

Coumarin-embedded [5]helicene derivatives: Synthesis, X-ray analysis and photoconducting properties

Hui Yang, Guofeng Chen,* Ran Zhang, Yanjie Zhu, and Jinchong Xiao*

College of Chemistry and Materials Science, Key Laboratory of Chemical Biology of Hebei Province, Hebei University, Baoding 071002, P. R. China

E-mail: chenguofeng@hbu.cn; jcxiaoicas@163.com

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Experimental details

Material and Instruments

All the chemical reagents were purchased from commercial suppliers and directly used without further purification unless otherwise specified. The experiments were performed in oil bath under a nitrogen atmosphere. Column chromatography was carried out on silica gel (200-300 mesh) by organic solvents as eluents. Thin layer chromatography was performed by using commercial silica gel plates and the dots were monitored with UV light (254 nm and 365 nm).

^1H NMR and ^{13}C NMR spectra were recorded on WNMN 400 and Bruker 600 MHz spectrometers. The proton chemical shifts are labelled in ppm with δ of CDCl_3 (7.26 ppm in ^1H NMR and 77.16 ppm in ^{13}C NMR) without any internal standard. Abbreviations in the NMR were described as follows: singlet = s; doublet = d; triplet = t; quartet = q; multiplet = m; broad = br. All the coupling constants were described in Hertz (Hz). MALDI-TOF mass spectra were carried out on Bruker Biflex III MALDI-TOF. The single crystal X-ray diffraction data were collected with a Bruker smart-1000 CCD diffractometer.

UV-vis absorption spectra were measured on Analytikjena SPECORD 210 PLUS and emission spectra were measured on Hitachi F-7000 spectrofluorometer in a 10 mm quartz cell. The cyclic voltammetry of the as-prepared compounds was tested on CHI 630A electrochemical analyzer at room temperature by using a three-electrode cell: glassy carbon as a working electrode; Pt wire as a counter electrode; Ag/AgNO_3 as a reference electrode. Tetrabutylammonium hexafluorophosphate in degassed dichloromethane (0.1 M) was used as the electrolyte. Scan rate: 0.1 V/s. The potential was calibrated against the Fc/Fc^+ couple. SEM measurements were carried out on a HITACHI SU8010 by drop casting the solutions on silica wafer. Photocurrent response was recorded on Salarton Analytical Modulab XM PhotoEchem testing system.

The preparation of 3a nanowire:

1 mL **3a**/THF (0.5 mM) solution was injected to hexadecyl trimethyl ammonium bromide (CTAB) aqueous solution (5 mL) with strong stirring for 5 min. The solution

was left to stand overnight to form nanowires. Then the solution was centrifugated to get the solid, which was further washed with pure water to remove the CTAB. The obtained sample was put on a silica wafer and dried overnight and then coated with gold in an ion coater.

The preparation of photoconductive devices

The photocurrent behaviors were measured by using a model Salartron Analytical (ModuLab XM) voltammetric analyzer with a three-electrode cell, where **3a**/C₆₀/ITO or **6a**/C₆₀/ITO were used as a working electrode, a platinum wire was used as a counter electrode and Ag/AgCl (saturated KCl solution) was used as a reference electrode. A solution of Na₂SO₄ (0.5 M) was used as a supporting electrolyte. The **3a**/C₆₀/ITO or **6a**/C₆₀/ITO films were prepared by spin coating of the mixture in toluene on ITO. The **3a**/C₆₀ or **6a**/C₆₀ films were prepared by spin coating of the mixture in toluene on ITO. The equimolar **3a**-nanowire and C₆₀ were mixed together in aqueous solution, which was dropped on ITO.

Table S1 Crystal data and structure refinement for **3a** and **5**.

| | 3a | 5 |
|---|--|--|
| Empirical formula | C ₄₇ H ₃₄ O ₂ | C ₃₇ H ₂₂ O ₂ |
| Formula weight | 630.26 | 498.16 |
| Temperature/K | 298(2) | 298(2) |
| Crystal system | monoclinic | triclinic |
| Space group | P2(1)/n | Pī |
| Unit cell dimensions | a = 15.0990(18)Å b = 15.0514(17)Å c = 15.4881(16)Å α = 90.00° β = 96.330(2)° γ = 90.00° | a = 18.0865(18)Å b = 18.3505(19)Å c = 19.254(2)Å α = 100.696(3)° β = 102.593(3)° γ = 93.475(2)° |
| Volume/Å ³ | 3498.4(7) | 6094.1(11) |
| Z | 4 | 8 |
| Absorption coefficient/mm ⁻¹ | 0.228 | 0.069 |
| F(000) | 1496 | 2180 |
| Crystal size/mm ³ | 0.23×0.20×0.15 | 0.21×0.16×0.10 |
| Radiation type | Mo K/a λ = 0.71073 | Mo K/a λ = 0.71073 |
| CCDC number | 2305620 | 2305621 |

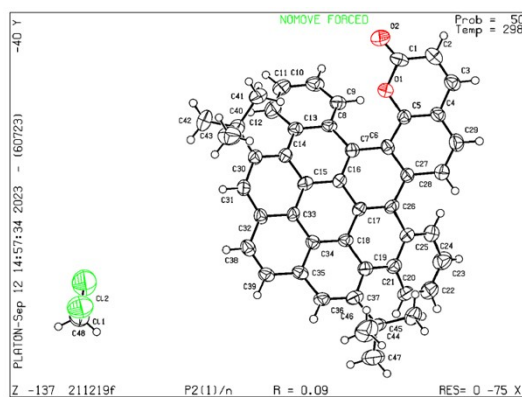


Figure S1 Crystal structure of **3a** with an ellipsoid contour at the 50% probability level.

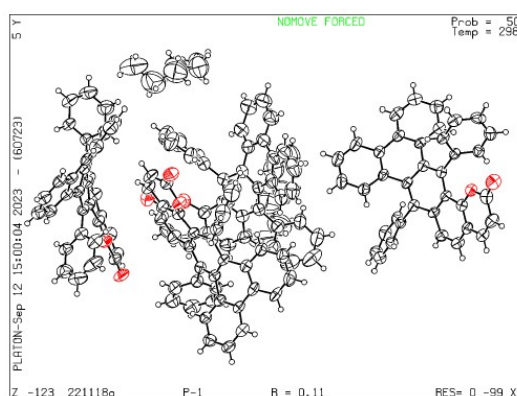


Figure S2 Crystal structure of **5** with an ellipsoid contour at the 50% probability level.

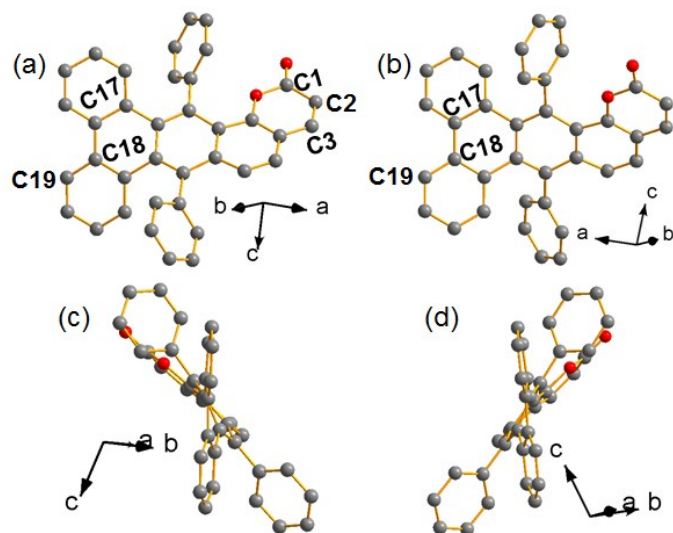


Figure S3 Single crystal of **5** (a)/(b) and side view (c)/(d). The hydrogen atoms are omitted for clarity.

The structure of compound **5** containing a coumarin unit is also evidenced by X-ray diffraction. It can form twisted configuration with the torsional angle of 52.27° between plane C1-C2-C3 and plane C17-C18-C19, which is larger than those of all carbon twistacenes.¹ Indeed, molecule **5** also includes two isomers (Fig. S3).

(1) (a) J. Xiao, H. M. Duong, Y. Liu, W. Shi, L. Ji, G. Li, S. Li, X. Liu, J. Ma, F. Wudl and Q. Zhang, *Angew. Chem. Int. Ed.*, 2012, **51**, 6094; (b) X. Zhang, S. Li, Z. Liu, S. Wang and J. Xiao, *NPG Asia Mater.*, 2015, **7**, e230; (c) B. Lv, J. Xiao, J. Zhou, X. Zhang, J. Duan, W. Su and J. Zhao, *ACS Appl. Mater. Interfaces*, 2016, **8**, 18998.

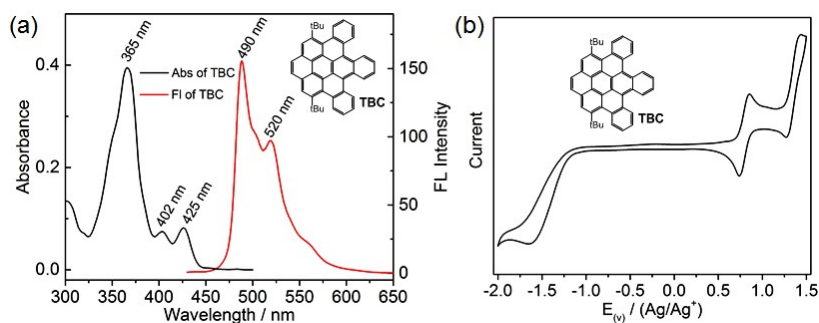


Figure S4 (a) UV-vis absorption and emission spectra of **TBC** in dilute dichloromethane ($c = 1 \times 10^{-5}$ M) and (b) Cyclic voltammetry of **TBC** in anhydrous dichloromethane.

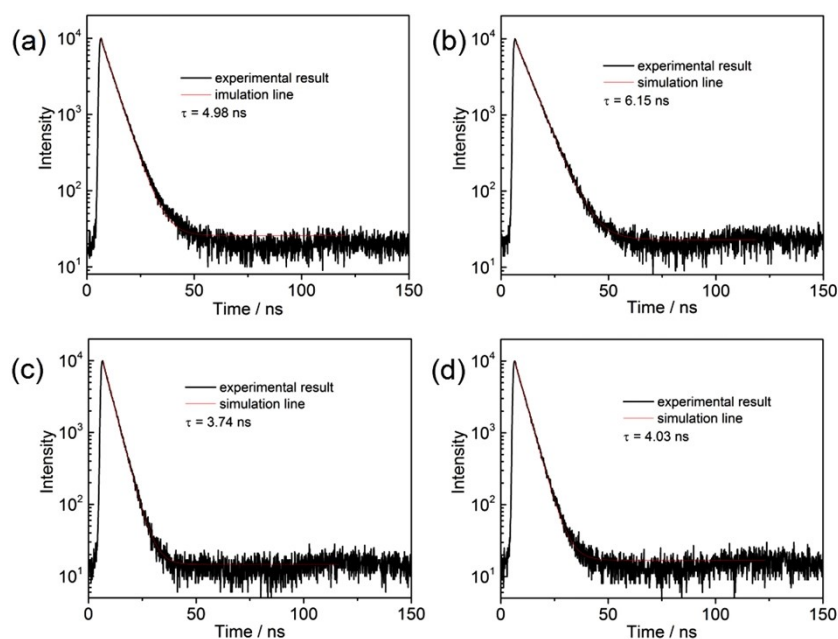


Figure S5 Fluorescence decay of **2** (a), **3a** (b), **5** (c), **6a** (d) in degassed dichloromethane.

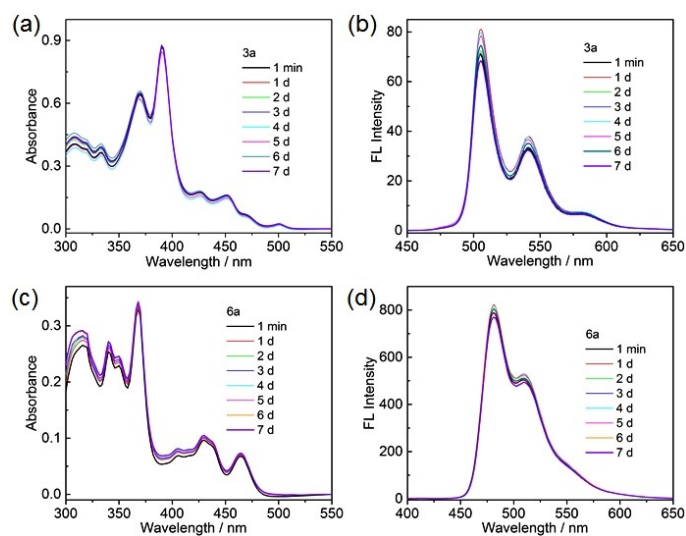


Figure S6 Changes of UV-vis absorption and emission spectra **3a** (a)/(b) and **6a** (c)/(d) in toluene under ambient light and air conditions.

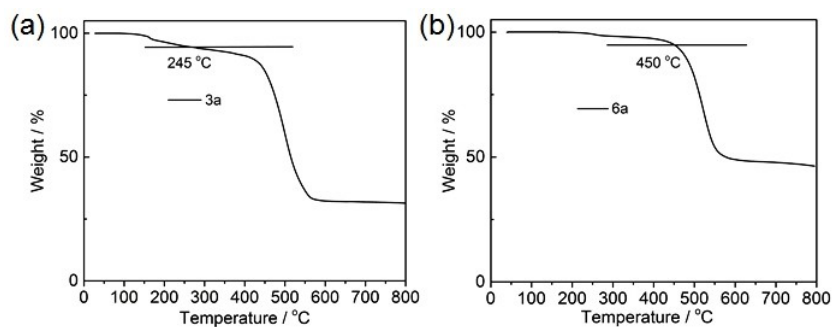


Figure S7 TGA data of (a) **3a** and (b) **6a** under nitrogen at a heating rate of 10 °C/min.

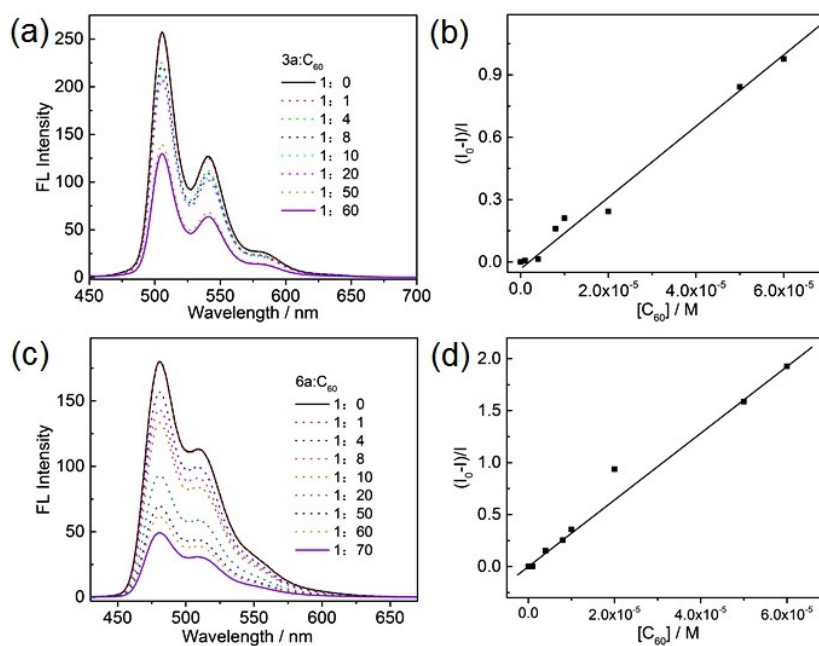


Figure S8 Fluorescence quenching spectra of **3a** (a) and **6a** (c) upon addition of C_{60} in toluene ($c = 1.0 \times 10^{-6}$ M). The Stern-Volmer plots for the fluorescence quenching of **3a** (b) and **6a** (d) by C_{60} .

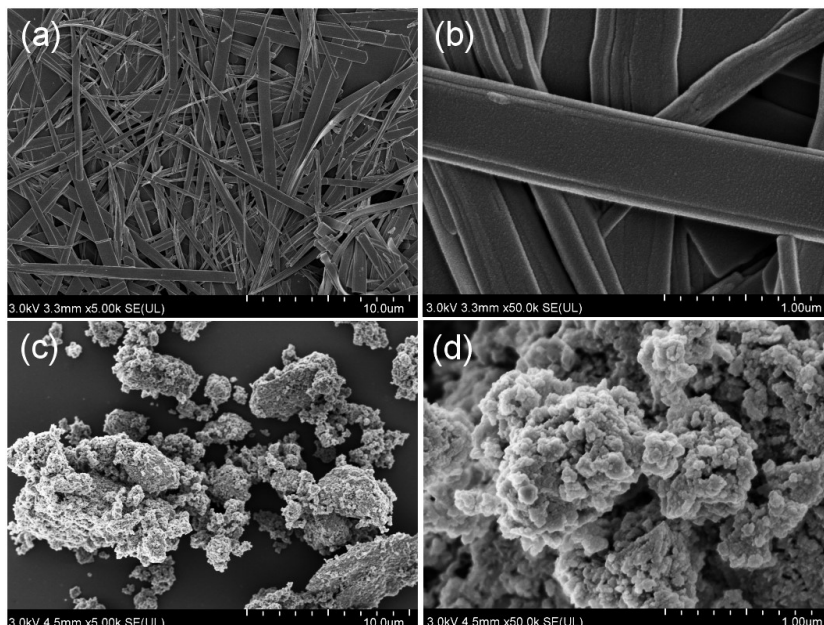


Figure S9 SEM images of **3a** nanowires film for the photocurrent test (a), magnified image (b) and from toluene solution (c), magnified image (d).

Synthesis of 2

A mixture of compound **1** (494 mg, 0.85 mmol), propiolic acid (72 μ L, 1.27 mmol), $\text{CF}_3\text{SO}_3\text{H}$ (68 μ L, 0.85 mmol) was stirred in chlorobenzene (6 mL) at 100 $^\circ\text{C}$ under nitrogen. After 10 h, methanol was added to quench the reaction and then NaHCO_3 solution was added. The mixture was partitioned between brine and dichloromethane. The organic solution was dried over Na_2SO_4 and removed under reduced pressure. The crude product was purified through silica gel column chromatography with petroleum ether (PE) and dichloromethane (v/v, 4:1) as an eluent to afford a yellow solid (**2**, 177 mg, 33%). ^1H NMR (600 MHz, 298 K, CDCl_3): δ 8.09 (d, $J = 1.2$ Hz, 1H), 8.02 (d, $J = 1.8$ Hz, 1H), 7.87-7.84 (m, 4H), 7.76 (d, $J = 9.0$ Hz, 1H), 7.67 (d, $J = 9.0$ Hz, 1H), 7.57-7.51 (m, 9H), 7.48-7.45 (m, 1H), 7.39 (d, $J = 8.4$ Hz, 1H), 6.33 (d, $J = 9.0$ Hz, 1H), 1.12 (s, 9H), 1.11 (s, 9H). ^{13}C NMR (150 MHz, 298 K, CDCl_3): δ 159.4, 152.8, 147.6, 147.3, 143.8, 143.5, 142.0, 135.7, 135.6, 133.8, 132.9, 132.6, 131.1, 130.9, 130.5, 130.4, 129.44, 129.41, 129.11, 129.06, 128.3, 128.1, 128.0, 127.8, 127.3, 126.9, 124.3, 124.2, 123.6, 123.4, 123.1, 122.9, 122.1, 115.5, 115.3, 34.9, 31.54, 31.52. HR-MS (MALDI-TOF) m/z : $[\text{M}]^+$ calcd for $\text{C}_{47}\text{H}_{38}\text{O}_2$ 634.2872, found 634.2864.

Synthesis of **3**

Trifluoromethanesulfonic acid (0.3 mL) was slowly dropped into a mixture of **2** (41 mg, 0.06 mmol) and DDQ (44 mg, 0.19 mmol) in anhydrous dichloromethane (15 mL) under nitrogen at 0 °C. After being stirred for 10 min, methanol was added to quench the reaction, and then saturated NaHCO₃ solution was added. The mixture was partitioned between brine and dichloromethane (40 mL × 3). The combined organic phase was dried over Na₂SO₄. After the organic solvent was removed under reduced pressure, the residue was purified through column chromatography (eluent, PE:CH₂Cl₂ = 4:1) to afford a yellow solid (**3**, 12 mg, 30%). ¹H NMR (400 MHz, 298 K, CDCl₃): δ 9.21 (d, *J* = 8.8 Hz, 1H), 8.93 (d, *J* = 8.4 Hz, 1H), 8.89 (d, *J* = 5.2 Hz, 2H), 8.65 (d, *J* = 8.0 Hz, 1H), 8.56 (d, *J* = 8.0 Hz, 1H), 8.44-8.37 (m, 3H), 7.98 (d, *J* = 9.2 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.54 (q, *J* = 7.2 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 1H), 6.58 (d, *J* = 9.2 Hz, 1H), 1.88 (s, 9H), 1.83 (s, 9H). ¹³C NMR (150 MHz, 298 K, CDCl₃): δ 160.1, 151.8, 146.3, 145.6, 144.2, 132.8, 132.0, 131.8, 130.8, 130.3, 130.2, 129.9, 129.7, 129.4, 129.2, 129.1, 128.7, 128.53, 128.49, 127.9, 127.2, 126.7, 126.4, 125.23, 125.18, 124.80, 124.77, 124.1, 123.5, 123.4, 123.2, 122.8, 122.5, 120.9, 120.8, 117.2, 116.7, 115.1, 38.8, 38.7, 35.3, 35.1. HR-MS (MALDI-TOF) *m/z*: [M]⁺ calcd for C₄₇H₃₄O₂ 630.2559, found 630.2552.

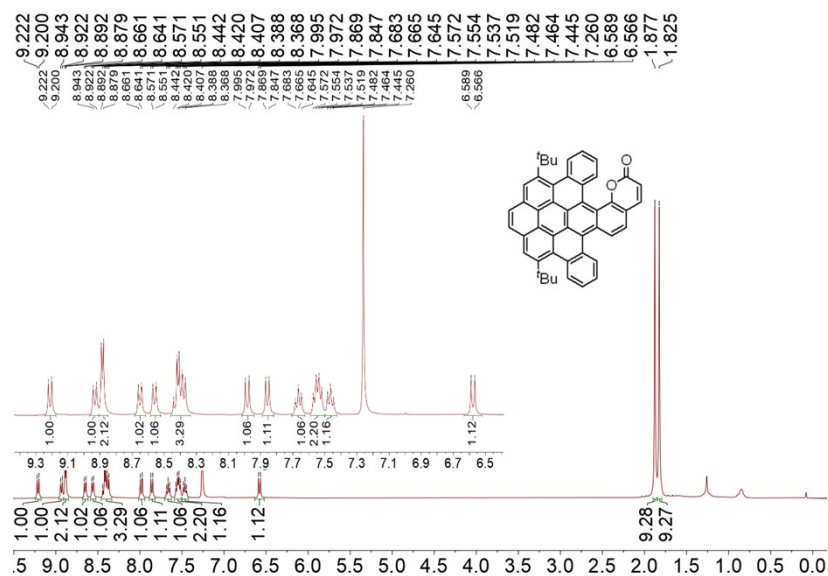


Figure S13 ¹H NMR spectrum of **3** (400 MHz).

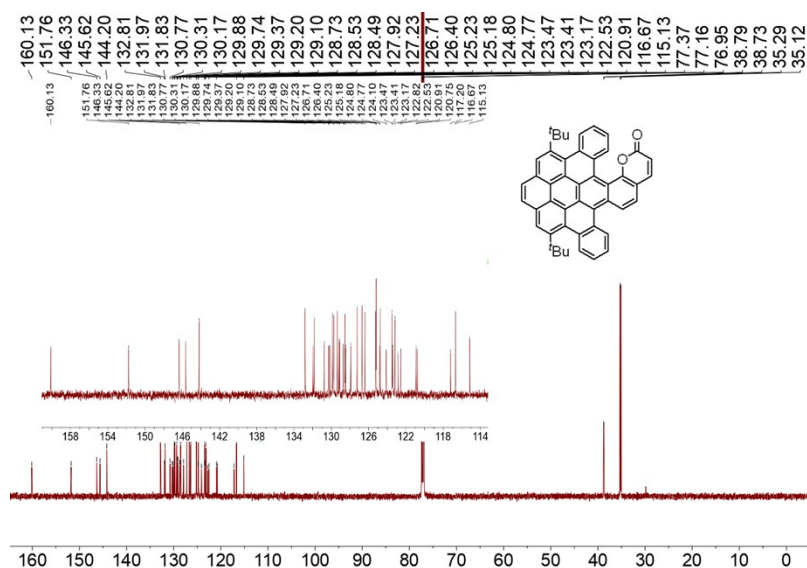


Figure S14 ^{13}C NMR spectrum of **3** (150 MHz).

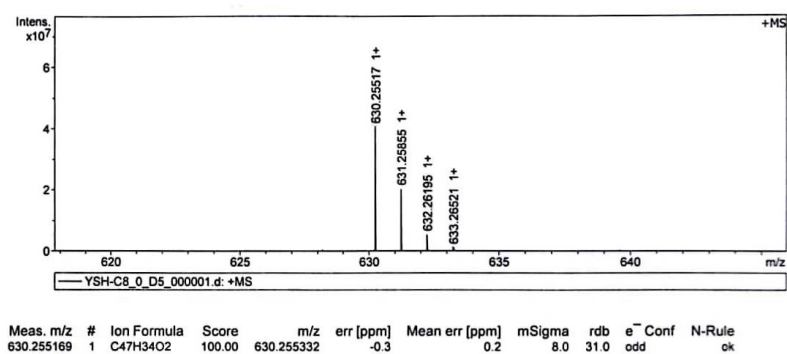


Figure S15 HR-MS spectrum of **3**.

Synthesis of **5**

A mixture of compound **4** (80 mg, 0.18 mmol), propiolic acid (20 μL , 0.32 mmol), TfOH (20 μL , 0.22 mmol) was stirred in chlorobenzene (6 mL) at 100 $^{\circ}\text{C}$ under nitrogen. After 10 h, methanol was added to quench the reaction, and then NaHCO_3 solution was added. The mixture was partitioned between brine and dichloromethane. The collected organic phase was dried over Na_2SO_4 and removed under reduced pressure. The crude product was purified through silica gel column chromatography with PE and dichloromethane (v/v, 6:1) as an eluent to afford an orange solid (**5**, 23 mg, 26%). ^1H NMR (400 MHz, 298 K, CDCl_3): δ 8.33-8.29 (m, 2H), 7.81-7.77 (m, 2H), 7.59-7.56 (m, 6H), 7.53-7.39 (m, 9H), 7.06-6.98 (m, 2H), 6.38 (d, $J = 9.6$ Hz, 1H). ^{13}C NMR (150 MHz, 298K, CDCl_3): δ 152.7, 143.7, 142.6, 140.9, 134.83, 134.80, 133.5, 133.0, 132.4, 132.3, 131.7, 131.1, 130.9, 130.7, 130.4, 130.2, 129.1, 128.9,

128.1, 127.9, 127.6, 127.2, 126.1, 125.7, 123.6, 123.5, 123.4, 123.3, 121.6, 115.7, 115.2. HR-MS (MALDI-TOF) m/z : $[M]^+$ calcd for $C_{37}H_{22}O_2$ 498.1620, found 498.1618.

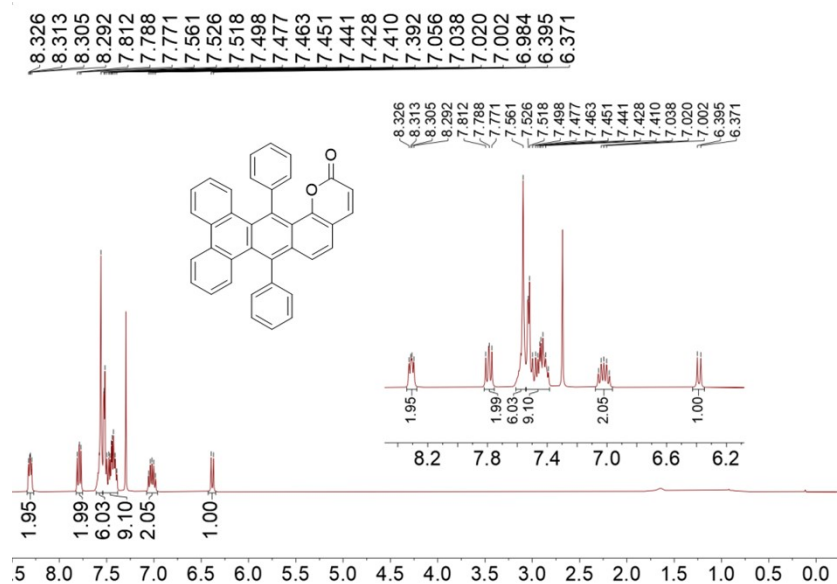


Figure S16 1H NMR spectrum of **5** (400 MHz).

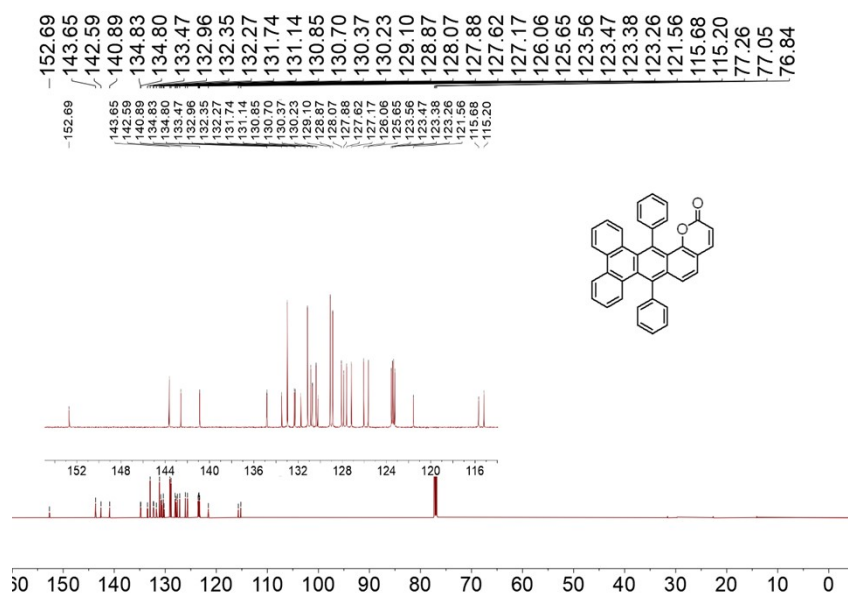


Figure S17 ^{13}C NMR spectrum of **5** (150 MHz).

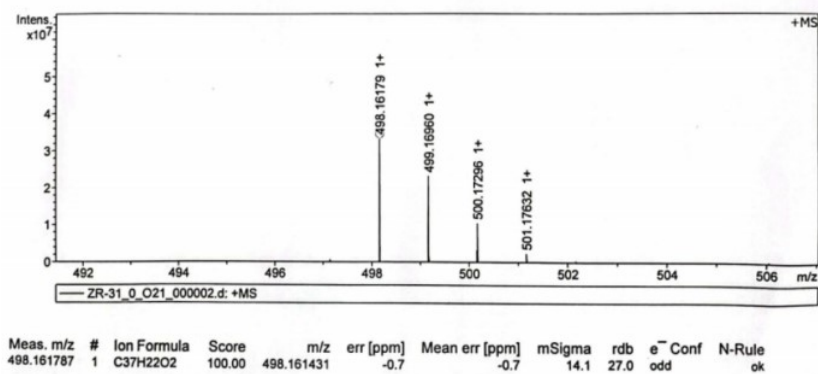


Figure S18 HR-MS spectrum of **5**.

Synthesis of **6**

Trifluoromethanesulfonic acid (0.3 mL) was slowly dropped into a mixture of **5** (63 mg, 0.13 mmol) and DDQ (115 mg, 0.50 mmol) in anhydrous dichloromethane (15 mL) under nitrogen at 0 °C. After being stirred for 10 min, methanol was added to quench the reaction, and then saturated NaHCO₃ solution was added to the reaction. The mixture was partitioned between brine and dichloromethane (30 mL × 3). The combined organic phase was dried over Na₂SO₄. After the organic solvent was removed under reduced pressure, the residue was purified through column chromatography (eluent, PE:CH₂Cl₂ = 3:1) to afford a yellow solid (**6**, 25 mg, 40%). ¹H NMR (400 MHz, 298 K, CDCl₃): δ 8.99 (d, *J* = 8.8 Hz, 1H), 8.90-8.84 (m, 3H), 8.81-8.72 (m, 4H), 8.23 (d, *J* = 8.0 Hz, 1H), 8.07-7.99 (m, 2H), 7.91 (d, *J* = 9.6 Hz, 1H), 7.77-7.70 (m, 4H), 7.60 (t, *J* = 8.0 Hz, 1H), 6.50 (d, *J* = 9.2 Hz, 1H). HR-MS (MALDI-TOF) *m/z*: [M]⁺ calcd for C₃₇H₁₈O₂ 494.1307, found 494.1305.

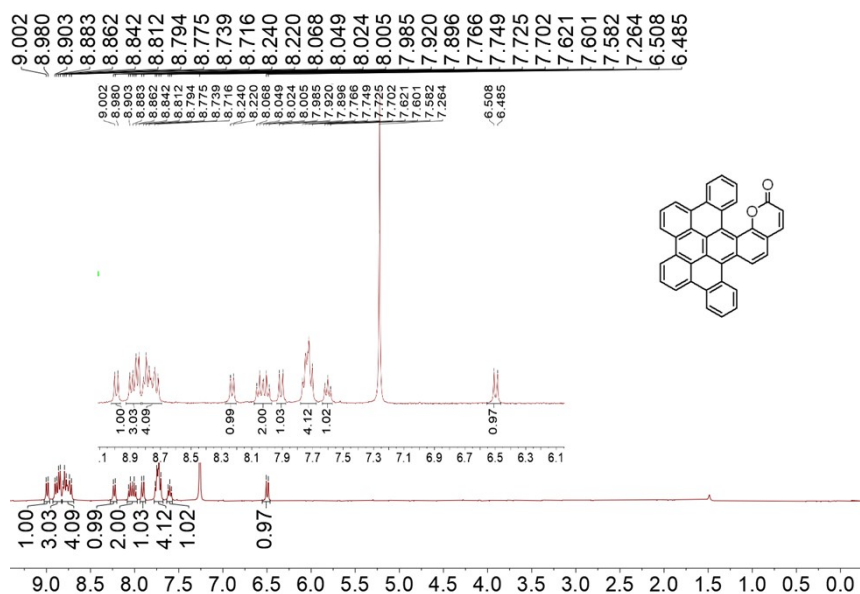


Figure S19 ^1H NMR spectrum of **6** (400 MHz).

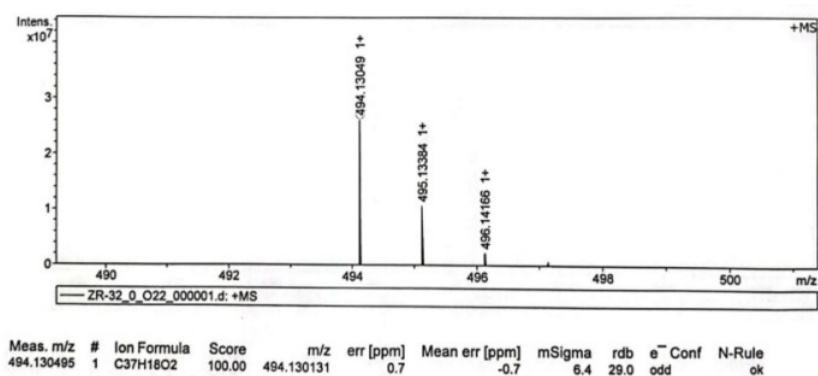


Figure S20 HR-MS spectrum of **6**.

Table S2 Cartesian coordinates of optimized species

| | | | |
|---|-------------|-------------|-------------|
| 2 | | | |
| 0 | | | |
| 1 | | | |
| C | 1.07658630 | -4.44229880 | -0.34595401 |
| C | -0.18510268 | -3.95763432 | 0.02325651 |
| C | -0.42160013 | -2.55453466 | 0.03535423 |
| C | 0.64754182 | -1.66204290 | -0.22891854 |
| C | 1.85980331 | -2.20571112 | -0.66725712 |
| C | 2.09801150 | -3.58481207 | -0.73896419 |
| C | -1.25022889 | -4.84528392 | 0.39243292 |
| C | -2.47369478 | -4.36952559 | 0.73537860 |
| C | -2.75979593 | -2.96393278 | 0.70101030 |
| C | -1.73341131 | -2.06095177 | 0.31589827 |
| C | -2.02698842 | -0.67692808 | 0.19009802 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.95348751 | 0.25358092 | -0.21527861 |
| C | 0.41119760 | -0.20537535 | -0.11397655 |
| C | -4.03400116 | -2.47175294 | 1.03232107 |
| C | -4.31395708 | -1.11401011 | 0.99904894 |
| C | -3.29769471 | -0.24403582 | 0.57035749 |
| C | -1.18603427 | 1.56582734 | -0.65522400 |
| C | -0.12063857 | 2.50696413 | -0.66212872 |
| C | 1.14321033 | 2.12494232 | -0.10286007 |
| C | 1.43511046 | 0.73904307 | 0.06387392 |
| C | -0.28436776 | 3.83391524 | -1.17212932 |
| C | 0.67576561 | 4.78339073 | -0.99191832 |
| C | 1.84497169 | 4.49197635 | -0.23930934 |
| C | 2.04785822 | 3.19266423 | 0.21770241 |
| C | 2.82737471 | 0.32656102 | 0.41508520 |
| C | -2.51525539 | 2.00490316 | -1.17728715 |
| C | 3.08612272 | -0.31800596 | 1.62617833 |
| C | 4.38610478 | -0.67219271 | 1.97342401 |
| C | 5.44414114 | -0.38708306 | 1.11327304 |
| C | 5.19320748 | 0.24882936 | -0.10151851 |
| C | 3.89412626 | 0.60056436 | -0.44827569 |
| C | -3.23252055 | 3.05403878 | -0.58558830 |
| C | -4.45709546 | 3.46199373 | -1.10721289 |
| C | -4.98154412 | 2.83304218 | -2.23547672 |
| C | -4.27610482 | 1.78994488 | -2.83242657 |
| C | -3.05454799 | 1.37867559 | -2.30652399 |
| O | 3.11109493 | 2.90903387 | 1.00648491 |
| C | 2.83410664 | 5.47918008 | 0.08633760 |
| C | 3.91831816 | 5.17180084 | 0.83229143 |
| C | 4.11415783 | 3.83006876 | 1.35059002 |
| O | 5.01956443 | 3.43535995 | 2.03273584 |
| C | 3.45906838 | -4.15359730 | -1.17494752 |
| C | 4.38191435 | -3.07513805 | -1.77018003 |
| C | 3.25989742 | -5.25303344 | -2.24145745 |
| C | 4.15449476 | -4.75675499 | 0.06721132 |
| C | -5.68242802 | -0.52873099 | 1.38334864 |
| C | -6.64843674 | -1.60335004 | 1.91166997 |
| C | -6.31575502 | 0.12822794 | 0.13616339 |
| C | -5.50027272 | 0.53825413 | 2.48683601 |
| H | 1.23293151 | -5.51507227 | -0.33504136 |
| H | 2.64517987 | -1.53582925 | -0.96290863 |
| H | -1.05212760 | -5.91205242 | 0.39860583 |
| H | -3.26742575 | -5.04941405 | 1.02691969 |
| H | -4.78953179 | -3.18865972 | 1.32691103 |
| H | -3.51498191 | 0.80931395 | 0.54958277 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.19077643 | 4.08289085 | -1.70394137 |
| H | 0.54492151 | 5.78382827 | -1.38945873 |
| H | 2.26293604 | -0.53377485 | 2.29694970 |
| H | 4.57474885 | -1.16017906 | 2.92291841 |
| H | 6.45799861 | -0.65198042 | 1.38977912 |
| H | 6.01124198 | 0.47425739 | -0.77628790 |
| H | 3.69821174 | 1.10108999 | -1.39043892 |
| H | -2.82682582 | 3.54189315 | 0.29341855 |
| H | -5.00245581 | 4.26911526 | -0.63112422 |
| H | -5.93519567 | 3.14954542 | -2.64206132 |
| H | -4.67807851 | 1.29369921 | -3.70846633 |
| H | -2.50908597 | 0.56291514 | -2.76627851 |
| H | 2.69447884 | 6.48931838 | -0.28614890 |
| H | 4.68244922 | 5.89343776 | 1.08619731 |
| H | 4.63474132 | -2.30390391 | -1.04096558 |
| H | 5.31704663 | -3.53660301 | -2.09913835 |
| H | 3.92530239 | -2.59099535 | -2.63834770 |
| H | 2.67123199 | -6.09231681 | -1.86508325 |
| H | 4.22940018 | -5.64779823 | -2.55953285 |
| H | 2.74920247 | -4.85173548 | -3.12103958 |
| H | 5.12804276 | -5.17584265 | -0.20629076 |
| H | 4.31277235 | -3.98804721 | 0.82817523 |
| H | 3.55463508 | -5.55498562 | 0.51169498 |
| H | -6.25133118 | -2.10192865 | 2.80024901 |
| H | -7.59897704 | -1.13892531 | 2.18691582 |
| H | -6.86165755 | -2.36375460 | 1.15557133 |
| H | -5.68943242 | 0.92741571 | -0.26214453 |
| H | -7.29148844 | 0.55674772 | 0.38681837 |
| H | -6.45976733 | -0.60964417 | -0.65793427 |
| H | -6.47192835 | 0.94969820 | 2.77653436 |
| H | -5.03367330 | 0.10367248 | 3.37494612 |
| H | -4.87677186 | 1.36941971 | 2.15071120 |

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| | | | |
|---|-------------|------------|-------------|
| C | -1.24847099 | 4.18491053 | -0.06331745 |
| C | 0.10049723 | 3.78741010 | 0.03801833 |
| C | 0.38403892 | 2.40611481 | 0.12795908 |
| C | -0.68591323 | 1.49224640 | 0.29700901 |
| C | -2.02229834 | 1.95414497 | 0.39562113 |
| C | -2.31814813 | 3.30733718 | 0.00465179 |
| C | 1.18380828 | 4.71337172 | -0.07021913 |
| C | 2.47521474 | 4.27908670 | -0.13264447 |
| C | 2.78339319 | 2.88414747 | -0.09070378 |

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|---|-------------|-------------|-------------|
| C | 1.73313047 | 1.95221386 | 0.06481764 |
| C | 2.04589115 | 0.57367174 | 0.17793266 |
| C | 0.96554410 | -0.37553880 | 0.26294199 |
| C | -0.39500370 | 0.08109956 | 0.30389072 |
| C | 4.08288143 | 2.38843155 | -0.32150480 |
| C | 4.40813778 | 1.04201306 | -0.31824943 |
| C | 3.39316650 | 0.13236939 | 0.14594972 |
| C | 1.24020489 | -1.74929684 | 0.31594893 |
| C | 0.18952366 | -2.66202262 | -0.04831315 |
| C | -1.16324420 | -2.19530393 | -0.05750568 |
| C | -1.44473266 | -0.84559469 | 0.36500502 |
| C | 0.47879438 | -3.97171598 | -0.52244355 |
| C | -0.50739326 | -4.79578216 | -0.99119434 |
| C | -1.84528254 | -4.34538666 | -1.06234626 |
| C | -2.14491985 | -3.05248169 | -0.62881056 |
| C | -2.68769892 | -0.38192312 | 0.95011395 |
| C | 2.56355925 | -2.13963464 | 0.76768569 |
| C | -3.53938839 | -1.26257806 | 1.65346861 |
| C | -4.59946242 | -0.79772378 | 2.40033086 |
| C | -4.82944834 | 0.58207555 | 2.49932377 |
| C | -4.01056800 | 1.46211733 | 1.82350231 |
| C | -2.95100696 | 1.01407975 | 1.00766287 |
| C | 3.62288020 | -1.18839938 | 0.71776844 |
| C | 4.81797330 | -1.48398259 | 1.40452734 |
| C | 5.01495027 | -2.69047674 | 2.04513435 |
| C | 3.99216185 | -3.64739124 | 2.04913021 |
| C | 2.78662853 | -3.36428406 | 1.43909028 |
| O | -3.39230985 | -2.54524575 | -0.81071812 |
| C | -2.90896809 | -5.12887215 | -1.62603770 |
| C | -4.15509945 | -4.62706942 | -1.76190447 |
| C | -4.46432888 | -3.26487707 | -1.35965860 |
| O | -5.52146542 | -2.70428618 | -1.45152360 |
| C | -3.68895518 | 3.83170597 | -0.52550494 |
| C | -3.41986513 | 4.59966411 | -1.85191254 |
| C | -4.34203177 | 4.81970870 | 0.46464223 |
| C | -4.68958232 | 2.71807126 | -0.90822606 |
| C | 5.76219212 | 0.65122402 | -0.98970698 |
| C | 5.88336964 | 1.46007541 | -2.31378340 |
| C | 5.85182220 | -0.82928342 | -1.42285780 |
| C | 6.96967469 | 1.02199697 | -0.10219892 |
| H | -1.43154033 | 5.23057329 | -0.27773459 |
| H | 0.95785991 | 5.77298961 | -0.12794970 |
| H | 3.28881491 | 4.98862164 | -0.24087779 |
| H | 4.83969792 | 3.11689532 | -0.58521278 |

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|---|-------------|-------------|-------------|
| H | 1.50803529 | -4.29645810 | -0.57123438 |
| H | -0.26596421 | -5.78399835 | -1.36682672 |
| H | -3.31994591 | -2.32097108 | 1.65002414 |
| H | -5.22540142 | -1.49613796 | 2.94336667 |
| H | -5.62627723 | 0.95946047 | 3.12995432 |
| H | -4.14469686 | 2.52458389 | 1.96004273 |
| H | 5.57621590 | -0.71884901 | 1.47328148 |
| H | 5.94174794 | -2.87698842 | 2.57545620 |
| H | 4.12218338 | -4.58459638 | 2.57806315 |
| H | 1.96987113 | -4.06513173 | 1.54307465 |
| H | -2.68713563 | -6.14180128 | -1.94734943 |
| H | -4.97593308 | -5.19235472 | -2.18111103 |
| H | -2.90847893 | 3.95791675 | -2.57352928 |
| H | -4.37128103 | 4.91477479 | -2.28840052 |
| H | -2.81699567 | 5.49745596 | -1.71135741 |
| H | -4.61499736 | 4.34146260 | 1.40672218 |
| H | -5.25467562 | 5.23857960 | 0.02980793 |
| H | -3.66700228 | 5.64787459 | 0.69588350 |
| H | -4.20786989 | 1.94357700 | -1.50992377 |
| H | -5.15171553 | 2.23065139 | -0.05532894 |
| H | -5.49325625 | 3.15608699 | -1.50562693 |
| H | 5.95787314 | 2.53564666 | -2.15132124 |
| H | 6.78597986 | 1.15116657 | -2.84775422 |
| H | 5.02233637 | 1.27511466 | -2.96067090 |
| H | 6.00233022 | -1.51970551 | -0.59836817 |
| H | 6.69892703 | -0.94719758 | -2.10353922 |
| H | 4.94789658 | -1.13673158 | -1.95469734 |
| H | 6.95153968 | 2.08262813 | 0.16105970 |
| H | 6.99231999 | 0.45076700 | 0.82734349 |
| H | 7.90397179 | 0.82233586 | -0.63582962 |

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| | | | |
|---|-------------|------------|-------------|
| C | 1.24294814 | 4.97696165 | 1.30130231 |
| C | 2.14241660 | 4.21507635 | 0.57841862 |
| C | 1.82963621 | 2.91048660 | 0.15559530 |
| C | 0.56348137 | 2.35979366 | 0.47244797 |
| C | -0.31903582 | 3.14540069 | 1.24198692 |
| C | 0.00547112 | 4.42943726 | 1.64276868 |
| C | 2.80050172 | 2.10135585 | -0.58254101 |
| C | 2.62783785 | 0.69814289 | -0.63704372 |
| C | 1.41076260 | 0.08736586 | -0.06692397 |
| C | 0.27253535 | 0.94707088 | 0.13483945 |
| C | 3.89308905 | 2.68665711 | -1.24756630 |

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|---|-------------|-------------|-------------|
| C | 4.80678502 | 1.92135496 | -1.94927694 |
| C | 4.63011980 | 0.53805600 | -2.02264962 |
| C | 3.55499880 | -0.05515222 | -1.38588101 |
| C | 1.28175361 | -1.27880387 | 0.21872155 |
| C | -0.01419733 | -1.84522480 | 0.36520494 |
| C | -1.16017869 | -1.02793643 | 0.08889399 |
| C | -1.01457965 | 0.39148989 | 0.08184669 |
| C | -2.22824066 | 1.25867959 | 0.04060999 |
| C | -3.17568874 | 1.21675453 | 1.07039477 |
| C | -4.30355019 | 2.02645722 | 1.02558712 |
| C | -4.50413958 | 2.88596151 | -0.05423828 |
| C | -3.56673274 | 2.93228062 | -1.08251603 |
| C | -2.43337276 | 2.12607252 | -1.03332078 |
| C | 2.47847020 | -2.14741675 | 0.41774432 |
| C | 3.41312518 | -1.81729006 | 1.40599706 |
| C | 4.54600138 | -2.60099549 | 1.60380731 |
| C | 4.76481784 | -3.72842589 | 0.81457103 |
| C | 3.83812446 | -4.07174429 | -0.16893604 |
| C | 2.70249602 | -3.29078439 | -0.36210519 |
| C | -0.20573786 | -3.21300372 | 0.73639739 |
| C | -1.43674784 | -3.79433498 | 0.67843251 |
| C | -2.55520970 | -3.06624995 | 0.19166432 |
| C | -2.40016230 | -1.71861203 | -0.12261859 |
| C | -3.84935275 | -3.65508055 | -0.00316048 |
| C | -4.88233467 | -2.93850840 | -0.49860123 |
| C | -4.71657243 | -1.54535758 | -0.87219498 |
| O | -3.42873865 | -1.02420325 | -0.66373703 |
| O | -5.54431222 | -0.81064093 | -1.33631215 |
| H | 1.51078884 | 5.97757906 | 1.62106938 |
| H | 3.12173162 | 4.62369830 | 0.36664991 |
| H | -1.26632438 | 2.74008350 | 1.55376246 |
| H | -0.70048187 | 4.99579544 | 2.23924181 |
| H | 4.00787335 | 3.76256307 | -1.24121555 |
| H | 5.63655697 | 2.39778568 | -2.45891583 |
| H | 5.31717125 | -0.07374444 | -2.59583656 |
| H | 3.41809936 | -1.11831585 | -1.49625284 |
| H | -3.02099787 | 0.54208068 | 1.90564571 |
| H | -5.03227530 | 1.98163514 | 1.82707658 |
| H | -5.39041536 | 3.50844223 | -0.09636320 |
| H | -3.72057670 | 3.59248188 | -1.92850687 |
| H | -1.70253231 | 2.16025235 | -1.83266880 |
| H | 3.24825541 | -0.93382634 | 2.01156002 |
| H | 5.25979799 | -2.32916210 | 2.37322297 |
| H | 5.64987928 | -4.33607123 | 0.96500104 |

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|---|-------------|-------------|-------------|
| H | 4.00158335 | -4.94610612 | -0.78900148 |
| H | 1.98939833 | -3.55167255 | -1.13580015 |
| H | 0.64630403 | -3.79097492 | 1.06315757 |
| H | -1.57312968 | -4.82989924 | 0.97004622 |
| H | -3.98449754 | -4.69918116 | 0.26177980 |
| H | -5.86903327 | -3.35429563 | -0.64920707 |

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|---|-------------|-------------|-------------|
| C | -0.22088582 | 5.05981450 | -0.67373960 |
| C | -1.39175154 | 4.32380289 | -0.81468903 |
| C | -1.42481900 | 2.95588691 | -0.52667062 |
| C | -0.22634851 | 2.32533063 | -0.09258704 |
| C | 0.95191311 | 3.09343308 | 0.11760390 |
| C | 0.93468277 | 4.45774422 | -0.20421930 |
| C | -2.65649842 | 2.16536571 | -0.64543506 |
| C | -2.64366482 | 0.78819836 | -0.28828700 |
| C | -1.39249614 | 0.12789177 | -0.01376382 |
| C | -0.18075615 | 0.89251389 | 0.05684013 |
| C | -3.85864790 | 2.72662366 | -1.08741536 |
| C | -5.02220726 | 1.96997474 | -1.15992069 |
| C | -5.02557911 | 0.64566987 | -0.75369732 |
| C | -3.85158674 | 0.03693014 | -0.28940253 |
| C | -1.35622541 | -1.25846603 | 0.19325177 |
| C | -0.09772859 | -1.92869923 | -0.01133240 |
| C | 1.10983601 | -1.16012774 | -0.00584085 |
| C | 1.04377128 | 0.25144368 | 0.29000469 |
| C | 2.13950573 | 1.03484535 | 0.83492543 |
| C | 3.17408296 | 0.43661204 | 1.58631905 |
| C | 4.19304859 | 1.18623501 | 2.13127269 |
| C | 4.20572821 | 2.57662849 | 1.95415387 |
| C | 3.17254239 | 3.19225003 | 1.27734299 |
| C | 2.11010122 | 2.44790411 | 0.72390324 |
| C | -2.59435925 | -1.94376484 | 0.53519226 |
| C | -3.83727596 | -1.31700581 | 0.25549138 |
| C | -5.02754730 | -1.99251886 | 0.59363078 |
| C | -5.00911733 | -3.22170595 | 1.22320270 |
| C | -3.78437827 | -3.80269978 | 1.57354243 |
| C | -2.60370249 | -3.16909812 | 1.24029220 |
| C | -0.04434554 | -3.30483853 | -0.37408294 |
| C | 1.13165765 | -3.91134415 | -0.71624852 |
| C | 2.33053551 | -3.16654876 | -0.77799629 |
| C | 2.29469509 | -1.80692158 | -0.46562209 |
| C | 3.57648089 | -3.72391695 | -1.22579324 |

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|---|-------------|-------------|-------------|
| C | 4.67778951 | -2.95694982 | -1.37107480 |
| C | 4.63733409 | -1.52967993 | -1.10004284 |
| O | 3.39466804 | -1.03787728 | -0.67266219 |
| O | 5.53891583 | -0.74511852 | -1.20720569 |
| H | -0.21677897 | 6.11465756 | -0.92351363 |
| H | -2.28144853 | 4.83315562 | -1.15794303 |
| H | 1.83183973 | 5.05228632 | -0.09649995 |
| H | -3.89916990 | 3.76337256 | -1.39101621 |
| H | -5.93568780 | 2.42419977 | -1.52646320 |
| H | -5.94676226 | 0.08158361 | -0.80945558 |
| H | 3.15281639 | -0.63107299 | 1.75523586 |
| H | 4.97620601 | 0.70145088 | 2.70202705 |
| H | 5.00685072 | 3.17239129 | 2.37624948 |
| H | 3.16467329 | 4.27202716 | 1.21015465 |
| H | -5.98336540 | -1.52469345 | 0.39890770 |
| H | -5.94074404 | -3.71180613 | 1.48154946 |
| H | -3.75972530 | -4.73471420 | 2.12647172 |
| H | -1.66644454 | -3.59887342 | 1.56547679 |
| H | -0.96353507 | -3.86559968 | -0.44834143 |
| H | 1.14654571 | -4.95574605 | -1.00771363 |
| H | 3.61319813 | -4.78555589 | -1.44942314 |
| H | 5.63016012 | -3.34797460 | -1.70140905 |

Table S3 Cartesian coordinates of optimized species

(P)-3a

| | | | |
|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 1.06731308 | 4.26776031 | -0.05862700 |
| C | -0.24344202 | 3.80501427 | -0.28696002 |
| C | -0.46903503 | 2.40814117 | -0.29165902 |
| C | 0.63900905 | 1.52950211 | -0.31156902 |
| C | 1.95683814 | 2.05193215 | -0.30113002 |
| C | 2.16000216 | 3.42926925 | 0.05367400 |
| C | -1.35571910 | 4.69082434 | -0.38814403 |
| C | -2.62793519 | 4.20519530 | -0.42868103 |
| C | -2.87947621 | 2.80311120 | -0.34465302 |
| C | -1.79555113 | 1.89894714 | -0.29469402 |
| C | -2.05307115 | 0.49930104 | -0.25707302 |
| C | -0.93825807 | -0.42326203 | -0.25179502 |
| C | 0.40388903 | 0.10522401 | -0.30096002 |
| C | -4.17904530 | 2.30183516 | -0.14651101 |
| C | -4.46401832 | 0.96466507 | 0.03968100 |
| C | -3.39253525 | 0.03238800 | -0.23642302 |
| C | -1.15662208 | -1.82177113 | -0.22697302 |

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|---|-------------|-------------|-------------|
| C | -0.01019100 | -2.70475419 | -0.22214102 |
| C | 1.28738309 | -2.14747616 | -0.02814000 |
| C | 1.50727411 | -0.75834906 | -0.28826102 |
| C | -0.06211900 | -4.11305929 | -0.46573703 |
| C | 1.00795907 | -4.93042536 | -0.22950002 |
| C | 2.20162116 | -4.40676632 | 0.32135302 |
| C | 2.31786316 | -3.02441822 | 0.41630503 |
| C | 2.77600320 | -0.23978802 | -0.77261306 |
| C | -2.53061518 | -2.30196617 | -0.25248402 |
| C | 3.71329227 | -1.07231908 | -1.42481210 |
| C | 4.81625035 | -0.55588004 | -2.06682015 |
| C | 5.00746636 | 0.83174406 | -2.11811215 |
| C | 4.09541530 | 1.66610412 | -1.51072811 |
| C | 2.98585522 | 1.16127009 | -0.80181206 |
| C | -3.58832026 | -1.37859510 | -0.48471703 |
| C | -4.80584835 | -1.87595113 | -0.99464807 |
| C | -5.08846836 | -3.22344023 | -1.01999307 |
| C | -4.17120430 | -4.10943630 | -0.43796803 |
| C | -2.92257021 | -3.65430727 | -0.06902101 |
| O | 3.41947925 | -2.45656418 | 0.96890707 |
| C | 3.31415324 | -5.20377038 | 0.74912205 |
| C | 4.42429032 | -4.63045633 | 1.26203709 |
| C | 4.52807533 | -3.18918623 | 1.41815910 |
| O | 5.44629039 | -2.57681118 | 1.88906914 |
| C | 3.43271825 | 4.01958029 | 0.72609905 |
| C | 2.96482822 | 4.77528034 | 2.00037515 |
| C | 4.14670630 | 5.03597336 | -0.18716701 |
| C | -5.82192141 | 0.65248705 | 0.75261706 |
| C | -5.78693444 | -0.64296905 | 1.59231012 |
| C | -6.09370442 | 1.77626613 | 1.79357413 |
| H | 1.18875709 | 5.33039640 | 0.11088601 |
| H | -1.17069808 | 5.75919142 | -0.40750703 |
| H | -3.47509325 | 4.88007935 | -0.48215203 |
| H | -4.96316136 | 3.03669422 | -0.02733900 |
| H | -0.94659907 | -4.54079633 | -0.90263406 |
| H | 0.94432907 | -5.99096344 | -0.44382303 |
| H | 3.53013225 | -2.13503716 | -1.48175510 |
| H | 5.50542939 | -1.22107509 | -2.57314419 |
| H | 5.84251244 | 1.24912009 | -2.66827919 |
| H | 4.19160930 | 2.73444920 | -1.62591912 |
| H | -5.52447739 | -1.16557509 | -1.36975510 |
| H | -6.02725346 | -3.58111026 | -1.42547210 |
| H | -4.42605732 | -5.15324337 | -0.29767902 |
| H | -2.23978516 | -4.34771331 | 0.39097403 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.24794023 | -6.28228848 | 0.64934705 |
| H | 5.28105438 | -5.20183438 | 1.59092811 |
| H | 2.41984117 | 4.10367130 | 2.66767819 |
| H | 2.31913517 | 5.62427339 | 1.77545213 |
| H | 3.83714828 | 5.15739837 | 2.53647118 |
| H | -6.66023946 | -0.65995305 | 2.24895916 |
| H | -5.80625544 | -1.55249311 | 1.00326607 |
| H | -4.89438835 | -0.66907805 | 2.22227416 |
| H | -6.32279646 | 2.73817220 | 1.33448710 |
| H | -5.23945638 | 1.90987314 | 2.46061318 |
| H | -6.96015950 | 1.49800511 | 2.39769817 |
| H | 4.55546133 | 4.57092233 | -1.08557808 |
| H | 3.46439125 | 5.82824439 | -0.50450104 |
| H | 4.97722736 | 5.50207039 | 0.35081303 |
| C | 4.43515132 | 2.96381821 | 1.23576609 |
| H | 5.13276237 | 3.44845825 | 1.92320214 |
| H | 5.02370036 | 2.50095818 | 0.44970903 |
| H | 3.92686728 | 2.16639116 | 1.78226413 |
| C | -7.02519851 | 0.65546805 | -0.21280902 |
| H | -7.01662351 | -0.17897101 | -0.91270806 |
| H | -7.04994353 | 1.58059911 | -0.79423706 |
| H | -7.95677759 | 0.59163204 | 0.35723503 |

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|---|-------------|-------------|-------------|
| C | -1.01478800 | 4.36667900 | 0.23144600 |
| C | 0.25121400 | 3.87416600 | -0.14573600 |
| C | 0.43321200 | 2.47637800 | -0.14492600 |
| C | -0.70409600 | 1.63341900 | -0.05987100 |
| C | -2.00260100 | 2.17546300 | 0.07096000 |
| C | -2.12056000 | 3.56875100 | 0.45434200 |
| C | 1.36027400 | 4.72459200 | -0.42625900 |
| C | 2.59719400 | 4.19823400 | -0.66380900 |
| C | 2.81818700 | 2.79436800 | -0.56001600 |
| C | 1.74213900 | 1.93708600 | -0.27206200 |
| C | 1.98728700 | 0.56071700 | -0.02672200 |
| C | 0.83547300 | -0.27731100 | 0.17269300 |
| C | -0.49904400 | 0.21092300 | -0.08893100 |
| C | 4.08402500 | 2.20923000 | -0.76517900 |
| C | 4.37541200 | 0.88195200 | -0.52029200 |
| C | 3.31379500 | 0.04710100 | 0.03634600 |
| C | 0.99361100 | -1.57324100 | 0.64253300 |
| C | -1.56660000 | -0.67804000 | -0.26211000 |
| C | -2.83399700 | -0.07307000 | -0.67584500 |

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|---|-------------|-------------|-------------|
| C | 2.31884700 | -2.11160900 | 0.84811800 |
| C | -3.85489500 | -0.76736000 | -1.35989000 |
| C | -5.04963000 | -0.17806000 | -1.71147200 |
| C | -5.30554000 | 1.14840400 | -1.35419700 |
| C | -4.32910200 | 1.86075800 | -0.69792400 |
| C | -3.06708700 | 1.30937100 | -0.38658300 |
| C | 3.46298600 | -1.30189800 | 0.56949700 |
| C | 4.72793000 | -1.85060300 | 0.89153500 |
| C | 4.89018400 | -3.15979700 | 1.29247100 |
| C | 3.77123300 | -3.99421200 | 1.40369100 |
| C | 2.51138600 | -3.46750600 | 1.21980200 |
| H | -1.08744400 | 5.43322200 | 0.39888100 |
| H | 1.19996700 | 5.79677300 | -0.45525000 |
| H | 3.43667100 | 4.84050300 | -0.90606100 |
| H | 4.84882800 | 2.86885400 | -1.13790600 |
| H | -3.68331400 | -1.77281200 | -1.67816400 |
| H | -5.77258500 | -0.74891500 | -2.28202400 |
| H | -6.25585300 | 1.61473000 | -1.58576900 |
| H | -4.54199400 | 2.84823700 | -0.42124800 |
| H | 5.59837700 | -1.22100000 | 0.84248500 |
| H | 5.88348100 | -3.53298900 | 1.51226100 |
| H | 3.88066300 | -5.03414300 | 1.68801800 |
| H | 1.67294800 | -4.11593900 | 1.40554500 |
| C | -3.28251400 | 4.28855600 | 1.22024400 |
| C | -4.00303700 | 5.30472000 | 0.30446700 |
| H | -4.82309400 | 5.78200200 | 0.84875600 |
| H | -3.31301300 | 6.08953200 | -0.01537700 |
| H | -4.41281900 | 4.85797700 | -0.60165300 |
| C | -4.30705400 | 3.34719500 | 1.87151400 |
| H | -4.87702000 | 3.89104400 | 2.62845100 |
| H | -4.98387300 | 2.91134300 | 1.18501900 |
| H | -3.80033900 | 2.51844200 | 2.37315500 |
| C | -2.66101300 | 5.09395700 | 2.39231900 |
| H | -2.07967400 | 4.44053200 | 3.04751500 |
| H | -2.01175100 | 5.90134300 | 2.05660200 |
| H | -3.46246800 | 5.54518100 | 2.98266000 |
| C | 5.80129000 | 0.40672100 | -0.94977500 |
| C | 6.75094700 | 0.18658400 | 0.27400700 |
| H | 7.30040000 | -0.75582800 | 0.20078100 |
| H | 7.49104700 | 0.98779300 | 0.31837400 |
| H | 6.22928200 | 0.21464600 | 1.23087000 |
| C | 5.68979200 | -0.82324600 | -1.89476900 |
| H | 5.05083000 | -1.62580600 | -1.54382700 |
| H | 5.27119900 | -0.48912800 | -2.84867200 |

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| H | 6.68312700 | -1.23597900 | -2.09029100 |
| C | 6.52877600 | 1.44315100 | -1.84749800 |
| H | 5.91458000 | 1.76112100 | -2.69194900 |
| H | 6.86980100 | 2.32473500 | -1.30135400 |
| H | 7.42579800 | 0.96245000 | -2.24575100 |
| C | -0.19754600 | -2.33878000 | 0.91803800 |
| C | -1.34763200 | -2.06928900 | 0.11676600 |
| C | -0.22651400 | -3.37661600 | 1.89610600 |
| C | -1.27950900 | -4.24363600 | 1.96336700 |
| C | -2.22554600 | -4.24443500 | 0.90639500 |
| C | -2.17825900 | -3.23027200 | -0.05514200 |
| O | -2.85005600 | -3.39923300 | -1.21950700 |
| C | -3.17986000 | -5.29693700 | 0.72042000 |
| C | -3.95391300 | -5.37050300 | -0.38525300 |
| C | -3.82666400 | -4.39459200 | -1.44382200 |
| O | -4.43341800 | -4.33447500 | -2.47786400 |
| H | 0.57783100 | -3.38842000 | 2.62835300 |
| H | -1.35735600 | -4.98147500 | 2.75261900 |
| H | -3.27689500 | -6.04165600 | 1.50365300 |
| H | -4.69672600 | -6.14148800 | -0.53372200 |

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|-----|-------------|-------------|-------------|
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| C | -1.06720933 | 4.26786020 | -0.05814994 |
| C | 0.24353879 | 3.80511226 | -0.28653895 |
| C | 0.46912390 | 2.40822817 | -0.29148395 |
| C | -0.63893312 | 1.52962303 | -0.31150696 |
| C | -1.95670325 | 2.05210498 | -0.30111496 |
| C | -2.15993035 | 3.42934806 | 0.05384907 |
| C | 1.35584881 | 4.69090939 | -0.38758896 |
| C | 2.62804594 | 4.20524244 | -0.42832696 |
| C | 2.87955405 | 2.80312736 | -0.34457096 |
| C | 1.79562803 | 1.89899022 | -0.29462795 |
| C | 2.05312214 | 0.49933114 | -0.25710595 |
| C | 0.93823813 | -0.42315500 | -0.25183095 |
| C | -0.40391601 | 0.10533794 | -0.30094196 |
| C | 4.17913518 | 2.30179541 | -0.14666094 |
| C | 4.46414329 | 0.96462733 | 0.03940707 |
| C | 3.39258827 | 0.03233619 | -0.23652895 |
| C | 1.15650924 | -1.82165109 | -0.22704495 |
| C | 0.01006421 | -2.70459723 | -0.22248795 |
| C | -1.28748392 | -2.14735027 | -0.02826194 |
| C | -1.50735503 | -0.75817719 | -0.28815595 |
| C | 0.06201431 | -4.11280733 | -0.46659797 |

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| C | -1.00805571 | -4.93025546 | -0.23058195 |
| C | -2.20163383 | -4.40675750 | 0.32063209 |
| C | -2.31786993 | -3.02444041 | 0.41607610 |
| C | -2.77615515 | -0.23954824 | -0.77235299 |
| C | 2.53042937 | -2.30196103 | -0.25231595 |
| C | -3.71379417 | -1.07198736 | -1.42415103 |
| C | -4.81678728 | -0.55539040 | -2.06599508 |
| C | -5.00761838 | 0.83227369 | -2.11769009 |
| C | -4.09519538 | 1.66654581 | -1.51074004 |
| C | -2.98576426 | 1.16152585 | -0.80178799 |
| C | 3.58826138 | -1.37871290 | -0.48454297 |
| C | 4.80583450 | -1.87635485 | -0.99399700 |
| C | 5.08833861 | -3.22387193 | -1.01893300 |
| C | 4.17080561 | -4.10968005 | -0.43704997 |
| C | 2.92212148 | -3.65432510 | -0.06857094 |
| O | -3.41938305 | -2.45675844 | 0.96908714 |
| C | -3.31409486 | -5.20389963 | 0.74833612 |
| C | -4.42413598 | -4.63075567 | 1.26165016 |
| C | -4.52791508 | -3.18953057 | 1.41823217 |
| O | -5.44603120 | -2.57733059 | 1.88956720 |
| C | -3.43287749 | 4.01944702 | 0.72595512 |
| C | -4.14641161 | 5.03631005 | -0.18711595 |
| C | -2.96546950 | 4.77452611 | 2.00080321 |
| C | 5.82226739 | 0.65240640 | 0.75201212 |
| C | 5.78666048 | -0.64218570 | 1.59293518 |
| C | 7.02536150 | 0.65389848 | -0.21366295 |
| H | -1.18865241 | 5.33046625 | 0.11156207 |
| H | 1.17086073 | 5.75928445 | -0.40672996 |
| H | 3.47522195 | 4.88010555 | -0.48175897 |
| H | 4.96325518 | 3.03664552 | -0.02753794 |
| H | 0.94653940 | -4.54032930 | -0.90365100 |
| H | -0.94449064 | -5.99071155 | -0.44531697 |
| H | -3.53095008 | -2.13476243 | -1.48095804 |
| H | -5.50626031 | -1.22053749 | -2.57198212 |
| H | -5.84254647 | 1.24971266 | -2.66798913 |
| H | -4.19081846 | 2.73488788 | -1.62649505 |
| H | 5.52468351 | -1.16616475 | -1.36901303 |
| H | 6.02722769 | -3.58170489 | -1.42403004 |
| H | 4.42547069 | -5.15350211 | -0.29654296 |
| H | 2.23903748 | -4.34758220 | 0.39122509 |
| H | -3.24789878 | -6.28238468 | 0.64819811 |
| H | -5.28083000 | -5.20224776 | 1.59052618 |
| H | -4.55464960 | 4.57167899 | -1.08597701 |
| H | -3.46395561 | 5.82877114 | -0.50368597 |

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| H | -4.97723270 | 5.50208801 | 0.35067909 |
| H | 6.66070556 | -0.65968764 | 2.24860623 |
| H | 4.89483243 | -0.66637775 | 2.22401022 |
| H | 5.80402157 | -1.55232476 | 1.00480114 |
| H | 7.04998544 | 1.57815355 | -0.79648999 |
| H | 7.01683857 | -0.18159558 | -0.91229600 |
| H | 7.95702054 | 0.59099054 | 0.35634509 |
| H | -2.42096342 | 4.10251310 | 2.66808926 |
| H | -2.31948152 | 5.62346719 | 1.77653120 |
| H | -3.83797459 | 5.15661508 | 2.53661425 |
| C | -4.43554249 | 2.96349488 | 1.23480515 |
| H | -5.13344657 | 3.44794087 | 1.92208420 |
| H | -3.92745940 | 2.16594985 | 1.78133819 |
| H | -5.02378550 | 2.50071081 | 0.44844310 |
| C | 6.09512436 | 1.77697650 | 1.79188019 |
| H | 5.24103828 | 1.91211945 | 2.45880424 |
| H | 6.32520528 | 2.73816559 | 1.33176716 |
| H | 6.96132444 | 1.49845454 | 2.39624224 |

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|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.60718118 | 5.02440637 | -0.98142013 |
| C | 1.74939924 | 4.26500428 | -0.75897912 |
| C | 1.65425518 | 2.94033719 | -0.32652808 |
| C | 0.37282207 | 2.35907619 | -0.15373607 |
| C | -0.78633199 | 3.17168429 | -0.27539408 |
| C | -0.64483593 | 4.49255138 | -0.72126611 |
| C | 4.08975935 | 2.72955708 | 0.15007495 |
| C | 2.84169424 | 2.13604408 | -0.04927906 |
| C | 2.72022418 | 0.72511799 | 0.05371095 |
| C | 1.41563106 | 0.10442799 | 0.05237095 |
| C | 0.24235301 | 0.93650110 | 0.05828595 |
| C | 5.21107040 | 1.95657899 | 0.42320797 |
| C | 5.11432835 | 0.57619489 | 0.45502497 |
| C | 3.88588624 | -0.06517211 | 0.24325196 |
| C | 1.30196001 | -1.29245410 | 0.15820895 |
| C | 0.00170989 | -1.87081410 | 0.35360297 |
| C | -1.15600316 | -1.05961800 | 0.16013195 |
| C | -1.03538210 | 0.36999810 | 0.18529595 |
| C | -0.19370317 | -3.22044819 | 0.77981800 |
| C | -1.42574728 | -3.80726119 | 0.75330200 |
| C | -2.53150434 | -3.10753310 | 0.20936896 |
| C | -2.37326628 | -1.76096101 | -0.10417607 |
| C | -2.15986315 | 1.25309020 | 0.47560598 |

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|---|-------------|-------------|-------------|
| C | 2.50095706 | -2.10914821 | -0.01839406 |
| C | -3.30002125 | 0.80684821 | 1.17634603 |
| C | -4.36195830 | 1.64483631 | 1.43516204 |
| C | -4.31383624 | 2.98000541 | 1.01499702 |
| C | -3.17144014 | 3.46497740 | 0.41392097 |
| C | -2.06351010 | 2.63030130 | 0.16442495 |
| C | 3.78066317 | -1.51241721 | 0.11941895 |
| C | 4.92780323 | -2.32289031 | 0.00537494 |
| C | 4.83951417 | -3.66390040 | -0.30592908 |
| C | 3.58641206 | -4.22579440 | -0.57135710 |
| C | 2.44725801 | -3.45823230 | -0.43869809 |
| O | -3.36808432 | -1.07915092 | -0.72263811 |
| C | -3.81144945 | -3.70610509 | -0.03518006 |
| C | -4.81782650 | -3.00138401 | -0.59597210 |
| C | -4.63603644 | -1.61698092 | -0.99462313 |
| O | -5.43994847 | -0.90301783 | -1.52701317 |
| H | 0.69763123 | 6.03988143 | -1.34855715 |
| H | 6.16541651 | 2.43593499 | 0.60659299 |
| H | 0.64994687 | -3.77272326 | 1.16293503 |
| H | -1.56310733 | -4.82258926 | 1.10656102 |
| H | -3.33099029 | -0.20713586 | 1.54699606 |
| H | -5.22527737 | 1.27244331 | 1.97308708 |
| H | -5.15049528 | 3.64221349 | 1.20320403 |
| H | -3.11296811 | 4.51822347 | 0.17647495 |
| H | 5.90803131 | -1.88098231 | 0.11562495 |
| H | 5.73941321 | -4.26048348 | -0.39691809 |
| H | 3.50690102 | -5.25350947 | -0.90551612 |
| H | 1.49758392 | -3.89148830 | -0.71035111 |
| H | -3.95673650 | -4.74492616 | 0.24285696 |
| H | -5.79447458 | -3.42341500 | -0.78748812 |
| H | -1.52112297 | 5.10638046 | -0.87669712 |
| H | 6.00294739 | -0.00570318 | 0.65429999 |
| H | 2.71926232 | 4.70006128 | -0.95789213 |
| H | 4.18330340 | 3.80662316 | 0.13214695 |

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|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 1.73125500 | -4.64629300 | -0.89714300 |
| C | 2.60032500 | -3.59040400 | -0.66713800 |
| C | 2.12423700 | -2.31921000 | -0.34211300 |
| C | 0.71871400 | -2.09570100 | -0.26998100 |
| C | -0.16012800 | -3.18380100 | -0.49575400 |
| C | 0.36871200 | -4.44679800 | -0.80531700 |
| C | 4.43581200 | -1.42511500 | -0.05494200 |

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|---|-------------|-------------|-------------|
| C | 3.05568800 | -1.21769500 | -0.11754000 |
| C | 2.54788300 | 0.10142200 | -0.01563600 |
| C | 1.12184600 | 0.32912800 | -0.03268700 |
| C | 0.18469800 | -0.77121400 | -0.03500400 |
| C | 5.31564900 | -0.35637100 | 0.03623600 |
| C | 4.83248000 | 0.93856800 | 0.07080300 |
| C | 3.45447400 | 1.19693100 | 0.06019800 |
| C | 0.64815300 | 1.63829000 | -0.11129700 |
| C | -0.75101800 | 1.82910500 | -0.34123200 |
| C | -1.67341500 | 0.83399900 | 0.10922100 |
| C | -1.20504500 | -0.55511700 | 0.17398000 |
| C | -1.21232200 | 2.97660200 | -1.04939000 |
| C | -2.53578900 | 3.28903900 | -1.10085800 |
| C | -3.42584500 | 2.56133700 | -0.27671100 |
| C | -2.97411800 | 1.40606300 | 0.36740000 |
| C | -2.08895300 | -1.74238900 | 0.15919800 |
| C | 1.53947200 | 2.76860800 | 0.11116300 |
| C | -3.44624200 | -1.74740700 | 0.55190300 |
| C | -4.29187100 | -2.81525200 | 0.33712000 |
| C | -3.82142400 | -3.96283300 | -0.30161300 |
| C | -2.48128200 | -4.03887100 | -0.60398700 |
| C | -1.58668000 | -2.98125300 | -0.33377700 |
| C | 2.93836500 | 2.55258300 | 0.17488800 |
| C | 3.78714400 | 3.65387000 | 0.40980300 |
| C | 3.28787100 | 4.92154000 | 0.62116300 |
| C | 1.90299500 | 5.12161100 | 0.64980400 |
| C | 1.05228800 | 4.06359700 | 0.41081000 |
| O | -3.74941500 | 0.87736300 | 1.34293000 |
| C | -4.76108700 | 3.00837200 | -0.01654000 |
| C | -5.55751400 | 2.39807400 | 0.88817900 |
| C | -5.07250800 | 1.26785400 | 1.64333100 |
| O | -5.64654200 | 0.62865300 | 2.48214300 |
| H | 2.12188200 | -5.62670500 | -1.14272200 |
| H | 6.38340500 | -0.53729800 | 0.07220100 |
| H | -0.48387900 | 3.57466400 | -1.57740400 |
| H | -2.90131200 | 4.12505000 | -1.68474700 |
| H | -3.83920500 | -0.91860800 | 1.09296200 |
| H | -5.31876600 | -2.74861200 | 0.67645800 |
| H | -4.48183300 | -4.79328800 | -0.52146400 |
| H | -2.10870800 | -4.94515600 | -1.05714800 |
| H | 4.85685700 | 3.50880100 | 0.45410400 |
| H | 3.96525800 | 5.74745600 | 0.80307900 |
| H | 1.49560300 | 6.09811700 | 0.88338800 |
| H | -0.01107300 | 4.22508100 | 0.49452500 |

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| H | -5.12266000 | 3.87010600 | -0.56796300 |
| H | -6.56978200 | 2.71588700 | 1.09407400 |
| H | -0.28680700 | -5.29075500 | -0.95505700 |
| H | 5.53832300 | 1.75480500 | 0.11593600 |
| H | 3.66188300 | -3.76459600 | -0.76125300 |
| H | 4.83893900 | -2.42677600 | -0.08154000 |

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| C | -0.60718173 | 5.02440945 | -0.98141409 |
| C | -1.74939986 | 4.26500647 | -0.75897507 |
| C | -1.65425594 | 2.94033737 | -0.32652804 |
| C | -0.37282289 | 2.35907624 | -0.15373603 |
| C | 0.78633125 | 3.17168622 | -0.27539204 |
| C | 0.64483533 | 4.49255333 | -0.72126207 |
| C | -4.08976213 | 2.72955551 | 0.15006699 |
| C | -2.84169508 | 2.13604339 | -0.04928202 |
| C | -2.72022516 | 0.72511728 | 0.05370998 |
| C | -1.41563111 | 0.10442815 | 0.05236998 |
| C | -0.24235297 | 0.93650213 | 0.05828398 |
| C | -5.21107226 | 1.95657653 | 0.42319901 |
| C | -5.11433034 | 0.57619342 | 0.45502001 |
| C | -3.88588629 | -0.06517370 | 0.24325000 |
| C | -1.30195919 | -1.29245396 | 0.15820799 |
| C | -0.00170913 | -1.87081309 | 0.35360301 |
| C | 1.15600400 | -1.05961710 | 0.16013099 |
| C | 1.03538209 | 0.37000001 | 0.18529399 |
| C | 0.19370479 | -3.22044620 | 0.77982004 |
| C | 1.42574884 | -3.80725932 | 0.75330403 |
| C | 2.53150597 | -3.10753234 | 0.20936900 |
| C | 2.37326604 | -1.76096023 | -0.10417703 |
| C | 2.15986323 | 1.25309100 | 0.47560601 |
| C | -2.50095533 | -2.10914894 | -0.01839302 |
| C | 3.30002128 | 0.80684789 | 1.17634506 |
| C | 4.36195741 | 1.64483588 | 1.43516309 |
| C | 4.31383549 | 2.98000598 | 1.01500005 |
| C | 3.17143844 | 3.46497809 | 0.41392501 |
| C | 2.06350931 | 2.63030310 | 0.16442699 |
| C | -3.78066238 | -1.51241881 | 0.11942099 |
| C | -4.92780152 | -2.32289380 | 0.00538098 |
| C | -4.83951160 | -3.66390490 | -0.30592204 |
| C | -3.58640954 | -4.22579702 | -0.57135406 |
| C | -2.44725641 | -3.45823305 | -0.43869705 |
| O | 3.36808416 | -1.07915025 | -0.72264207 |

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| C | 3.81145102 | -3.70610447 | -0.03517902 |
| C | 4.81782714 | -3.00138348 | -0.59597306 |
| C | 4.63603522 | -1.61698137 | -0.99462809 |
| O | 5.43994731 | -0.90301937 | -1.52702013 |
| H | -0.69763267 | 6.03988455 | -1.34854812 |
| H | -6.16542032 | 2.43593263 | 0.60658103 |
| H | -0.64994430 | -3.77272018 | 1.16293906 |
| H | 1.56310879 | -4.82258640 | 1.10656506 |
| H | 3.33098922 | -0.20713619 | 1.54699309 |
| H | 5.22527645 | 1.27244180 | 1.97308812 |
| H | 5.15049359 | 3.64221397 | 1.20320907 |
| H | 3.11296651 | 4.51822517 | 0.17648199 |
| H | -5.90802956 | -1.88098870 | 0.11563299 |
| H | -5.73940972 | -4.26048888 | -0.39690905 |
| H | -3.50689761 | -5.25351210 | -0.90551309 |
| H | -1.49758137 | -3.89148713 | -0.71035207 |
| H | 3.95673796 | -4.74492455 | 0.24286000 |
| H | 5.79447516 | -3.42341458 | -0.78748907 |
| H | 1.52112143 | 5.10638332 | -0.87669108 |
| H | -6.00294946 | -0.00570456 | 0.65429303 |
| H | -2.71926390 | 4.70006456 | -0.95788509 |
| H | -4.18330807 | 3.80662059 | 0.13213499 |