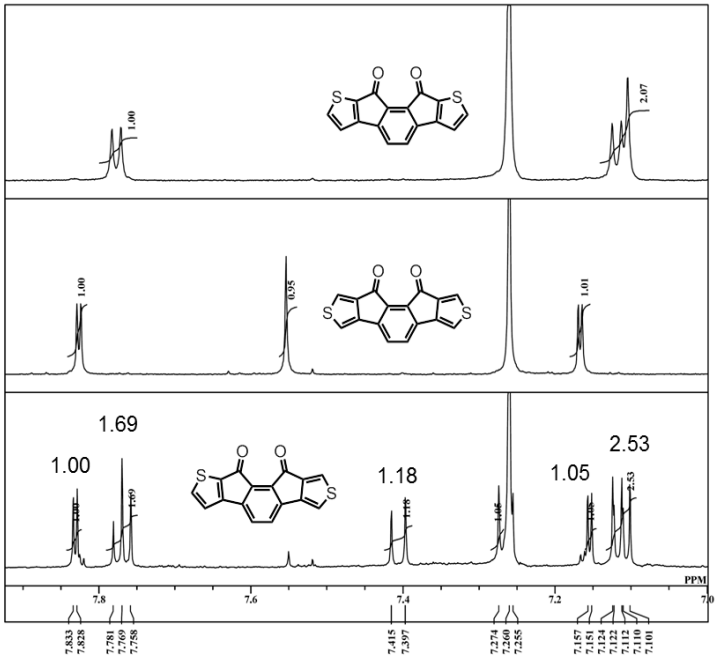


Figure S2. Partial [1]H NMR spectra of (a) **3**, (b) **5**, and (c) a mixture of **3** and the isomer most likely derived by α, β-cyclization, obtained by cyclization of diester **8a** with PPA. In (c), integration values relative to the lowest field signal at 7.83 ppm are also shown. The signals due to **3** overlap at 7.77 (ca. 0.7 H) and 7.10–7.12 (ca. 1.5 H) to those of the isomer of α, β-cyclization.

## 3. Differential Scanning Calorimetry of 1–5

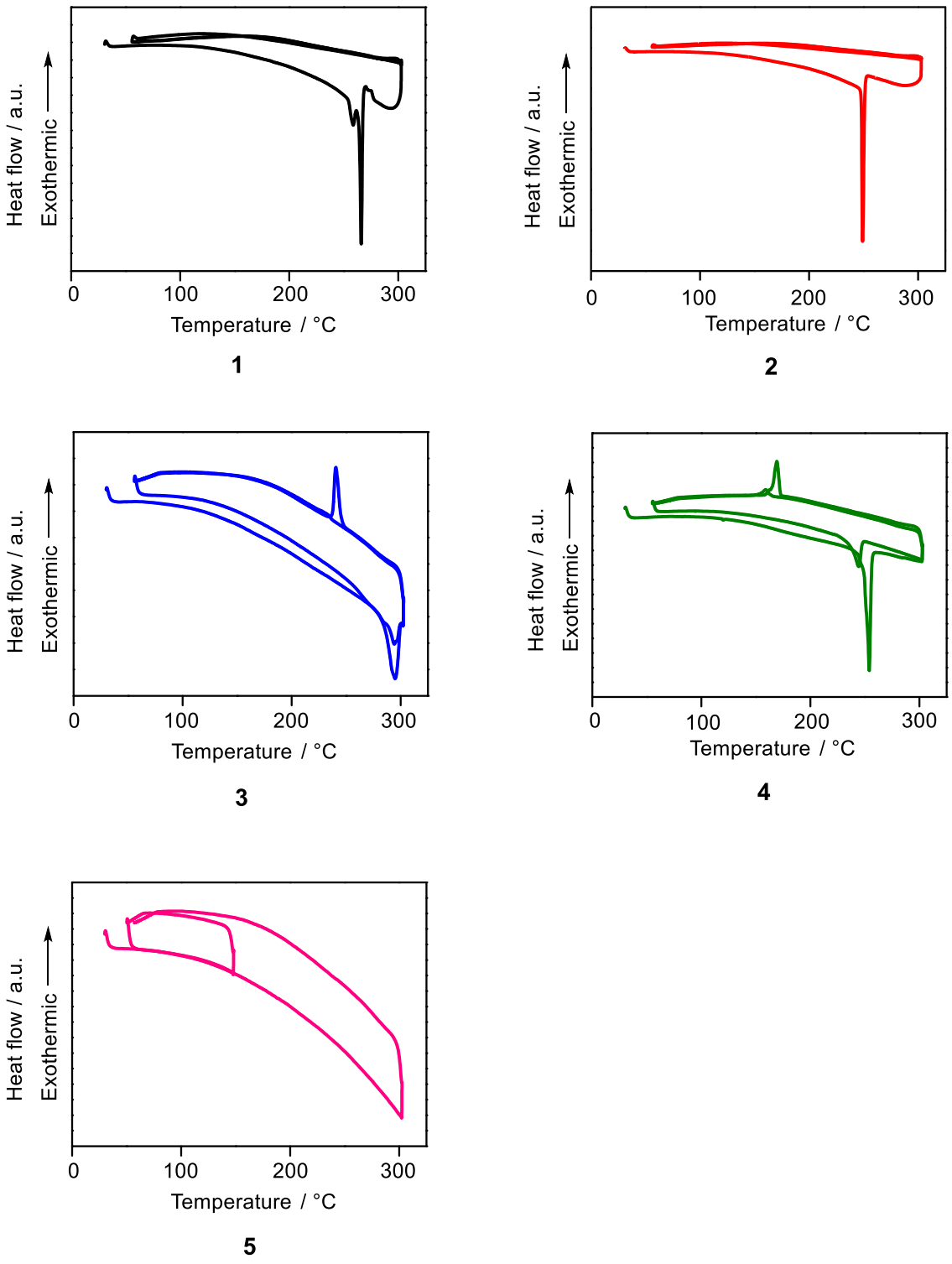


Figure S3. Differential scanning calorimetry traces for **1** (black), **2** (red), **3** (blue), **4** (green), and **5** (pink). The DSC measurements were performed under purified nitrogen at a heating or cooling rate of 10 °C $min^{-1}$.

## 4. Additional UV-vis Absorption Spectra of 1–5

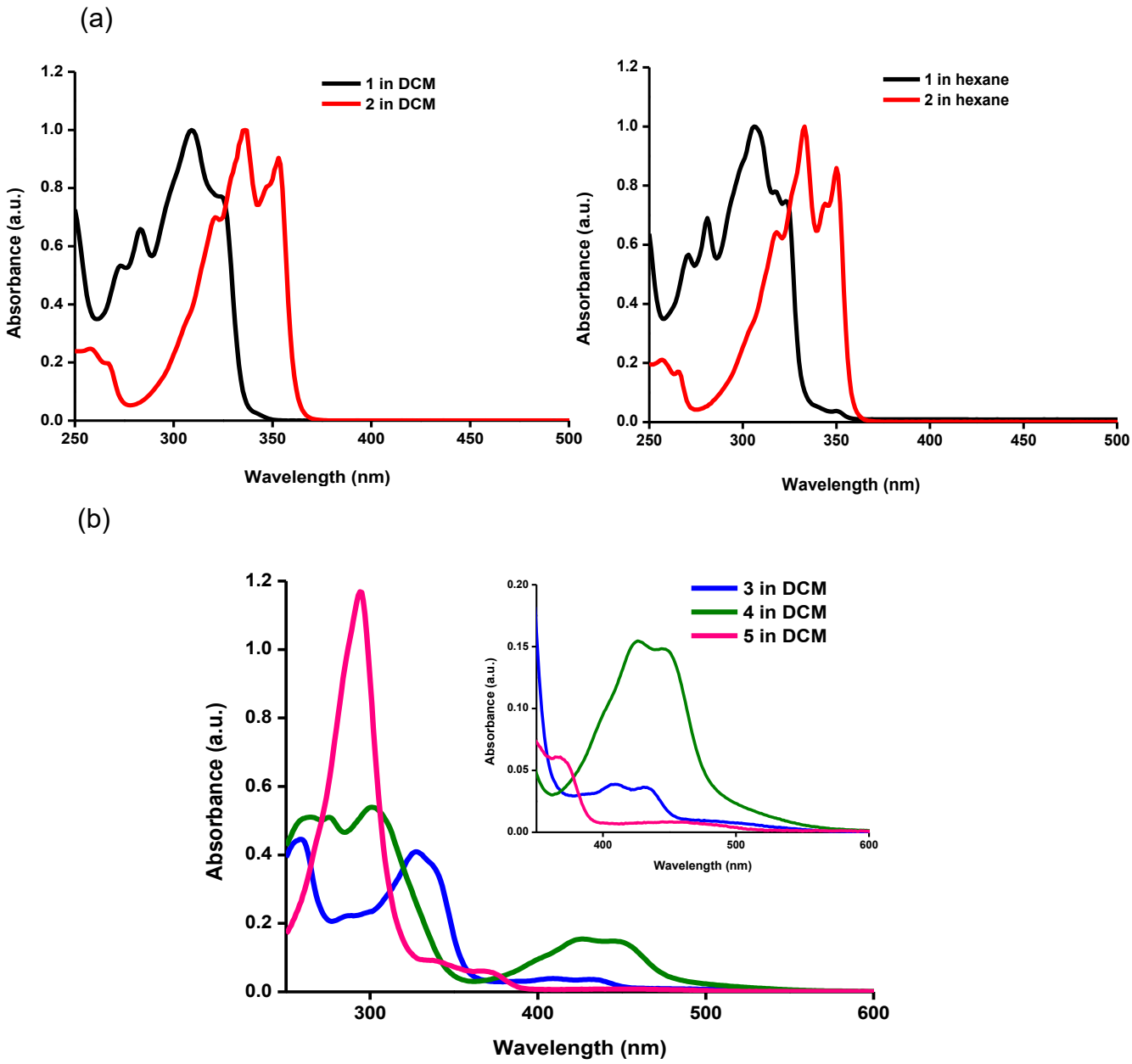


Figure S4. (a) UV-vis spectra for **1** (black curves) and **2** (red curves) in DCM (left) and hexane (right). In DCM concentrations of **1** and **2** are $4.16 \times 10^{-5}$ mol $L^{-1}$ and $6.12 \times 10^{-5}$ mol $L^{-1}$, respectively. In hexane concentrations of **1** and **2** are $1.12 \times 10^{-5}$ mol $L^{-1}$ and $1.15 \times 10^{-5}$ mol $L^{-1}$, respectively. (b) UV-vis spectra for **3** (blue curves), **4** (green curves), and **5** (pink curves). Inset: Long wavelength region with expanded longitudinal axis. Concentrations of **3**–**5** are $1.21 \times 10^{-5}$ mol $L^{-1}$, $1.80 \times 10^{-5}$ mol $L^{-1}$, and $2.51 \times 10^{-5}$ mol $L^{-1}$, respectively.

**Table S1.** Absorption Spectral Data for **1**–**5** in Different Solvents.

| Compd | $\lambda_{abs}$ (ε) (nm) in THF ($\times 10^4$ L mol$^{-1}$ cm$^{-1}$) | $\lambda_{abs}$ (ε) (nm) in DCM ($\times 10^4$ L mol$^{-1}$ cm$^{-1}$) | $\lambda_{abs}$ (ε) (nm) in hexane ($\times 10^4$ L mol$^{-1}$ cm$^{-1}$) |
|---|---|---|---|
| **1** | 281 (1.28), 307 (1.93), 323 (1.45) | 283 (1.29), 309 (1.95), 325 (1.51) | 281 (1.21), 306 (1.84), 318 (1.38), 323 (1.34) |
| **2** | 334 (3.54), 345 (2.62), 352 (3.08) | 336 (3.65), 347 (2.67), 353 (3.11) | 333 (3.34), 344 (2.46), 350 (2.91) |
| **3** | 404 (0.25), 426 (0.24), 496 (0.05) | 409 (0.26), 431 (0.27), 500 (0.08) | not measured |
| **4** | 421 (1.21), 442 (1.11), 505 (0.12) | 426 (1.31), 446 (1.18), 509 (0.13) | not measured |
| **5** | 366 (0.42), 445 (0.04) | 368 (0.48), 456 (0.07) | not measured |

## 5. Additional Fluorescence Spectra of 1 and 2

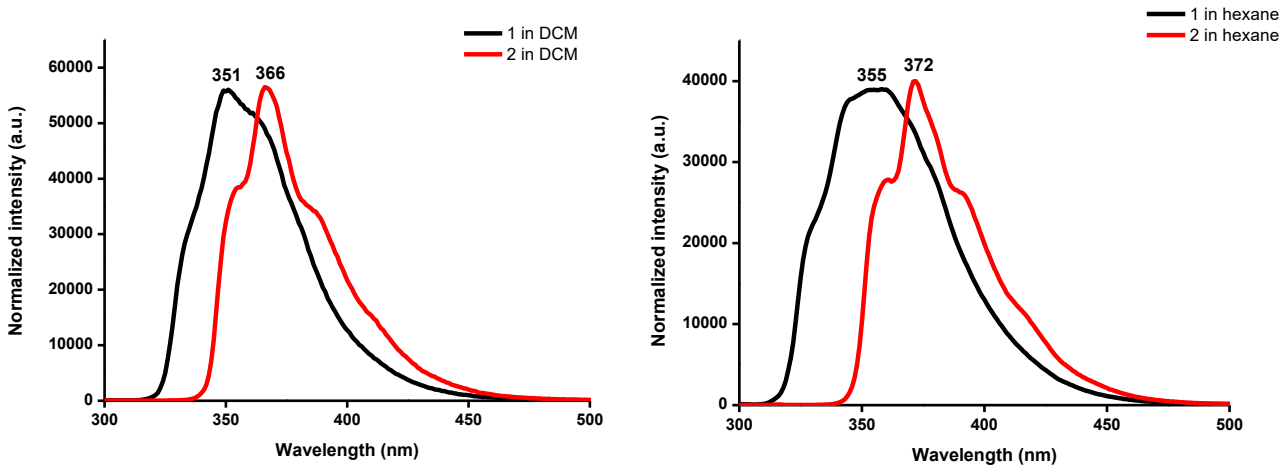


Figure S5. Fluorescence spectra of **1** (black curves) and **2** (red curves) in DCM (left) and hexane (right). In DCM concentrations of **1** and **2** are $4.16 \times 10^{-5}$ mol $L^{-1}$ and $6.12 \times 10^{-5}$ mol $L^{-1}$, respectively. In hexane concentrations of **1** and **2** are $1.12 \times 10^{-5}$ mol $L^{-1}$ and $1.15 \times 10^{-5}$ mol $L^{-1}$, respectively. In both solvents, excitation wavelengths of **1** and **2** are 308 and 335 nm, respectively.

## 6. Stability and Aromaticity Parameters for 1, 2, 7a, and 8a

**Table S2.** Stability and Aromaticity Parameters for **1**, **2**, **7a**, and **8a**.

| | Compound | | | |
|---|---|---|---|---|
| Parameter | **1** | **2** | **7a** | **8a** |
| Relative stability (kcal/mol)[a] | 1.82 | 0.06 | 0 | 0.40 |
| NICS(1)[b] | | | | |
| benzene | −10.1 | −10.1 | −10.1 | −10.0 |
| thiophene | −8.8 | −8.7 | −8.7 | −8.7 |
| HOMA[c] | | | | |
| benzene | 0.918 | 0.911 | 0.912 | 0.918 |
| thiophene | 0.595 | 0.608 | 0.602 | 0.608 |

[a] Relative energy of the DFT calculations at the B3LYP/6-311+G(d,p) level taking the energy of **7a** as a standard. [b] Nucleus independent chemical shift 1 Å above the center of the ring Nucleus independent chemical shift 1 Å above the center of the ring calculated by the GIAO method at the HF/6-311+G(d,p) level for the geometry optimized by the B3LYP/6-311+G(d,p) level. [c] Harmonic oscillator model of aromaticity.

## 7. TD-DFT Calculations for 1−5

**Table S3.** Excitation energies of **1** calculated at the TD-B3LYP/6-311+G(d,p) level of theory.

| Exited State | Transition Energy / eV (Wavelength / nm) | Main CI Coefficient | Oscillator Strength, *f* |
|---|---|---|---|
| 1 | 4.39 (283) | 0.68611 (HOMO — LUMO) | 0.5284 |
| 2 | 4.56 (272) | –0.10955 (HOMO–4 — LUMO) | 0.0001 |
| | | 0.12692 (HOMO–3 — LUMO) | |
| | | 0.65614 (HOMO — LUMO+2) | |
| | | –0.14131 (HOMO — LUMO+10) | |
| 3 | 4.94 (251) | 0.63850 (HOMO — LUMO+1) | 0.0000 |
| | | 0.22705 (HOMO — LUMO+8) | |
| 4 | 5.37 (231) | 0.16057 (HOMO–1 — LUMO+1) | 0.0104 |
| | | 0.60398 (HOMO — LUMO+3) | |
| | | –0.14183 (HOMO — LUMO+7) | |
| | | –0.14304 (HOMO–3 — LUMO+9) | |
| | | –0.17695 (HOMO — LUMO+12) | |
| 5 | 5.44 (228) | 0.12443 (HOMO–4 — LUMO+2) | 0.0668 |
| | | –0.13052 (HOMO–2 — LUMO) | |
| | | –0.11256 (HOMO–1 — LUMO+2) | |
| | | 0.64128 (HOMO — LUMO+6) | |
| | | –0.12883(HOMO — LUMO+13) | |
| 6 | 5.49 (226) | 0.65440 (HOMO — LUMO+4) | 0.0000 |
| | | 0.18906 (HOMO — LUMO+5) | |
| 7 | 5.55 (223) | 0.46731 (HOMO–3 — LUMO) | 0.0142 |
| | | –0.10118 (HOMO–1 — LUMO) | |
| | | 0.11063 (HOMO–1 — LUMO+6) | |
| | | –0.17418 (HOMO — LUMO+2) | |
| | | –0.39781 (HOMO — LUMO+10) | |
| | | 0.17638 (HOMO — LUMO+14) | |

| | | | |
|---|---|---|---|
| 8 | 5.77 (215) | –0.15039 (HOMO–1 — LUMO+3) | 0.0000 |
| | | –0.17071 (HOMO — LUMO+4) | |
| | | 0.61851 (HOMO — LUMO+5) | |
| | | 0.14981 (HOMO — LUMO+8) | |
| 9 | 5.86 (212) | –0.10712 (HOMO–4 — LUMO+6) | 0.0052 |
| | | –0.18107 (HOMO–2 — LUMO+2) | |
| | | –0.1084(HOMO–2 — LUMO+10) | |
| | | 0.58659 (HOMO–1 — LUMO) | |
| | | –0.12606 (HOMO — LUMO+10) | |
| | | 0.18958(HOMO — LUMO+18) | |
| 10 | 5.87 (211) | 0.12369 (HOMO–1 — LUMO+4) | 0.0020 |
| | | 0.21828 (HOMO — LUMO+3) | |
| | | 0.59118 (HOMO — LUMO+7) | |
| | | 0.12850 (HOMO — LUMO+9) | |

**Table S4.** Excitation energies of **2** calculated at the TD-B3LYP/6-311+G(d,p) level of theory.

| Exited State | Transition Energy / eV (Wavelength / nm) | Main CI Coefficient | Oscillator Strength, *f* |
|---|---|---|---|
| 1 | 4.23 (293) | 0.68926 (HOMO — LUMO) | 0.6722 |
| 2 | 4.51 (274) | 0.12038 (HOMO–2 — LUMO) | 0.0095 |
| | | –0.10326 HOMO–1 — LUMO) | |
| | | 0.65022 (HOMO — LUMO+2) | |
| | | –0.15920 (HOMO — LUMO+10) | |
| 3 | 4.86 (255) | 0.61920 (HOMO — LUMO+1) | 0.00000 |
| | | 0.19823 (HOMO — LUMO+5) | |
| | | 0.20881 (HOMO — LUMO+8) | |
| 4 | 5.25 (236) | –0.17624 (HOMO–1 — LUMO+1) | 0.0134 |
| | | 0.61800 (HOMO — LUMO+3) | |
| | | 0.20060 (HOMO — LUMO+9) | |
| | | –0.14099 (HOMO— LUMO+12) | |
| 5 | 5.42 (228) | 0.61992 (HOMO— LUMO+4) | 0.0000 |
| | | –0.24160 (HOMO — LUMO+5) | |
| | | 0.16952 (HOMO — LUMO+8) | |
| 6 | 5.51 (225) | –0.10179 (HOMO–2 — LUMO) | 0.0046 |
| | | –0.30422 (HOMO–1 — LUMO) | |
| | | 0.11309 (HOMO—– LUMO+2) | |
| | | 0.56618 (HOMO — LUMO+10) | |
| | | –0.17305 (HOMO — LUMO+14) | |
| 7 | 5.54 (224) | 0.15928 (HOMO–1 — LUMO+3) | 0.0000 |
| | | –0.17069 (HOMO — LUMO+1) | |
| | | 0.24886 (HOMO — LUMO+4) | |
| | | 0.58678 (HOMO — LUMO+5) | |

| | | | |
|---|---|---|---|
| 8 | 5.55 (223) | 0.14657 (HOMO–1 — LUMO+2) | 0.0045 |
| | | 0.65410 (HOMO — LUMO+6) | |
| | | –0.10924 (HOMO — LUMO+19) | |
| 9 | 5.81 (213) | –0.21991 (HOMO — LUMO+1) | 0.0000 |
| | | –0.16479 (HOMO — LUMO+4) | |
| | | 0.61741 (HOMO — LUMO+8) | |
| 10 | 5.82 (213) | –0.18188 (HOMO–1 — LUMO+5) | 0.0024 |
| | | –0.22418 (HOMO — LUMO+3) | |
| | | –0.15843 (HOMO — LUMO+7) | |
| | | –0.56538 (HOMO — LUMO+9) | |
| | | –0.14286 (HOMO — LUMO+12) | |

**Table S5.** Excitation energies of diketone **3** calculated at the TD-B3LYP/6-311+G(d,p) level of theory.

| Exited State | Transition Energy / eV (Wavelength / nm) | Main CI Coefficient | Oscillator Strength, *f* |
|---|---|---|---|
| 1 | 2.65 (468) | 0.69408 (HOMO — LUMO) | 0.0004 |
| 2 | 2.77 (447) | –0.22566 (HOMO–5 — LUMO+1) | 0.0000 |
| | | 0.65465 (HOMO–1 — LUMO) | |
| 3 | 3.09 (401) | –0.12492 (HOMO–4 — LUMO) | 0.0654 |
| | | 0.23933 (HOMO–2 — LUMO) | |
| | | 0.64755 (HOMO — LUMO+1) | |
| 4 | 3.18 (390) | 0.48955 (HOMO–5 — LUMO) | 0.0000 |
| | | –0.48126 (HOMO–1 — LUMO+1) | |
| 5 | 4.41 (281) | 0.14771 (HOMO–6 — LUMO+1) | 0.0108 |
| | | –0.22157 (HOMO–4 — LUMO+1) | |
| | | 0.33593 (HOMO–3 — LUMO) | |
| | | 0.52599 (HOMO–2 — LUMO+1) | |
| | | 0.14622 (HOMO — LUMO+7) | |
| 6 | 4.61 (269) | 0.22928 (HOMO–3 — LUMO+1) | 0.8383 |
| | | 0.60912 (HOMO–2 — LUMO) | |
| | | –0.23115 (HOMO — LUMO+1) | |
| 7 | 4.61 (268) | 0.49001 (HOMO–5 — LUMO) | 0.0000 |
| | | 0.50135 (HOMO–1 — LUMO+1) | |
| 8 | 4.89 (253) | 0.22980 (HOMO–6 — LUMO) | 0.0457 |
| | | 0.50900 (HOMO–4 — LUMO) | |
| | | 0.32160 (HOMO–3 — LUMO+1) | |
| | | –0.16497 (HOMO–2 — LUMO) | |
| | | 0.13921 (HOMO — LUMO+1) | |
| | | 0.15947 (HOMO — LUMO+5) | |
| 9 | 4.97 (250) | 0.35461 (HOMO–4 — LUMO+1) | 0.0220 |
| | | 0.55401 (HOMO–3 — LUMO) | |

| | | | |
|---|---|---|---|
| | | –0.15920 (HOMO–2 — LUMO+1) | |
| | | –0.13683 (HOMO — LUMO+7) | |
| 10 | 5.02 (247) | 0.64575 (HOMO–5 — LUMO+1) | 0.0001 |
| | | 0.24097 (HOMO–1 — LUMO) | |
| | | 0.11790 (HOMO–1 — LUMO+7) | |

**Table S6.** Excitation energies of diketone **4** calculated at the TD-B3LYP/6-311+G(d,p) level of theory.

| Exited State | Transition Energy / eV (Wavelength / nm) | Main CI Coefficient | Oscillator Strength, *f* |
|---|---|---|---|
| 1 | 2.48 (500) | 0.69364 (HOMO — LUMO) | 0.0000 |
| 2 | 2.64 (468) | 0.22218 (HOMO–4 — LUMO+1) | 0.0000 |
| | | 0.65608 (HOMO–1 — LUMO+1) | |
| 3 | 2.95 (420) | 0.25196 (HOMO–2 — LUMO) | 0.1088 |
| | | 0.65114 (HOMO — LUMO+1) | |
| 4 | 3.05 (406) | 0.50956 (HOMO–4 — LUMO) | 0.0000 |
| | | 0.45474 (HOMO–1 — LUMO+1) | |
| | | 0.10726 (HOMO–1 — LUMO+6) | |
| 5 | 4.44 (278) | 0.23555 (HOMO–6 — LUMO+1) | 0.0099 |
| | | –0.15349 (HOMO–5 — LUMO+1) | |
| | | 0.23728 (HOMO–3 — LUMO) | |
| | | 0.53939 (HOMO–2 — LUMO+1) | |
| | | 0.22879 (HOMO — LUMO+3) | |
| 6 | 4.49 (276) | –0.47155 (HOMO–4 — LUMO) | 0.0000 |
| | | 0.51996 (HOMO–1 — LUMO+1) | |
| 7 | 4.63 (267) | 0.64895 (HOMO–2 — LUMO) | 0.6219 |
| | | –0.25682 (HOMO — LUMO+1) | |
| 8 | 4.80 (258) | –0.19229 (HOMO–6 — LUMO) | 0.3047 |
| | | 0.57874 (HOMO–5 — LUMO) | |
| | | –0.30848 (HOMO–3 — LUMO+1) | |
| | | 0.11419 (HOMO — LUMO+6) | |
| 9 | 4.88 (254) | 0.64242 (HOMO–4 — LUMO+1) | 0.0000 |
| | | –0.24328 (HOMO–1 — LUMO) | |
| | | 0.10555 (HOMO–1 — LUMO+3) | |
| 10 | 5.01 (247) | –0.10310 (HOMO–7 — LUMO) | 0.0280 |
| | | –0.25255 (HOMO–5 — LUMO+1) | |
| | | 0.57717 (HOMO–3 — LUMO) | |

–0.24638 (HOMO–2 — LUMO+1)

**Table S7.** Excitation energies of diketone **5** calculated at the TD-B3LYP/6-311+G(d,p) level of theory.

| Exited State | Transition Energy / eV (Wavelength / nm) | Main CI Coefficient | Oscillator Strength, *f* |
|---|---|---|---|
| 1 | 2.72 (454) | –0.17922 (HOMO–4 — LUMO+1) | 0.0000 |
| | | 0.63861 (HOMO–1 — LUMO) | |
| | | 0.12657 (HOMO–1 — LUMO+1) | |
| 2 | 2.73 (453) | 0.69263 (HOMO — LUMO) | 0.0001 |
| 3 | 3.20 (386) | 0.25547 (HOMO–7 — LUMO) | 0.0000 |
| | | 0.43332 (HOMO–4 — LUMO) | |
| | | 0.13024 (HOMO–1 — LUMO) | |
| | | –0.43184 (HOMO–1 — LUMO+1) | |
| | | 0.11558 (HOMO–1 — LUMO+3) | |
| 4 | 3.22 (384) | –0.25124 (HOMO–3 — LUMO) | 0.0773 |
| | | 0.64278 (HOMO — LUMO+1) | |
| 5 | 4.47(277) | –0.11065 (HOMO–6 — LUMO+1) | 0.0257 |
| | | –0.13953 (HOMO–5 — LUMO+1) | |
| | | –0.12566 (HOMO–3 — LUMO) | |
| | | 0.36281 (HOMO–3 — LUMO+1) | |
| | | 0.45655 (HOMO–2 — LUMO) | |
| | | 0.25909 (HOMO–2 — LUMO+1) | |
| | | –0.13425 (HOMO — LUMO+6) | |
| 6 | 4.56 (271) | 0.45817 (HOMO–4 — LUMO) | 0.0002 |
| | | –0.14343 (HOMO–4 — LUMO+1) | |
| | | 0.49642 (HOMO–1 — LUMO+1) | |
| 7 | 471 (263) | –0.10459 (HOMO–6 — LUMO) | 0.5371 |
| | | 0.10598 (HOMO–6 — LUMO+1) | |
| | | 0.16490 (HOMO–5 — LUMO) | |
| | | 0.36213 (HOMO–3 — LUMO) | |
| | | –0.33328 (HOMO–3 — LUMO+1) | |

| | | | |
|---|---|---|---|
| | | 0.36077 (HOMO–2 — LUMO) | |
| | | 0.12079 (HOMO–2 — LUMO+1) | |
| | | 0.18448 (HOMO — LUMO+1) | |
| 8 | 4.82 (257) | 0.10492 (HOMO–6 — LUMO) | 0.4043 |
| | | –0.25042 (HOMO–5 — LUMO) | |
| | | 0.50265 (HOMO–3 — LUMO) | |
| | | 0.25568 (HOMO–3 — LUMO+1) | |
| | | –0.11996 (HOMO–2 — LUMO) | |
| | | 0.20762 (HOMO — LUMO+1) | |
| | | 0.13749 (HOMO — LUMO+3) | |
| 9 | 4.95 (250) | 0.28406 (HOMO–7 — LUMO) | 0.0002 |
| | | 0.58449 (HOMO–4 — LUMO+1) | |
| | | 0.16673 (HOMO–1 — LUMO) | |
| | | 0.14007 (HOMO–1 — LUMO+1) | |
| 10 | 5.07 (244) | 0.53166 (HOMO–5 — LUMO) | 0.0468 |
| | | –0.30587 (HOMO–5 — LUMO+1) | |
| | | 0.11588 (HOMO–3 — LUMO) | |
| | | 0.14202 (HOMO–3 — LUMO+1) | |
| | | –0.17805 (HOMO–2 — LUMO) | |
| | | –0.10234 (HOMO — LUMO+3) | |

## 8. $^{1}H$ and $^{13}C\{^{1}H\}$ NMR Spectra of **1-5** and **12-16.**

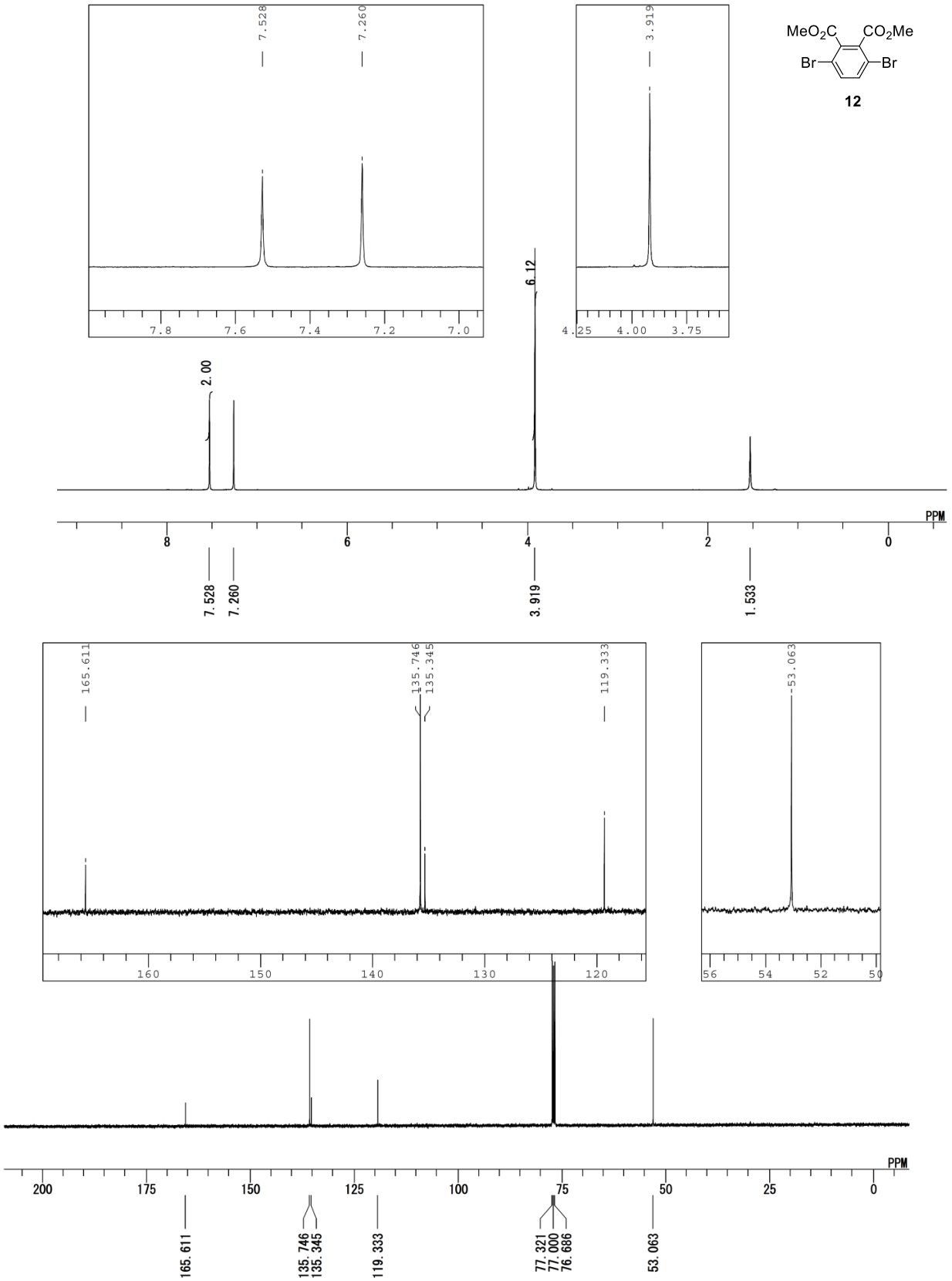


Figure S6. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of dimethyl 3,6-dibromophthalate (**12**) at 30 °C in $CDCl_3$.

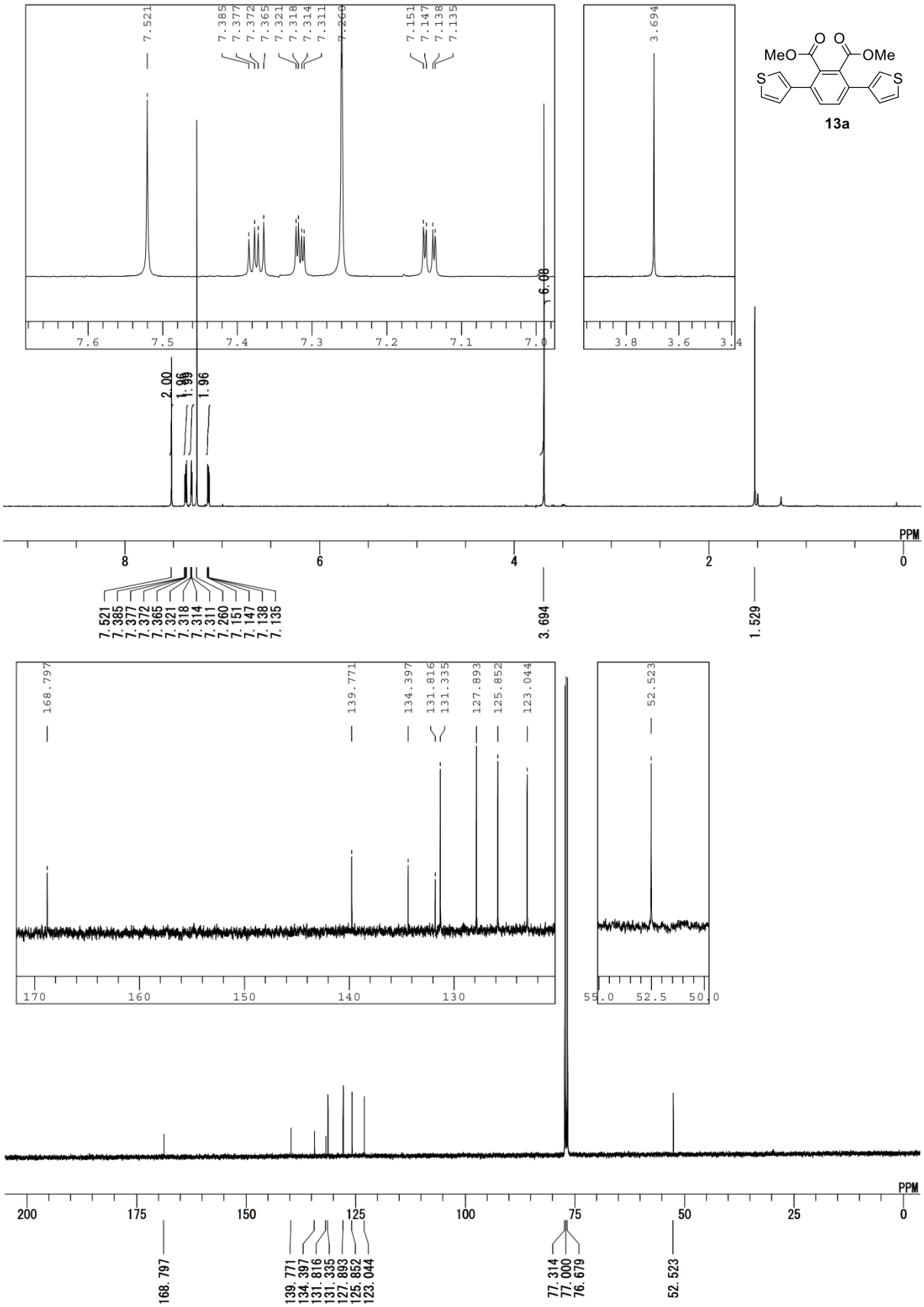


Figure S7. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of dimethyl 3,6-di(thiophen-3-yl)phthalate (**13a**)at 30 °C in $CDCl_3$.

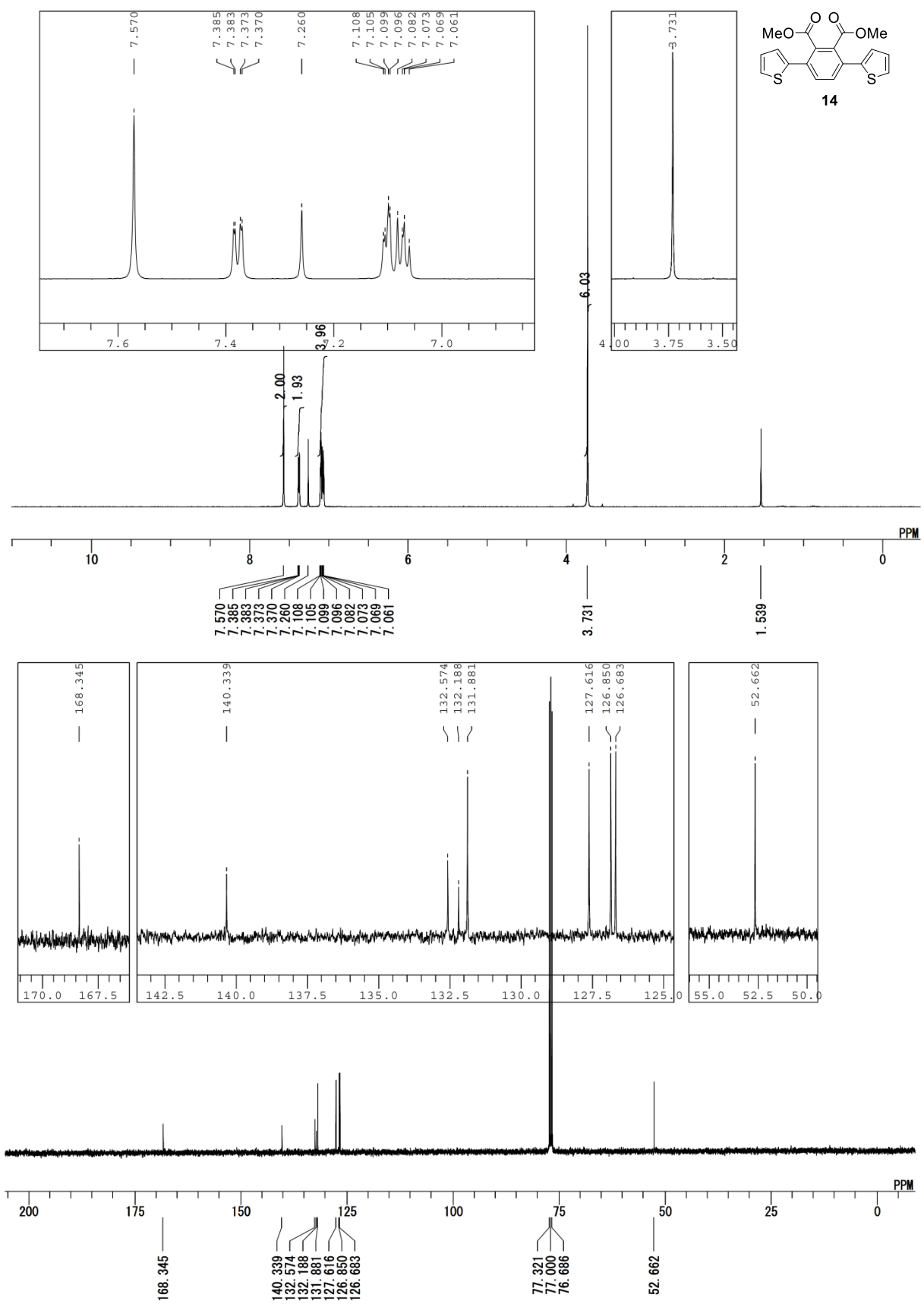


Figure S8. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of dimethyl 3,6-di(thiophen-2-yl)phthalate (**14**)at 30 °C in $CDCl_3$.

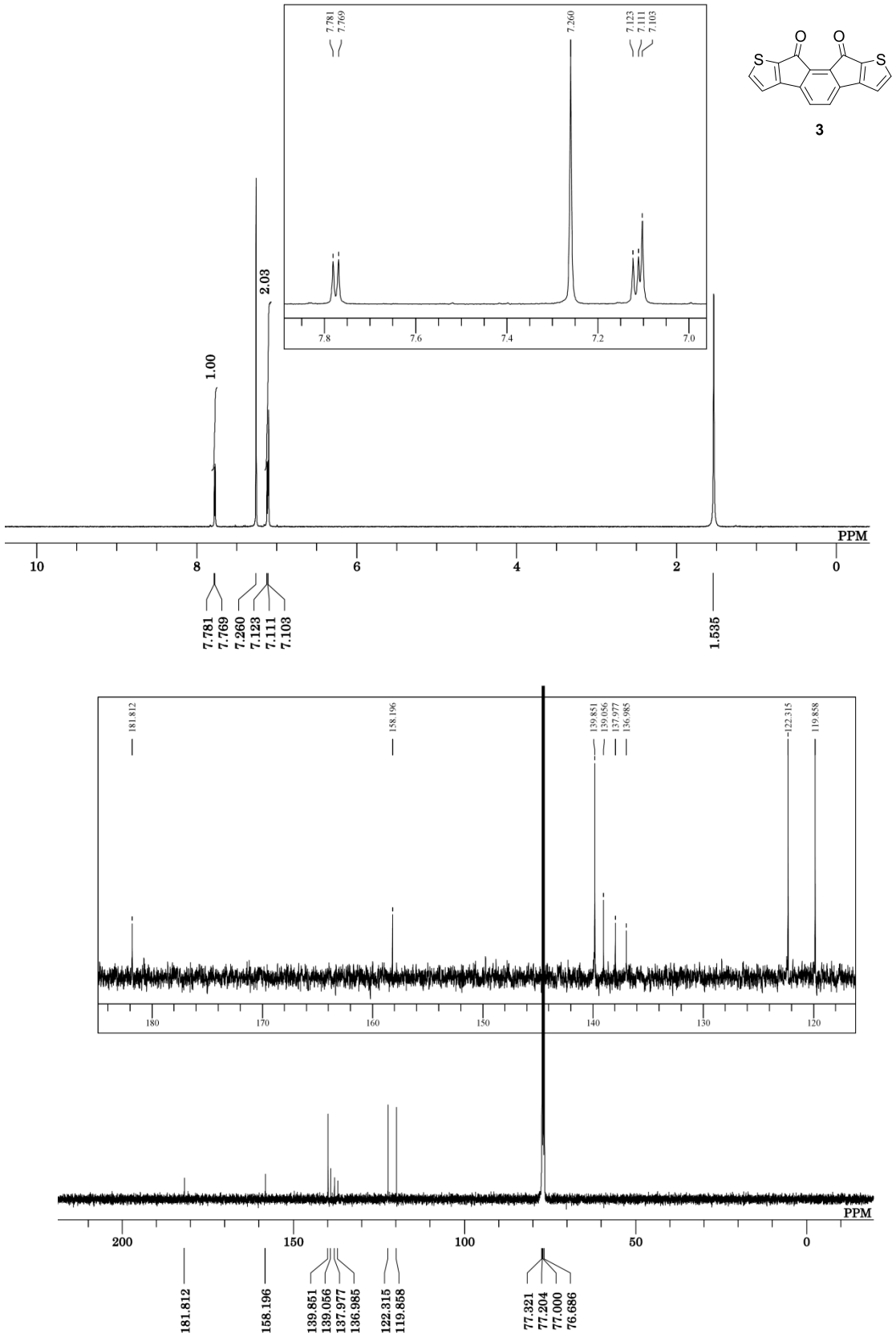


Figure S9. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of *as*-indaceno[2,3-*b*:7,6-*b*']dithiophene-9,10-dione (**3**)at 30 °C in $CDCl_3$.

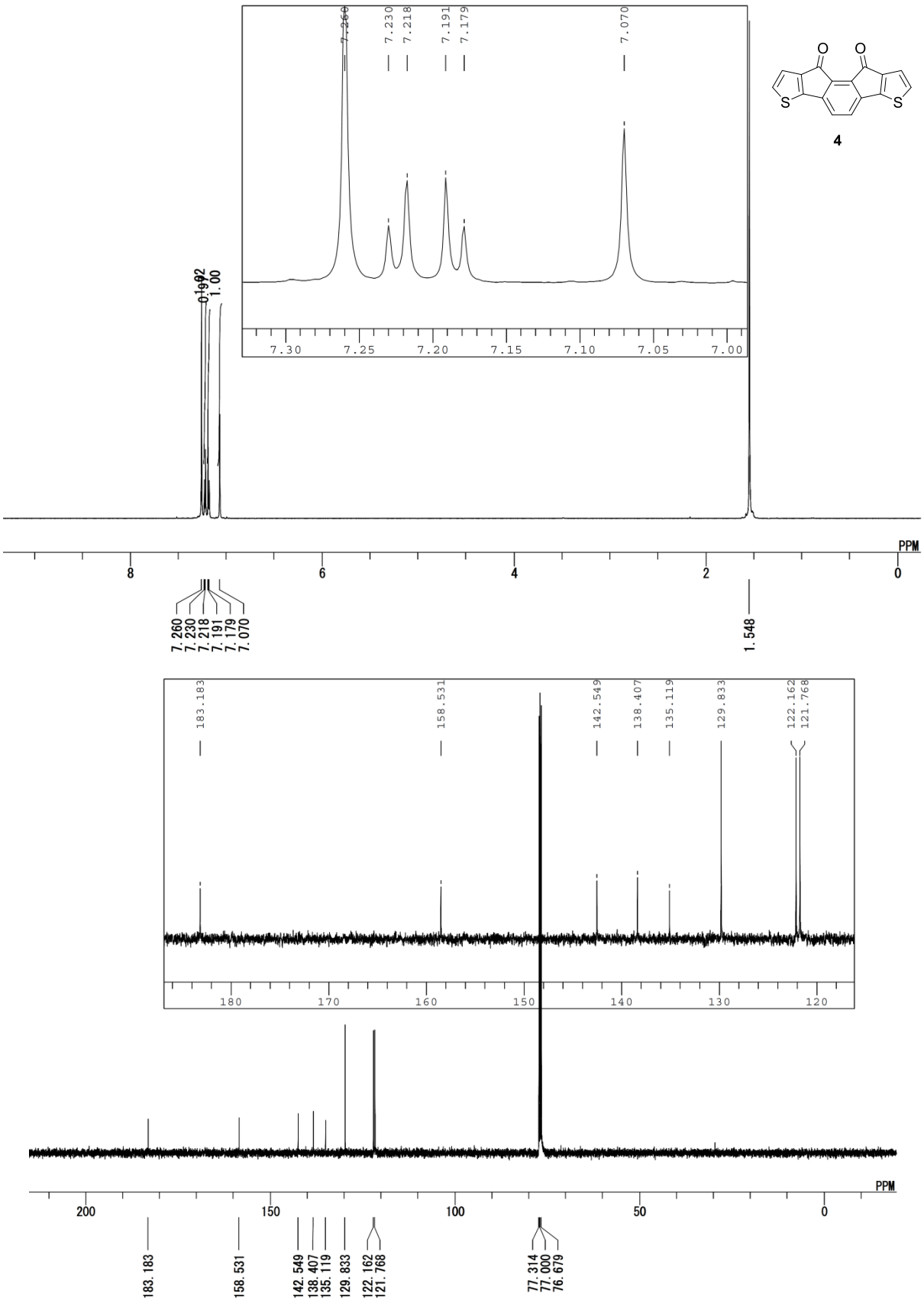


Figure 10. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of *as*-indaceno[3,2-*b*:6,7-*b*']dithiophene-9,10-dione (**4**)at 30 °C in $CDCl_3$.

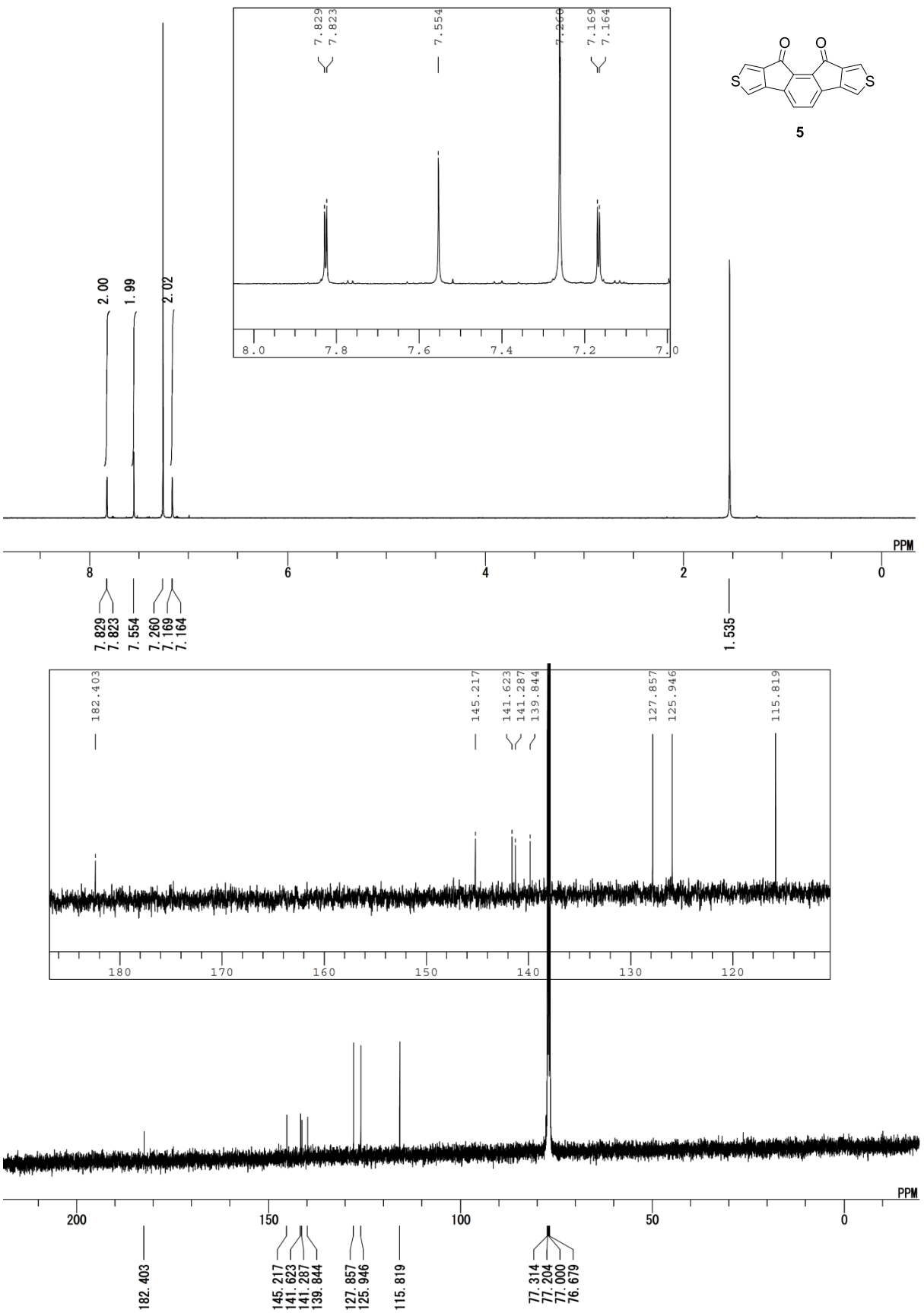


Figure 11. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of *as*-indaceno[2,3-*c*:6,7-*c*']dithiophene-9,10-dione (**5**)at 30 °C in $CDCl_3$.

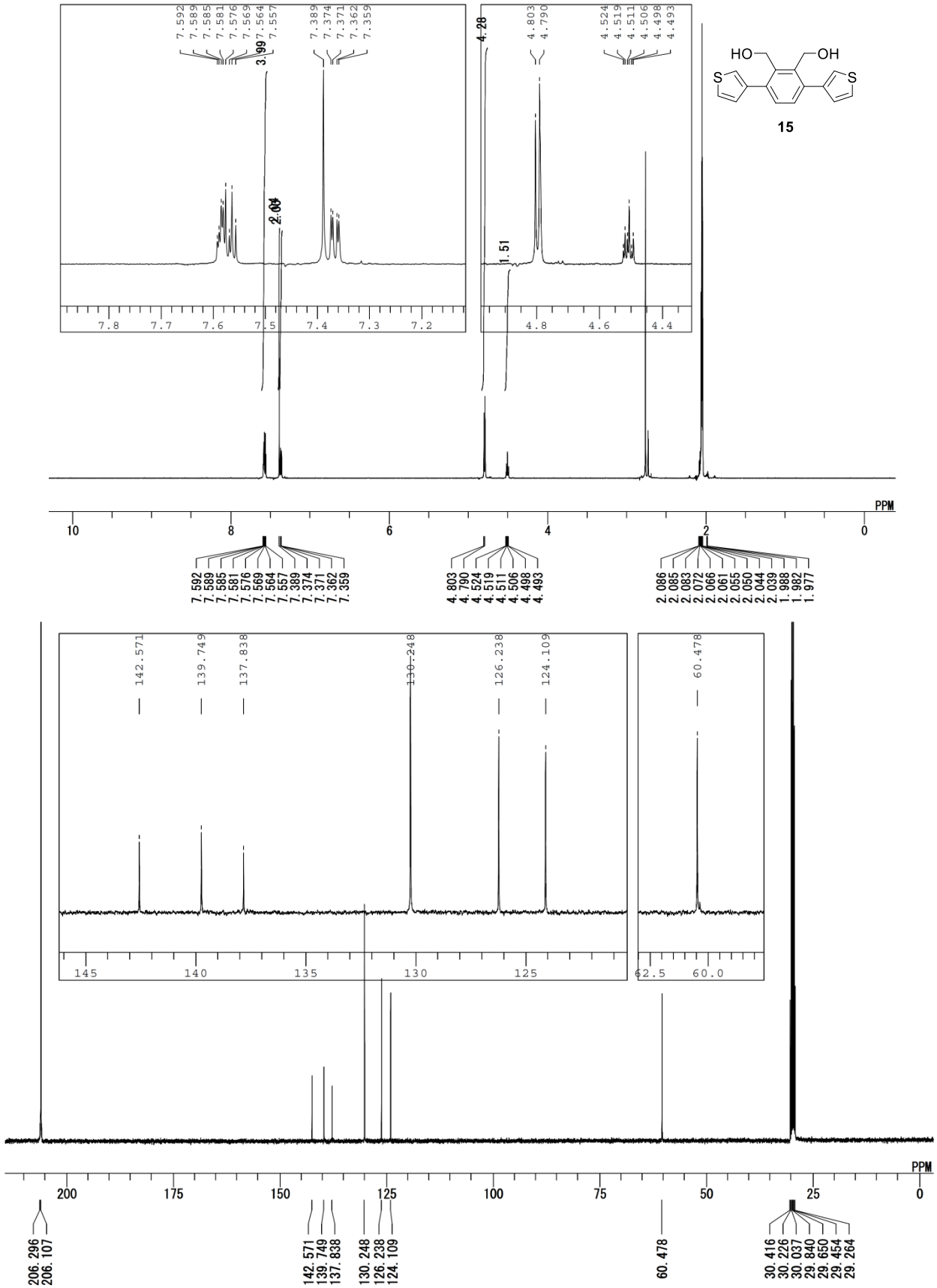


Figure S12. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of [3,6-di(thiophen-3-yl)-1,2-phenylene]dimethanol (**15**)at 30 °C in Acetone-$d_6$.

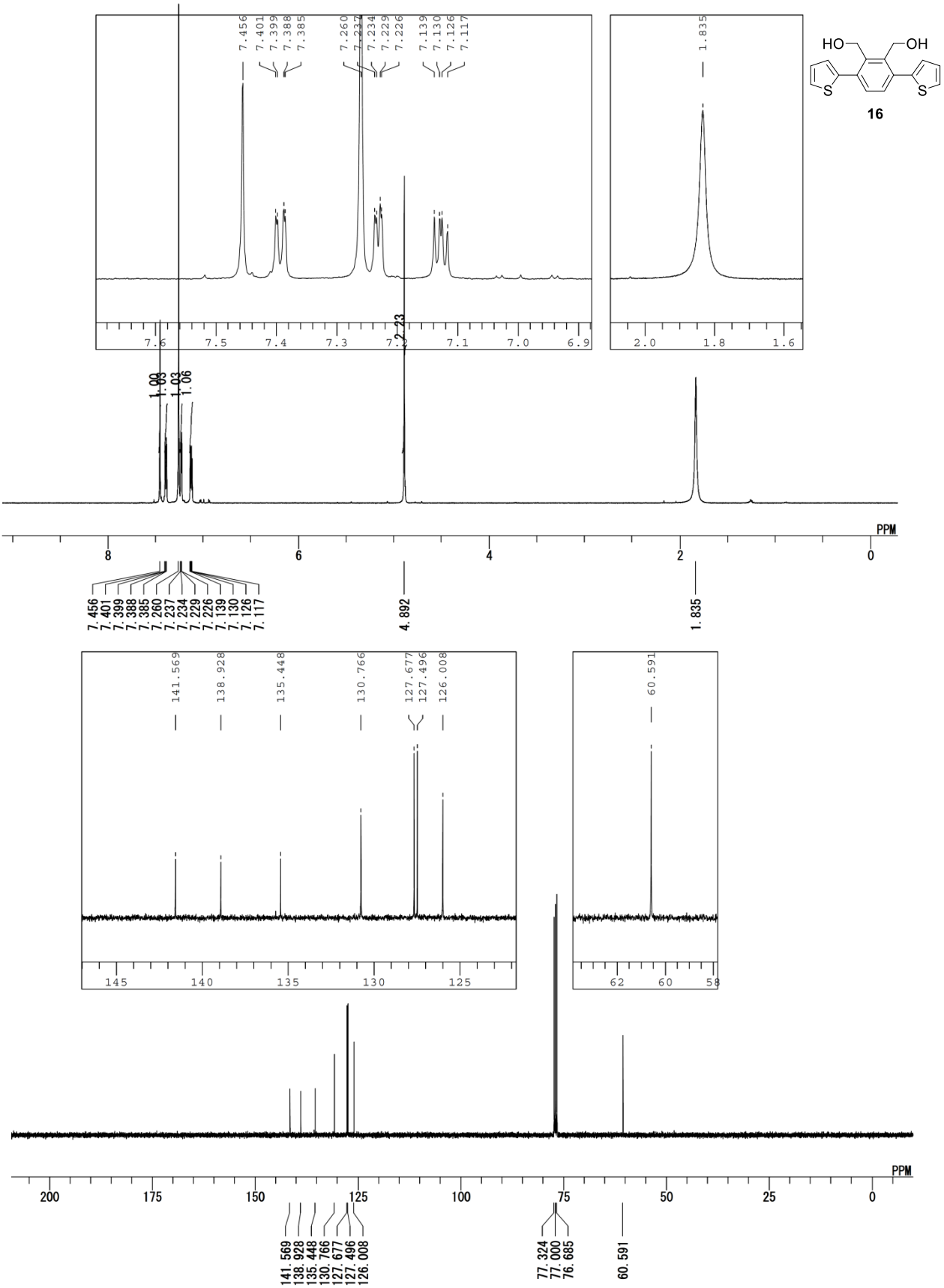


Figure S13. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of [3,6-di(thiophen-2-yl)-1,2-phenylene]dimethanol (**16**)at 30 °C in $CDCl_3$.

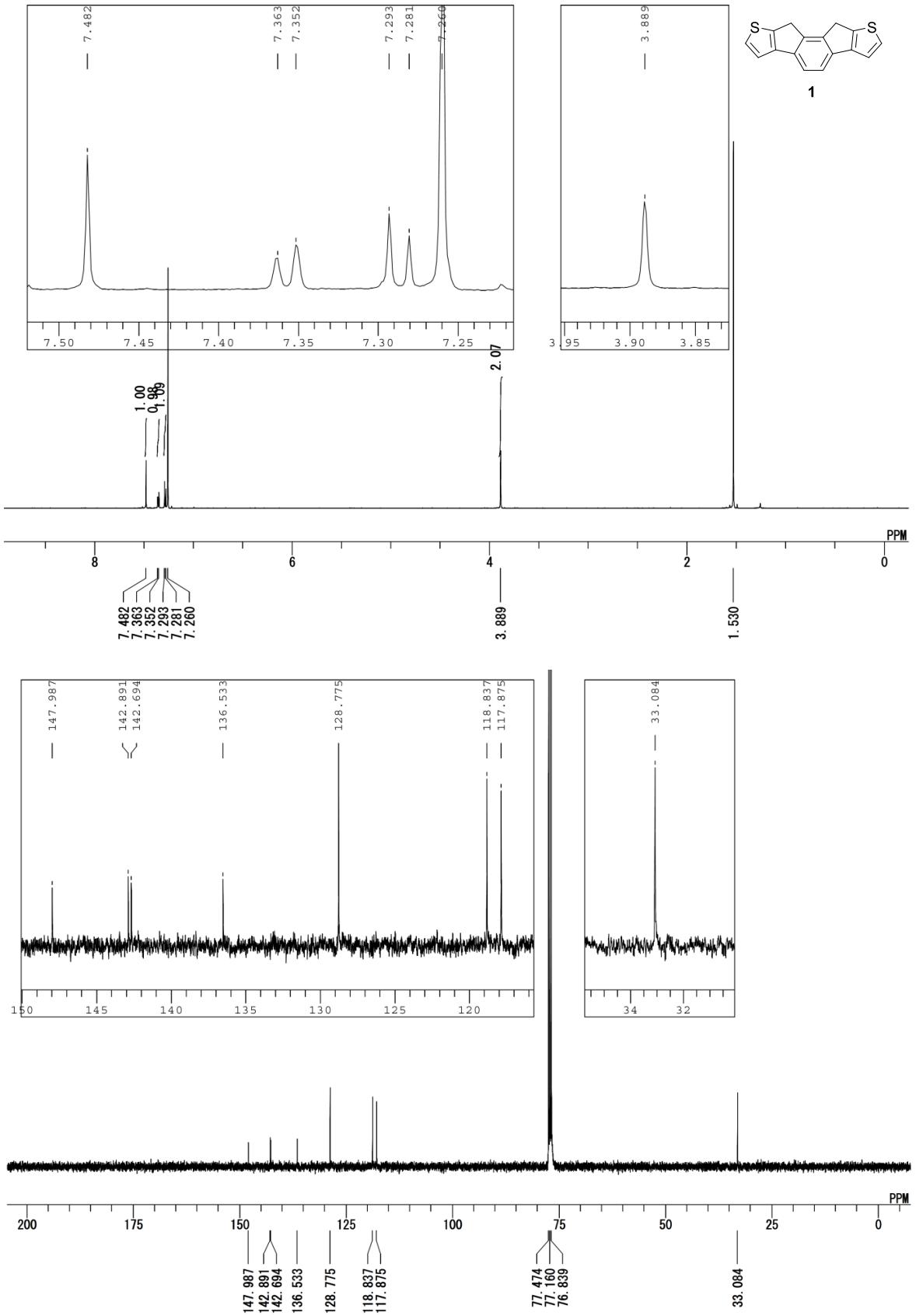


Figure S14. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of 9,10-dihydro-*as*-indaceno[2,3-*b*:7,6-*b*']dithiophene (**1**) at 30 °C in $CDCl_3$.

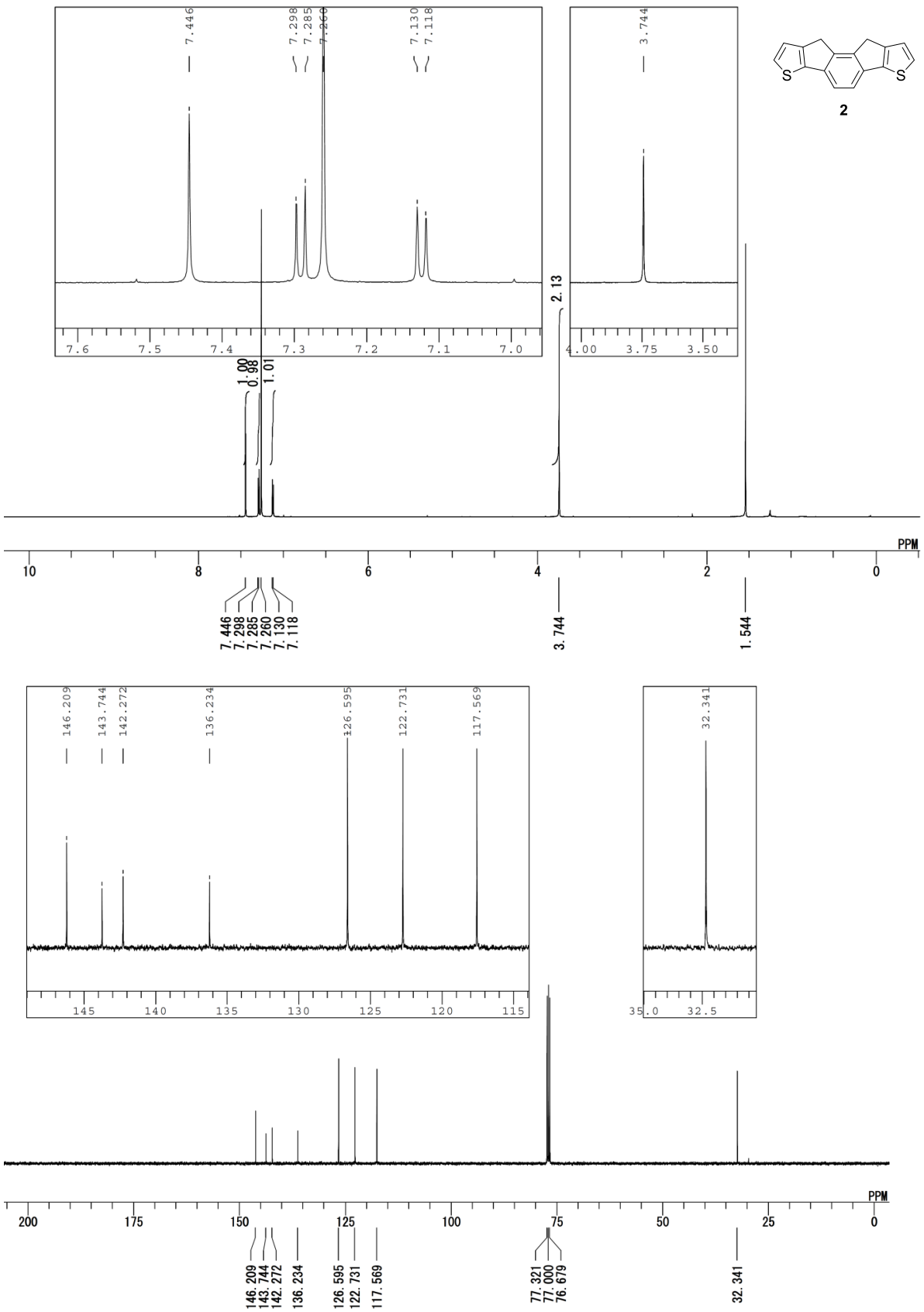


Figure S15. $^{1}H$ (top) and $^{13}C\{^{1}H\}$ (bottom) NMR spectra of 9,10-dihydro-*as*-indaceno[3,2-*b*:6,7-*b*']dithiophene (**2**)at 30 °C in $CDCl_3$.

## 9. Cartesian Coordinates for Theoretically Optimized Structures of **1–6** and **7a**–**10a**

**Compound 1**

Total E(RB3LYP) = -1412.28535895 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | 0.315053 | 0.000339 | 0.6695 | 15 | 1.062853 | -0.0002 | 4.2696 |
| 2 | 0.315053 | 0.000339 | -0.6695 | 16 | 1.062853 | -0.0002 | -4.2696 |
| 3 | -0.86715 | 0.000171 | -1.3156 | 17 | -0.33335 | -0.00033 | -4.747 |
| 4 | -2.04375 | 0.000196 | -0.6725 | 18 | -1.26555 | -0.00018 | -3.7797 |
| 5 | -2.04375 | 0.000196 | 0.6725 | 19 | -2.99235 | 0.000165 | -1.2329 |
| 6 | -0.86715 | 0.000171 | 1.3156 | 20 | -2.99235 | 0.000165 | 1.2329 |
| 7 | -0.60195 | 0.000072 | 2.625 | 21 | 2.132896 | 0.925492 | 1.4654 |
| 8 | 0.713253 | -9E-06 | 2.8472 | 22 | 2.133212 | -0.92471 | 1.4652 |
| 9 | 1.525953 | 0.000275 | 1.5829 | 23 | 2.132896 | 0.925492 | -1.4654 |
| 10 | 1.525953 | 0.000275 | -1.5829 | 24 | 2.133212 | -0.92471 | -1.4652 |
| 11 | 0.713253 | -9E-06 | -2.8472 | 25 | -2.35445 | -0.00025 | 3.9136 |
| 12 | -0.60195 | 0.000072 | -2.625 | 26 | -0.58005 | -0.00065 | 5.8185 |
| 13 | -1.26555 | -0.00018 | 3.7797 | 27 | -0.58005 | -0.00065 | -5.8185 |
| 14 | -0.33335 | -0.00033 | 4.747 | 28 | -2.35445 | -0.00025 | -3.9136 |

**Compound 2**

Total E(RB3LYP) = -1412.28815990 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | 0.601714 | 0.000308 | 0.6696 | 15 | 1.279714 | -0.00027 | 4.13 |
| 2 | 0.601714 | 0.000308 | -0.6696 | 16 | 1.279714 | -0.00027 | -4.13 |
| 3 | -0.57709 | 0.000252 | -1.3234 | 17 | 0.097613 | -0.00042 | -4.767 |
| 4 | -1.75049 | 0.00029 | -0.6724 | 18 | -1.08339 | -0.00017 | -3.8832 |
| 5 | -1.75049 | 0.00029 | 0.6724 | 19 | -2.70349 | 0.000277 | -1.2257 |
| 6 | -0.57709 | 0.000252 | 1.3234 | 20 | -2.70349 | 0.000277 | 1.2257 |
| 7 | -0.31949 | 0.000059 | 2.6365 | 21 | 2.423872 | 0.927031 | 1.4653 |
| 8 | 1.000914 | 0.000053 | 2.8268 | 22 | 2.424058 | -0.92637 | 1.465 |
| 9 | 1.818414 | 0.000221 | 1.5727 | 23 | 2.423872 | 0.927031 | -1.4653 |
| 10 | 1.818414 | 0.000221 | -1.5727 | 24 | 2.424058 | -0.92637 | -1.465 |
| 11 | 1.000914 | 0.000053 | -2.8268 | 25 | 0.004212 | -0.00071 | 5.8624 |
| 12 | -0.31949 | 0.000059 | -2.6365 | 26 | 2.277714 | -0.0005 | 4.5848 |
| 13 | -1.08339 | -0.00017 | 3.8832 | 27 | 2.277714 | -0.0005 | -4.5848 |
| 14 | 0.097613 | -0.00042 | 4.767 | 28 | 0.004212 | -0.00071 | -5.8624 |

**Compound 3**

Total E(RB3LYP) = -1560.34852564 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | 0.687818 | -0.118796 | -0.000006 | 14 | 5.126268 | 0.712342 | 0.000018 |
| 2 | -0.687818 | -0.118796 | -0.000007 | 15 | 4.676294 | -0.964748 | 0.000007 |
| 3 | -1.383351 | 1.128704 | -0.000007 | 16 | -4.676293 | -0.964748 | 0.000009 |
| 4 | -0.705908 | 2.330571 | -0.000009 | 17 | -5.126269 | 0.712342 | 0.000011 |
| 5 | 0.705908 | 2.330571 | -0.000008 | 18 | -4.047266 | 1.563229 | 0.000003 |
| 6 | 1.383351 | 1.128705 | -0.000006 | 19 | -1.528119 | -2.441331 | 0.000006 |
| 7 | 2.827793 | 0.839978 | -0.000005 | 20 | 1.528119 | -2.441331 | -0.000012 |
| 8 | 3.010432 | -0.52621 | -0.000009 | 21 | -1.244863 | 3.271157 | -0.00001 |
| 9 | 1.719745 | -1.250151 | -0.000011 | 22 | 1.244862 | 3.271157 | -0.000008 |
| 10 | -1.719746 | -1.250151 | -0.000006 | 23 | 4.142849 | 2.640571 | 0.000016 |
| 11 | -3.010433 | -0.52621 | -0.000006 | 24 | 6.173503 | 0.976881 | 0.000027 |
| 12 | -2.827793 | 0.839978 | -0.000005 | 25 | -6.173503 | 0.976881 | 0.000017 |
| 13 | 4.047266 | 1.563229 | 0.000011 | 26 | -4.142849 | 2.640571 | 0.000005 |

**Compound 4**

Total E(RB3LYP) = -1560.34838948 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | -0.68699 | 0.383439 | -0.000002 | 14 | -5.206896 | 0.045668 | 0.000001 |
| 2 | 0.68699 | 0.383439 | 0 | 15 | -4.40869 | 1.155437 | 0.000003 |
| 3 | 1.381667 | -0.868235 | -0.000001 | 16 | 4.40869 | 1.155437 | -0.000003 |
| 4 | 0.704839 | -2.072004 | -0.000002 | 17 | 5.206895 | 0.045667 | 0.000003 |
| 5 | -0.704839 | -2.072004 | -0.000001 | 18 | 4.285478 | -1.445064 | 0.000004 |
| 6 | -1.381667 | -0.868235 | -0.000001 | 19 | 1.53209 | 2.699745 | 0.000002 |
| 7 | -2.809803 | -0.558023 | 0.000001 | 20 | -1.532091 | 2.699745 | 0 |
| 8 | -3.033642 | 0.800468 | 0.000001 | 21 | 1.243921 | -3.012454 | -0.000003 |
| 9 | -1.725056 | 1.50891 | -0.000001 | 22 | -1.243921 | -3.012453 | -0.000001 |
| 10 | 1.725055 | 1.50891 | 0.000002 | 23 | -6.285036 | -0.007544 | 0.000001 |
| 11 | 3.033642 | 0.800468 | -0.000006 | 24 | -4.78494 | 2.169117 | 0.000005 |
| 12 | 2.809803 | -0.558022 | -0.000004 | 25 | 4.784941 | 2.169116 | -0.000005 |
| 13 | -4.285477 | -1.445065 | 0 | 26 | 6.285036 | -0.007545 | 0.000006 |

**Compound 5**

Total E(RB3LYP) = -1560.35329160 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | -0.69492 | 0.251927 | -0.000001 | 14 | -5.3631 | -0.337429 | 0.000001 |
| 2 | 0.694775 | 0.252003 | -0.000003 | 15 | -4.33948 | 1.064885 | 0.000005 |
| 3 | 1.385368 | -0.989257 | -0.000002 | 16 | 4.338844 | 1.065242 | -0.000002 |
| 4 | 0.69864 | -2.198868 | -0.000004 | 17 | 5.363707 | -0.337268 | 0.00001 |
| 5 | -0.69888 | -2.198861 | -0.000005 | 18 | 3.996414 | -1.427556 | 0.000008 |
| 6 | -1.38551 | -0.989197 | -0.000003 | 19 | 1.505359 | 2.577114 | -0.000025 |
| 7 | -2.83019 | -0.723234 | -0.000003 | 20 | -1.50505 | 2.577231 | 0.000021 |
| 8 | -3.02963 | 0.692944 | 0.000003 | 21 | 1.24022 | -3.137994 | -0.000004 |
| 9 | -1.70975 | 1.388087 | 0.000009 | 22 | -1.24046 | -3.137981 | -0.000007 |
| 10 | 1.709606 | 1.387873 | -0.000012 | 23 | -4.16823 | -2.492613 | -0.000009 |
| 11 | 3.029496 | 0.692632 | -0.000008 | 24 | -4.76647 | 2.056468 | 0.000008 |
| 12 | 2.8301 | -0.72346 | -0.000002 | 25 | 4.766438 | 2.056495 | -0.000004 |
| 13 | -3.99683 | -1.426973 | -0.000004 | 26 | 4.168063 | -2.493115 | 0.000015 |

**Compound 6**

Total E(RB3LYP) = -770.77836507 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | -0.000005 | 0.473097 | 0.691529 | 18 | 0.00001 | -0.781662 | 5.210701 |
| 2 | -0.000005 | 0.473097 | -0.691529 | 19 | 0.000007 | 0.603736 | 5.393651 |
| 3 | -0.000002 | -0.755803 | -1.386962 | 20 | -0.000001 | 1.464361 | 4.292178 |
| 4 | -0.000001 | -1.971592 | -0.696875 | 21 | 0 | -2.911536 | -1.237888 |
| 5 | -0.000001 | -1.971592 | 0.696875 | 22 | 0 | -2.911536 | 1.237888 |
| 6 | -0.000002 | -0.755803 | 1.386962 | 23 | -0.879324 | 2.269141 | 1.547911 |
| 7 | -0.000001 | -0.47346 | 2.827076 | 24 | 0.879289 | 2.269157 | 1.547909 |
| 8 | -0.000004 | 0.92325 | 3.013705 | 25 | -0.879324 | 2.269141 | -1.547911 |
| 9 | -0.000011 | 1.625649 | 1.6718 | 26 | 0.879289 | 2.269157 | -1.547909 |
| 10 | -0.000011 | 1.625649 | -1.6718 | 27 | -0.000003 | 2.539482 | -4.440747 |
| 11 | -0.000004 | 0.92325 | -3.013705 | 28 | 0.00001 | 1.013322 | -6.397498 |
| 12 | -0.000001 | -0.47346 | -2.827076 | 29 | 0.000017 | -1.436164 | -6.075302 |
| 13 | -0.000001 | 1.464361 | -4.292178 | 30 | 0.00001 | -2.406812 | -3.796551 |
| 14 | 0.000007 | 0.603736 | -5.393651 | 31 | 0.00001 | -2.406812 | 3.796551 |
| 15 | 0.00001 | -0.781662 | -5.210701 | 32 | 0.000017 | -1.436164 | 6.075302 |
| 16 | 0.000007 | -1.330341 | -3.92892 | 33 | 0.00001 | 1.013322 | 6.397498 |
| 17 | 0.000007 | -1.330341 | 3.92892 | 34 | -0.000003 | 2.539482 | 4.440747 |

**Compound 7a**

Total E(RB3LYP) = -1412.28826638 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | 1.056125 | 0.906172 | 0 | 15 | 1.386042 | -4.10848 | 0 |
| 2 | -0.28924 | 1.354874 | 0 | 16 | 1.149875 | 4.682758 | 0 |
| 3 | -1.35449 | 0.447967 | 0 | 17 | -0.08588 | 5.274751 | 0 |
| 4 | -1.05613 | -0.90617 | 0 | 18 | -1.38604 | 4.108481 | 0 |
| 5 | 0.289237 | -1.35487 | 0 | 19 | -2.38264 | 0.795365 | 0 |
| 6 | 1.354493 | -0.44797 | 0 | 20 | 2.382639 | -0.79537 | 0 |
| 7 | -2.00652 | -2.0943 | 0 | 21 | -2.65932 | -2.08767 | 0.880468 |
| 8 | -1.05613 | -3.26604 | 0 | 22 | -2.65932 | -2.08767 | -0.88047 |
| 9 | 0.241948 | -2.80697 | 0 | 23 | 2.659321 | 2.087665 | 0.880468 |
| 10 | 2.006519 | 2.094303 | 0 | 24 | 2.659321 | 2.087665 | -0.88047 |
| 11 | 1.056125 | 3.266038 | 0 | 25 | -2.073 | -5.24797 | 0 |
| 12 | -0.24195 | 2.806965 | 0 | 26 | 0.323219 | -6.32766 | 0 |
| 13 | -1.14988 | -4.68276 | 0 | 27 | 2.072999 | 5.247973 | 0 |
| 14 | 0.085877 | -5.27475 | 0 | 28 | -0.32322 | 6.327662 | 0 |

**Compound 8a**

Total E(RB3LYP) = -1412.28762484 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | 0.000005 | -1.474118 | 1.195278 | 15 | 0.000005 | -1.99937 | -2.622451 |
| 2 | 0.000005 | -0.056599 | 1.192316 | 16 | -0.000006 | 1.856207 | -3.458442 |
| 3 | 0.000006 | 0.667461 | 0 | 17 | -0.000011 | 0.992514 | -4.975873 |
| 4 | 0.000005 | -0.056599 | -1.192316 | 18 | -0.000004 | -0.367046 | -4.806356 |
| 5 | 0.000005 | -1.474118 | -1.195278 | 19 | 0.000008 | 1.751704 | 0 |
| 6 | 0.000006 | -2.185506 | 0 | 20 | 0.000007 | -3.271741 | 0 |
| 7 | 0.000005 | -1.99937 | 2.622451 | 21 | -0.880571 | -2.620286 | 2.824915 |
| 8 | 0.000006 | -0.726518 | 3.432338 | 22 | 0.880579 | -2.620288 | 2.824914 |
| 9 | 0.000007 | 0.359125 | 2.586876 | 23 | -0.000005 | -1.063644 | 5.634792 |
| 10 | -0.000004 | -0.367046 | 4.806356 | 24 | -0.000016 | 1.551131 | 5.899442 |
| 11 | -0.000011 | 0.992514 | 4.975873 | 25 | -0.880571 | -2.620286 | -2.824915 |
| 12 | -0.000006 | 1.856207 | 3.458442 | 26 | 0.880579 | -2.620288 | -2.824914 |
| 13 | 0.000007 | 0.359125 | -2.586876 | 27 | -0.000016 | 1.551131 | -5.899442 |
| 14 | 0.000006 | -0.726518 | -3.432338 | 28 | -0.000005 | -1.063644 | -5.634792 |

**Compound 9a**

Total E(RB3LYP) = -1560.35609206 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | -0.963094 | -0.974675 | 0.000004 | 14 | 5.272396 | -0.395929 | -0.00001 |
| 2 | -1.332708 | 0.386805 | 0.000001 | 15 | 4.026 | -1.625886 | -0.000002 |
| 3 | -0.361317 | 1.388494 | 0.000002 | 16 | -4.756799 | -0.871139 | -0.000007 |
| 4 | 0.963094 | 0.974675 | 0.000005 | 17 | -5.272397 | 0.395927 | -0.000007 |
| 5 | 1.332708 | -0.386805 | 0.000005 | 18 | -4.026 | 1.625887 | -0.000004 |
| 6 | 0.361317 | -1.388494 | 0.000003 | 19 | -6.307644 | 0.701312 | -0.00001 |
| 7 | 2.217421 | 1.829102 | 0.000015 | 20 | 6.307643 | -0.701313 | -0.000014 |
| 8 | 3.337501 | 0.849825 | -0.000001 | 21 | -2.26306 | -3.039047 | 0.000007 |
| 9 | 2.800857 | -0.420986 | 0 | 22 | 2.26306 | 3.039047 | 0.000008 |
| 10 | -2.217421 | -1.829102 | 0.000007 | 23 | -0.607263 | 2.444477 | 0.000002 |
| 11 | -3.337501 | -0.849825 | -0.000001 | 24 | 0.607262 | -2.444477 | 0.000002 |
| 12 | -2.800857 | 0.420986 | -0.000002 | 25 | 5.362156 | 1.767072 | -0.000017 |
| 13 | 4.756799 | 0.871138 | -0.000013 | 26 | -5.362155 | -1.767073 | -0.000008 |

**Compound 10a**

Total E(RB3LYP) = -1560.35669978 hartree

| Number | X | Y | Z | Number | X | Y | Z |
|---|---|---|---|---|---|---|---|
| 1 | 1.184425 | 1.204734 | 0.000003 | 14 | -2.594398 | -0.625882 | -0.000004 |
| 2 | 1.187058 | -0.208357 | -0.000001 | 15 | -3.440971 | 0.461099 | -0.000005 |
| 3 | 0 | -0.939756 | -0.000004 | 16 | -2.608975 | 1.702474 | -0.00001 |
| 4 | -1.187058 | -0.208357 | -0.000003 | 17 | -3.465201 | -2.109289 | 0.000002 |
| 5 | -1.184425 | 1.204734 | -0.000001 | 18 | -4.985179 | -1.244353 | 0.000008 |
| 6 | 0 | 1.930429 | 0.000004 | 19 | -4.815943 | 0.114322 | 0.000006 |
| 7 | 2.608974 | 1.702474 | 0.000002 | 20 | -5.906456 | -1.806925 | 0.000011 |
| 8 | 3.44097 | 0.461099 | 0.000001 | 21 | 2.979355 | 2.85517 | 0.000005 |
| 9 | 2.594398 | -0.625881 | -0.000001 | 22 | -2.979356 | 2.855169 | -0.000005 |
| 10 | 4.815943 | 0.114323 | 0.000003 | 23 | 0 | -2.023722 | -0.000006 |
| 11 | 4.985179 | -1.244352 | 0.000001 | 24 | 0 | 3.014809 | 0.000004 |
| 12 | 3.465202 | -2.10929 | -0.000003 | 25 | 5.633079 | 0.822405 | 0.000005 |
| 13 | 5.906456 | -1.806924 | 0 | 26 | -5.633079 | 0.822404 | 0.000008 |