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Synthesis, Mesomorphism, Photophysics and Device Performance of Liquid-crystalline Pincer Complexes of Gold(III)

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Supplementary Information

Instrumentation

^{1}H NMR spectra were measured on a Jeol ECS400 spectrometer operating at 400 MHz with chemical shifts referred to residual non-deuterated $CHCl_3$ signals. Concentration-dependent ^{1}H spectra were measured on a Bruker 500 AVANCE II spectrometer operating at 500 MHz.

Mass spectra (ESI and APCI) were collected on Bruker compact time of flight mass spectrometer; spectra were internally calibrated using sodium formate as the calibrant. Samples were transferred to the spectrometer an Agilent 1260 Infinity LC system.

Cyclic Voltammetry was performed using an EmStat3+. A glassy carbon working electrode and platinum wire counter electrode were used to study solutions containing 1 mM of [Au], where [Au] is the gold complex in question, and 0.1 M $[NBu_4][PF_6]$ in a CH_2Cl_2 solution. Ferrocene was used as an internal reference. Cyclic voltammetry was performed between +0.7 and -2.5 V for 3 scans at a scan rate of (100 mV s^{-1}).

Elemental analysis was carried out using an Exeter Analytical Inc. CE-440 Analyser and Sartorius S2 analytical balance; calibration was performed against acetanilide standards and checked by the use of *S*-benzyl thiouronium chloride as internal standard.

Polarising optical microscopy was carried out using an Olympus BX50 polarising microscope equipped with a Linkam scientific LTS350 heating stage, Linkam LNP2 cooling pump, and Linkam TMS92 controller, differential scanning calorimetry was performed on a Mettler DSC822^e using Mettler STAR-E software, which was calibrated before use against indium and zinc standards under an atmosphere of dry nitrogen. Small-angle X-ray scattering was recorded using a Bruker D8 Discover equipped with a temperature controlled, bored graphite rod furnace, custom built at the University of York. Cu-K_α (λ = 0.154056 nm) radiation was used, generated from a 1 µS microfocus source. Diffraction patterns were recorded on a 2048 × 2048 pixel Bruker VANTEC 500 area detector set at a distance of 121 mm from the sample, allowing simultaneous collection of small angle and wide angle scattering data. Samples were measured in 1 mm capillary tubes in a magnetic field of *ca* 1 T.

The absorption spectra of the complexes were measured in solution in CH_2Cl_2 in 1 cm pathlength quartz cuvettes using a Biotek Instruments XS spectrometer. Emission spectra were recorded using a Jobin Yvon Fluoromax-2 spectrometer equipped with a Hamamatsu R928 photomultiplier tube (PMT). For the measurements at 298 K, the solutions were contained within 1 cm pathlength quartz cuvettes modified for connection to a vacuum line. Degassing was achieved via a minimum of three freeze-pump-thaw cycles whilst connected to the vacuum manifold; final vapour pressure at 77 K was < 5 x 10^{-2} mbar, as monitored using a Pirani gauge. Luminescence quantum yields were determined using aqueous $[Ru(bipy)_3]Cl_2$ as the standard (ϕ = 0.040 in air-equilibrated aqueous solution).[1] Emission spectra at 77 K were recorded in a glass of EPA (= diethyl ether / isopentane / ethanol, 2:2:1 v/v) in 4 mm diameter tubes held within a

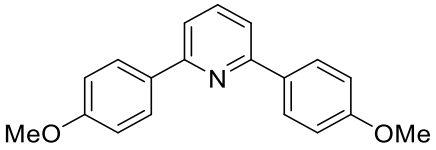
liquid-nitrogen-cooled quartz dewar. The luminescence lifetimes of the complexes in deoxygenated solution and at 77 K were measured by multi-channel scaling following excitation into the lowest-energy absorption band using a microsecond pulsed xenon lamp; an appropriate excitation wavelength corresponding to the low-energy absorption band of the complexes was selected by means of a monochromator. The emitted light was detected at 90˚ using a Peltier-cooled R928 PMT after passage through a monochromator. The lifetimes in air-equilibrated solution (< 10 μs) were measured by time-correlated single photon counting (TCSPC), following excitation at 374 nm with a pulsed laser diode.

Diffraction data were collected at 110 K on an Oxford Diffraction SuperNova dual-source X-ray diffractometer with CuKα radiation (λ = 1.54184) using a EOS CCD camera. The crystal was cooled with an Oxford Instruments Cryojet. Diffractometer control, data collection, initial unit cell determination, frame integration and unit-cell refinement was carried out with 'Crysalis'.[2] Face-indexed absorption corrections were applied using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.[3] OLEX2[4] was used for overall structure solution, refinement and preparation of computer graphics and publication data. Within OLEX2, the algorithm used for structure solution was ShelXT.[5] Refinement by full-matrix least-squares used the SHELXL-97[6] algorithm within OLEX2.[4] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using a 'riding model' and included in the refinement at calculated positions.

Device fabrication and Measurements: The patterned ITO substrates were rinsed with acetone and isopropyl alcohol using sonication for 15 min, followed by 15 min UV-ozone-treatment. After surface treatment, the PEDOT:PSS layer was spin-coated onto the ITO substrate as the hole-injecting layer, and then annealed at 150 °C for 15 min. The emissive layers were prepared by spin-coating onto the PEDOT:PSS and then annealed at 80 °C for 15 min. The hole blocking layer, electron-transporting and the cathode materials were thermally evaporated onto the emitter layer in a vacuum chamber. The thermally evaporated deposition rates are 0.6^{-1} Å s^{-1} for organic layers, 0.1 Å s^{-1} for Liq and 1.5-1.8 Å s^{-1} for Al electrode, respectively. The current-voltage-luminance (*J-V-L*) characteristics and the electroluminescence spectra of the devices were simultaneously obtained by using a spectroradiometer (PR735) and Keithley 2400 sourcemeter unit under ambient atmosphere at room temperature.

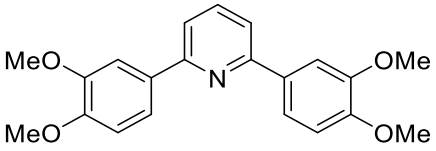
Synthesis

Cyclometallating Ligands



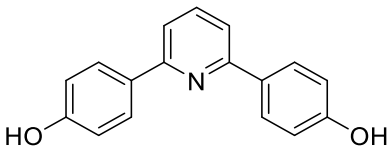
2,6-Bis(4-methoxyphenyl)pyridine (1): 2,6-dibromopyridine (2.59 g, 10.9 mmol) and 4-methoxyphenyl boronic acid (5.01 g, 32.9 mmol) were added to a flask containing $Pd(OAc)_2$ (13.1 mg, 0.5 mol%) and K_3PO_4 (6.99 g, 32.9 mmol). Ethylene glycol (80 cm^3) was added, and the reaction mixture heated to 80 °C for 1.5 hours with vigorous stirring. The reaction mixture was cooled to room temperature, isolated by filtration and washed with water (150 cm^3), after which it was air dried. The resulting grey solid was dissolved in CH_2Cl_2 and filtered through Celite®. The filtrate was collected and the solvent removed under reduced pressure. The solid, off-white residue was crystallised from ethanol to give the pure product as colourless crystals. 2.16 g (68 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.09 (4H, AA'XX'), 7.73 (1H, t, $^3J_{HH}$ = 7.6 Hz), 7.56 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.0 (4H, AA'XX'), 3.87 (6H, s) ppm; CHN elemental analysis: observed (calculated): %C 78.0 (78.3), %H 5.9 (5.9), %N 4.8 (4.8).



2,6-Bis(3,4-dimethoxyphenyl)pyridine (1): Synthesised as for 2,6-bis(4-methoxyphenyl)-pyridine, using 2,6-dibromopyridine (2.21 g, 9.21 mmol), 3,4-dimethoxyphenyl boronic acid (5.02 g, 27.4 mol) and crystallised from ethanol to give colourless crystals. 2.94 g (91 %).

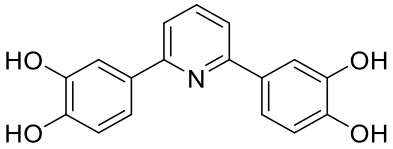
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (2H, d, $^4J_{HH}$ = 2.0 Hz), 7.74 (1H, t, $^3J_{HH}$ = 7.2 Hz), 7.64 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 1.6 Hz), 7.67 (2H, d, $^3J_{HH}$ = 7.6 Hz), 6.97 (2H, d, $^3J_{HH}$ = 8.4 Hz), 4.01 (6H, s), 3.96 (6H, s) ppm. CHN elemental analysis: observed (calculated): %C 71.8 (71.8), %H 6.1 (6.0), %N 4.0 (4.0).



2,6-Bis(4-hydroxyphenyl)pyridine (2): 2,6-bis(4-methoxyphenyl)pyridine (1.52 g, 5.13 mmol) was added to molten pyridinium chloride (7.47 g, 64.6 mmol) at 200 °C and stirred for 16 hours. The still molten mixture was added to distilled water (100 cm^3) and the resulting yellow

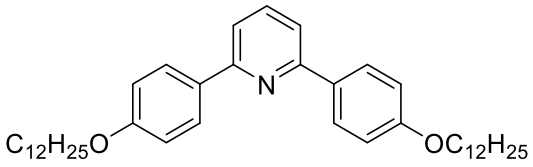
precipitate was isolated by filtration and air-dried. It was used without further purification. 952 mg (71 %).

^{1}H NMR (400 MHz, d_6-DMSO): δ = 9.74 (2H, s), 7.99 (4H, AA'XX'), 7.77 (1H, t, $^3J_{HH}$ = 7.6 Hz), 7.64 (2H, d, $^3J_{HH}$ = 7.6 Hz), 6.85 (4H, AA'XX') ppm.



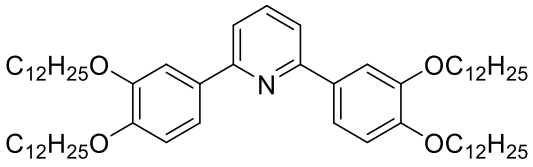
2,6-Bis(3,4-dihydroxyphenyl)pyridine (2): Synthesised as for 2,6-bis(4-hydroxyphenyl)pyridine using 2,6-bis(3,4-dimethoxyphenyl)pyridine (1.21 g, 3.40 mmol). 743 mg (73 %).

^{1}H NMR (400 MHz, d_6-DMSO): δ = 9.20 (2H, s), 9.06 (2H, s), 7.72 (1H, t, $^3J_{HH}$ = 7.6 Hz), 7.63 (2H, d, $^4J_{HH}$ = 2.0 Hz), 7.55 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.41 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.0 Hz), 6.82 (2H, d, $^3J_{HH}$ = 8.0 Hz) ppm.



2,6-bis(4-dodecyloxyphenyl)pyridine (3): 2,6-bis(4-hydroxyphenyl)pyridine (0.903 g, 3.42 mmol), 1-bromododecane (2.06 cm^3, 8.63 mmol), K_2CO_3 (1.41 g, 10.2 mmol) were heated to 90 °C in DMF (50 cm^3) for 16 hours. The reaction mixture was cooled to room temperature and the solid isolated by filtration and washed with water (150 cm^3) and acetone (60 cm^3) and left to air dry. 1.67 g (82 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.06 (4H, AA'XX'), 7.71 (1H, t, $^3J_{HH}$ = 7.6 Hz), 7.55 (2H, d, $^3J_{HH}$ = 7.6 Hz), 6.98 (4H, AA'XX'), 4.0 (4H, t, $^3J_{HH}$ = 6.8 Hz), 1.79 (4H, m), 1.47 (4H, m), 1.21 (32H, broad m), 0.87 (6H, t, $^3J_{HH}$ = 7.2 Hz) ppm; CHN elemental analysis: observed (calculated): %C 82.0 (82.0), %H 10.1 (10.3), %N 2.3 (2.3)



2,6-Bis(3,4-bis-dodecyloxyphenyl)pyridine (3): Synthesised as for 2,6-bis(4-dodecyloxyphenyl)pyridine using 2,6-bis(3,4-dihydroxyphenyl)pyridine (1.02 g, 3.41 mmol), 1-bromododecane (5.22 cm^3, 21.6 mmol), K_2CO_3 (5.91 g, 42.6 mmol). 2.27 g (70 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (2H, d, $^4J_{HH}$ = 2.0 Hz), 7.71 (1H, t, $^3J_{HH}$ = 7.6 Hz), 7.61 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.4 Hz), 7.55 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.95 (2H, d, $^3J_{HH}$ = 8.4 Hz), 4.11 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz) 1.84 (8H, m), 1.47 (8H, m), 1.24 (64H, broad m), 0.87 (6H, t,

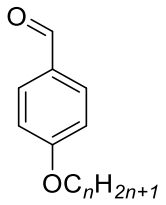
$^3J_{HH}$ = 6.8 Hz), 0.87 (6H, t, $^3J_{HH}$ = 7.2 Hz) ppm; CHN elemental analysis: observed (calculated): %C 80.4 (80.6), %H 11.2 (11.3), %N 1.5 (1.5)

Phenylalkynyl Ligands

4-Ethynyl-1,2-bisalkoxybenzene ligands were synthesised *via* literature procedure, 4-ethynyl-1-alkoxybenzene and 5-ethynyl-1,2,3-tri(alkoxy)benzene ligands synthesised partially by modification of the same.[7]

General Procedure for the Synthesis of 4-Octyloxybenzaldehyde:

Under at atmosphere of nitrogen, the appropriate 1-bromoalkane (1.1 eq.) was added to a flask of 4-hydroxybenzaldehyde (1.0 eq.) and K_2CO_3 (1.1 eq.), along with a catalytic amount of KI. DMF (70 cm^3) was added and the reaction mixture was heated to 90 °C for 16 hours. The reaction mixture was then cooled to room temperature and insoluble salts were removed *via* by filtration and the solvent removed *in vacuo* from the filtrate. The residue was extracted into hexane and washed with 2M NaOH(aq) solution, brine and saturated $LiCl_{(aq)}$ solution, dried over $MgSO_4$ and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel using CH_2Cl_2 as the eluent.



4-Octyloxybenzaldehyde: As above, with 4-hydroxybenzaldehyde (2.99 g, 24.5 mmol), 1-bromooctane (5.95 cm^3, 6.71 g, 34.7 mmol) and K_2CO_3 (4.43 g, 32.0 mmol). 4.71 g. (82%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.88 (1H, s), 7.82 (2H, AA'XX'), 6.99 (2H, AA'XX'), 4.03 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (8H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-Decyloxybenzaldehyde: As above, with 4-hydroxybenzaldehyde (3.00 g, 24.5 mmol), 1-bromodecane (7.62 cm^3, 8.12 g, 36.7 mmol) and K_2CO_3 (6.79 g, 49.1 mmol). 4.81 g. (74%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.87 (1H, s), 7.82 (2H, AA'XX'), 6.99 (2H, AA'XX'), 4.03 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (10H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-Dodecyloxybenzaldehyde: As above, with 4-hydroxybenzaldehyde (2.92 g, 23.7 mmol), 1-bromododecane (8.85 cm^3, 9.19 g, 36.9 mmol) and K_2CO_3 (6.74 g, 48.8 mmol). 3.6 g. (50%).

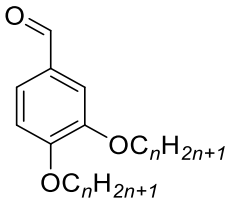
^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.87 (1H, s), 7.82 (2H, AA'XX'), 6.99 (4H, AA'XX'), 4.03 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (12H, m), 0.88 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-Tetradecyloxybenzaldehyde: As above, with 4-hydroxybenzaldehyde (3.02 g, 24.5 mmol), 1-bromotetradecane (11.0 cm^3, 10.3 g, 37.0 mmol) and K_2CO_3 (6.74 g, 48.8 mmol). 4.83 g. (62%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.87 (1H, s), 7.82 (2H, AA'XX'), 6.99 (2H, AA'XX'), 4.03 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (14H, m), 0.88 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

General Procedure for the Synthesis of 3,4-Bis(alkyloxy)benzaldehyde:

Under an atmosphere of nitrogen, the appropriate 1-bromoalkane (2.2 eq.) was added to a flask of 4-hydroxybenzaldehyde (1.0 eq.) and K_2CO_3 (2.2 eq.), along with a catalytic amount of KI. DMF (70 cm^3) was added and the reaction mixture was heated to 90 °C for 16 hours. The reaction mixture was then cooled to room temperature and poured into aqueous 1M HCl**.** The product was extracted into CH_2Cl_2, washed with brine, dried over $MgSO_4$ and the solution concentrated *in vacuo*. The residue was purified by column chromatography on silica gel.



3,4-Bis(octyloxy)benzaldehyde: As above, using 3,4-dihydroxybenzaldehyde (1.52 g, 10.9 mmol), 1-bromooctane (4.21 cm^3, 23.3 mmol) and potassium carbonate (3.32 g, 23.9 mmol), using CH_2Cl_2 as the eluent. 2.50 g. (63 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (1H, s), 7.41 (1H, dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.0 Hz), 7.39 (1H, m), 6.95 (1H, d, $^3J_{HH}$ = 8.2 Hz), 4.08 (2H, t, $^3J_{HH}$ = 6.5 Hz), 4.05 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (16H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

3,4-Bis(decyloxy)benzaldehyde: As above, using 3,4-dihydroxybenzaldehyde (1.98 g, 14.5 mmol), 1-bromooctane (7.32 cm^3, 35.2 mmol) and potassium carbonate (4.50 g, 32.6 mmol), using petroleum ether (40-60):ethyl acetate as the eluent. 5.91 g. (97 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (1H, s), 7.41 (1H, dd, $^3J_{HH}$ = 8.2 Hz), $^4J_{HH}$ = 2.0 Hz), 7.39 (1H, m), 6.95 (1H, d, $^3J_{HH}$ = 8.2 Hz), 4.08 (2H, t, $^3J_{HH}$ = 6.5 Hz), 4.05 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (32H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

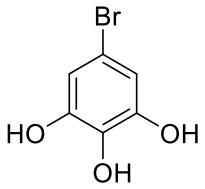
3,4-Bis(dodecyloxy)benzaldehyde: As above, using 3,4-dihydroxybenzaldehyde (2.01 g, 14.5 mmol), 1-bromododecane (7.92 cm^3, 31.9 mmol) and potassium carbonate (4.42 g, 31.9 mmol), using hexane:ethyl acetate (85 : 15) as the eluent. 6.71 g. (97 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (1H, s), 7.41 (1H, dd, $^3J_{HH}$ = 8.2 Hz), $^4J_{HH}$ = 2.0 Hz), 7.39 (1H, m), 6.95 (1H, d, $^3J_{HH}$ = 8.2 Hz), 4.08 (2H, t, $^3J_{HH}$ = 6.5 Hz), 4.05 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (40H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

3,4-Bis(tetradecyloxy)benzaldehyde: As above, using 3,4-dihydroxybenzaldehyde (2.00 g, 14.5 mmol), 1-bromotetradecane (9.50 cm^3, 31.9 mmol), and potassium carbonate (4.41 g, 31.9 mmol), using hexane– ethyl acetate (85 : 15) as the eluent. 6.20 g (77 %).

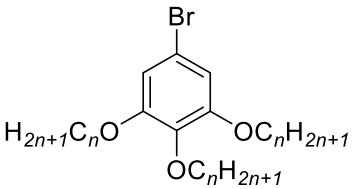
^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (1H, s), 7.41 (1H, dd, $^3J_{HH}$ = 8.2 Hz), $^4J_{HH}$ = 2.0 Hz), 7.39 (1H, m), 6.95 (1H, d, $^3J_{HH}$ = 8.2 Hz), 4.08 (2H, t, $^3J_{HH}$ = 6.5 Hz), 4.05 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (48H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

Synthesis of 3,4,5-Tris(alkoxy)benzaldehyde from Bromoaryl precursor



5-Bromo-1,2,3-trihydroxybenzene: 5-bromo-1,2,3-trimethoxybenzene (15.0 g, 60.7 mmol) in CH_2Cl_2 (50 cm^3) was cooled to -78 °C under an atmosphere of nitrogen. BBr_3 (1M in CH_2Cl_2, 200 cm^3, 200 mmol) was added dropwise and stirred at -78 °C for 1 hour. The solution was warmed to room temperature and stirred for 24 hours. The reaction was quenched with water, and the resulting precipitate removed *via* filtration and washed with CH_2Cl_2. The filtrate was separated and the aqueous layer washed with ethyl acetate (2 x 35 cm^3), brine (35 cm^3) and a further portion of ethyl acetate (35 cm^3). The organic layers were combined, dried over $MgSO_4$ and concentrated *in vacuo* to give the product. 12.1 g (97 %).

^{1}H NMR (400 MHz, CD_3OD): δ = 6.43 (2H, s) ppm; CHN elemental analysis: observed (calculated): %C 35.6 (35.2), %H 2.4 (2.5).



1-Bromo-3,4,5-trioctyloxybenzene: Under an atmosphere of nitrogen, 5-bromo-1,2,3-trihydroxybenzene (2.01 g, 9.80 mmol), 1-bromododecane (9.21 cm^3, 53.2 mmol) and K_2CO_3 (12.4 g, 89.7 mmol) in DMF was heated to 90 °C for 16 hours. The solution was cooled to room temperature and the product extracted into hexane, dried over $MgSO_4$ and the solution concentrated *in vacuo* to give a brown oil. The residue was purified flash chromatography on silica gel with CH_2Cl_2/petroleum ether (40-60) as eluent (7:3). 2.89 g (55 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.67 (2H, s), 3.92 (4H, t, $^3J_{HH}$ = 6.6 Hz), 3.91 (2H, t, $^3J_{HH}$ = 7.2 Hz), 1.78 (4H, m), 1.72 (2H, m), 1.45 (6H, m), 1.26 (24H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.1 Hz) ppm.

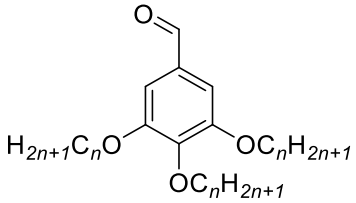
1-Bromo-3,4,5-tridodecyloxybenzene: Under an atmosphere of nitrogen, 5-bromo-1,2,3-trihydroxybenzene (2.00 g, 9.81 mmol), 1-bromododecane (14.0 cm^3, 47.9 mmol) and K_2CO_3 (12.3 g, 88.9 mmol) in DMF was heated to 90 °C for 16 hours. The solution was cooled to room temperature and the solid isolated by filtration. The solid was washed with water (100 cm^3) and

acetone (50 cm^3) to give the product as an off-white solid which was used without further purification. 6.74 g (95 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.67 (2H, s), 3.93 (4H, t, $^3J_{HH}$ = 6.6 Hz), 3.91 (2H, t, $^3J_{HH}$ = 7.2 Hz), 1.78 (4H, m), 1.72 (2H, m), 1.45 (6H, m), 1.26 (48H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.1 Hz) ppm.

General Procedure for Synthesis of 3,4,5-Tris(alkyloxy)benzaldehyde

1-Bromo-3,4,5-trisalkoxybenzene in diethyl ether was cooled to -15 °C under a nitrogen atmosphere. n-BuLi (2.7 M in hexane, 1.0 equiv.) was added dropwise and the solution stirred at -15 °C for 15 minutes. DMF (1.3 equiv.) was added and the reaction mixture warmed to room temperature and stirred for 1 hour, after which HCl (10 %) was added. The solution was separated and the aqueous layer washed with diethyl ether. The organic layers were combined, dried over $MgSO_4$ and concentrated to give a brown oil.



3,4,5-Tris(octyloxy)benzaldehyde: As above, using 1-bromo-3,4,5-tris(octyloxy)benzene (2.11 g, 3.88 mmol), BuLi (2.7 M in hexane, 1.50 cm^3, 3.90 mmol), DMF (0.5 cm^3, 6.51 mmol) and HCl (10 %, 6.79 cm^3) in diethyl ether (70 cm^3). The residue was purified by column chromatography on silica gel with petroleum ether (40-60)/ethyl acetate (9:1) as eluent to give a colourless oil. 911 mg (46 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (1H, s), 7.08 (2H, s), 4.05 (2H, t, $^3J_{HH}$ = 6.6 Hz), 4.03 (4H, t, $^3J_{HH}$ = 6.6 Hz), 1.82 (4H, m), 1.75 (2H, m), 1.47 (6H, m), 1.26 (24H, broad m), 0.87 (9H, m) ppm.

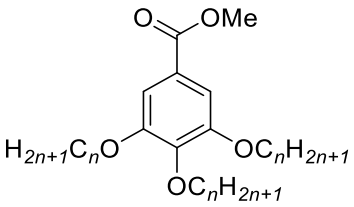
3,4,5-Tris(dodecyloxy)benzaldehyde: As above, using 1-bromo-3,4,5-tris(dodecyloxy)benzene (3.68 g, 5.10 mmol), n-BuLi (2.7 M in hexane, 1.9 cm^3, 5.13 mmol), DMF (0.7 cm^3, 9.0 mmol) and HCl (10 %, 9.0 cm^3) in diethyl ether (100 cm^3). The brown oil crystallised on standing. The residue was purified by column chromatography on silica gel with petroleum ether (40-60)/ethyl acetate (95:5) as eluent to give a colourless oil which crystallised on standing to give a white amorphous solid. 2.61 g (76 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (1H, s), 7.08 (2H, s), 4.05 (2H, t, $^3J_{HH}$ = 6.8 Hz), 4.03 (4H, t, $^3J_{HH}$ = 6.5 Hz), 1.82 (4H, m), 1.75 (2H, m), 1.47 (6H, m), 1.26 (48H, broad m), 0.87 (9H, m) ppm; CHN elemental analysis: observed (calculated): %C 78.2 (78.4), %H 11.9 (11.9).

General Procedure for Synthesis of Methyl 3,4,5-Tris(alkoxy)benzoate

Methyl 3,4,5-trihydroxybenzoate and K_2CO_3 (3.3 equiv.) were heated to reflux in 2-pentanone (80 cm^3). 1-bromoalkane was added and the mixture heated for 24 hours at reflux. The reaction

mixture was cooled to room temperature, filtered through a pad of Celite® and the filtrate concentrated *in vacuo*.



Methyl 3,4,5-tris(decyloxy)benzoate: As above, using methyl 3,4,5-trihydroxybenzoate (3.09 g, 16.8 mmol), 1-bromodecane (11.9 cm^3, 56.8 mmol) and K_2CO_3 (13.5 g, 96.9 mmol). The brown residue was purified by column chromatography on silica gel with CH_2Cl_2 as the eluent to give a colourless oil. 6.02 g (46 %).

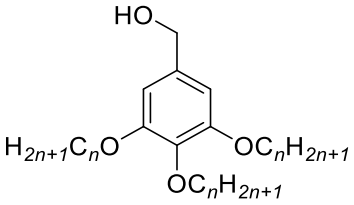
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.25 (2H, s), 4.01 (2H, t, $^3J_{HH}$ = 6.6 Hz), 4.01 (4H, t, $^3J_{HH}$ = 6.6 Hz), 1.80 (4H, m), 1.74 (2H, m), 1.46 (6H, m), 1.26 (36H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 6.9 Hz) ppm.

Methyl 3,4,5-tris(tetradecyloxy)benzoate: As above, using methyl 3,4,5-trihydroxybenzoate (3.10 g, 16.8 mmol), 1-bromotetradecane (16.5 cm^3, 55.4 mmol) and K_2CO_3 (13.4 g, 97.8 mmol). The brown residue was crystallised from ethanol to give a colourless solid. 3.31 g (34 %) ppm.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.25 (2H, s), 4.00 (6H, t, $^3J_{HH}$ = 6.6 Hz), 1.80 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (60H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 6.9 Hz).

General Procedure for Synthesis of 3,4,5-Trialkoxybenzyl Alcohol

Under at atmosphere of dinitrogen, methyl 3,4,5-trialkoxybenzoate was dissolved in dry THF and the mixture cooled to 0 °C. Lithium aluminium hydride (1M in THF, 1 equiv.) was added dropwise with stirring and the mixture was allowed to slowly warm to room temperature and stirred for 16 hours. The reaction was quenched with ethyl acetate (20 cm^3), followed by ethanol (20 cm^3) and water (20 cm^3). The volatiles were removed *in vacuo*, the product extracted with CH_2Cl_2, washed with water and dried over $MgSO_4$. The solvent was removed *in vacuo* to give a light brown oil.



3,4,5-Tris(decyloxy)benzyl alcohol: As above, with methyl 3,4,5-tris(decyloxy)benzoate (5.87 g, 9.68 mmol) and lithium aluminium hydride (1M in THF, 10.0 cm^3, 10.0 mmol) in THF (100 cm^3). The residue was crystallised from hexane to give a colourless solid. 2.86 g (52 %).

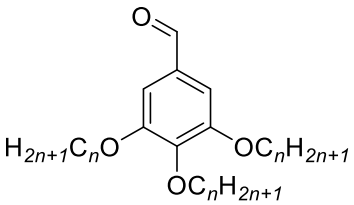
^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.56 (2H, s), 4.59 (2H, d, $^3J_{HH}$ = 6.0 Hz) 3.97 (4H, t, $^3J_{HH}$ = 6.6 Hz), 3.93 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.80 (4H, m), 1.74 (2H, m), 1.46 (6H, m), 1.26 (36H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 6.9 Hz) ppm.

3,4,5-Tris(tetradecyloxy)benzyl alcohol: As above, with methyl 3,4,5-tris(tetradecyloxy)benzoate (2.27 g, 2.91 mmol) and lithium aluminium hydride (1M in THF, 2.90 cm^3, 2.89 mmol) in THF (50 cm^3). The residue was crystallised from ethanol to give a colourless solid. 1.05 g (49 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.56 (2H, s), 4.59 (2H, d, $^3J_{HH}$ = 6.0 Hz) 3.97 (4H, t, $^3J_{HH}$ = 6.6 Hz), 3.93 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.80 (4H, m), 1.74 (2H, m), 1.46 (6H, m), 1.26 (60H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 6.9 Hz) ppm.

General Procedure for Synthesis of 3,4,5-Tris(alkoxy)benzaldehyde from the Methyl Ester

3,4,5-Trialkoxybenzyl alcohol was dissolved in CH_2Cl_2. Manganese dioxide (10.0 equiv.), was added and the mixture stirred at room temperature for 36 hours. $MgSO_4$ was added and the mixture stirred for 15 minutes. The solution was filtered through Celite® and the filtrate concentrated *in vacuo* to give a light yellow oil.



3,4,5-Tris(decyloxy)benzaldehyde: As above, using 3,4,5-tris(decyloxy)benzyl alcohol (2.77 g, 4.81 mmol) and manganese dioxide (4.21 g, 48.3 mmol) in CH_2Cl_2 (130 cm^3). The residue was purified by column chromatography on silica gel using CH_2Cl_2 as the eluent to give a colourless oil. 2.41 g (88 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (1H, s), 7.08 (2H, s), 4.05 (2H, t, $^3J_{HH}$ = 6.8 Hz), 4.03 (4H, t, $^3J_{HH}$ = 6.5 Hz), 1.82 (4H, m), 1.75 (2H, m), 1.47 (6H, m), 1.26 (36H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 6.9 Hz).

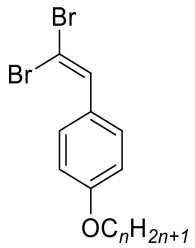
3,4,5-Tris(tetradecyloxy)benzaldehyde: As above, using 3,4,5-tris(tetradecyloxy)benzyl alcohol (952 mg, 1.31 mmol) and manganese dioxide (1.11 g, 12.7 mmol) in CH_2Cl_2 (100 cm^3). The residue was crystallised from acetone to give a colourless, waxy solid. 923 mg (97 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (1H, s), 7.08 (2H, s), 4.05 (2H, t, $^3J_{HH}$ = 6.8 Hz), 4.03 (4H, t, $^3J_{HH}$ = 6.5 Hz), 1.82 (4H, m), 1.75 (2H, m), 1.47 (6H, m), 1.26 (60H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 6.9 Hz) ppm.

General Procedure for Synthesis of 4-(2,2-dibromovinyl)-1-(alkyloxy)benzene, 4-(2,2-dibromovinyl)-1,2-bis(alkyloxy)benzene and 5-(2,2-dibromovinyl)-1,2,3-tris(alkyloxy)benzene:

Under a nitrogen atmosphere and cooled in an ice bath to 0 °C, a solution of tetrabromomethane (1.3 equiv.) in CH_2Cl_2 (20 cm^3) was added to a solution of triphenylphosphine (2.6 equiv.) in CH_2Cl_2 (60 cm^3), with the temperature maintained below 15 °C. After full addition the mixture was cooled again to 0 °C. A solution of the appropriate (alkyloxy)benzaldehyde and triethylamine (1.0 equiv.) in CH_2Cl_2 was added dropwise and the mixture stirred for 30 minutes. The mixture was warmed to room temperature and poured into hexane (100 cm^3). The mixture was filtered through a Celite® plug and the filtrate concentrated *in vacuo* to give a brown oil which was purified by column chromatography on silica gel.

4-(2,2-Dibromovinyl)-1-(alkyloxy)benzene:



4-(2,2-Dibromovinyl)-1-(octyloxy)benzene: As above, with 4-octyloxybenzaldehyde (4.38 g, 18.8 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (12.9 g, 49.2 mmol) and tetrabromomethane (8.09 g, 24.4 mmol), purified with 7:3 petroleum ether(40-60):DCM as eluent. 3.36 g. (46%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.50 (2H, AA'XX'), 7.40 (1H, s), 6.87 (2H, AA'XX'), 3.96 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (8H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-(2,2-Dibromovinyl)-1-(decyloxy)benzene: As above, with 4-decyloxybenzaldehyde (4.47 g, 17.2 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (12.1 g, 46.1 mmol) and tetrabromomethane (7.61 g, 22.9 mmol), purified with 7:3 petroleum ether(40-60):DCM as eluent. 5.87 g. (82%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49 (4H, AA'XX'), 7.40 (1H, s), 6.87 (4H, AA'XX'), 3.96 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (10H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

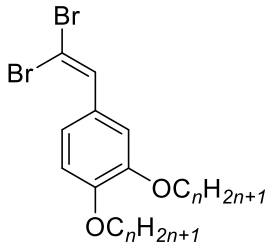
4-(2,2-Dibromovinyl)-1-(dodecyloxy)benzene: As above, with 4-dodecyloxybenzaldehyde (3.59 g, 12.4 mmol) in CH_2Cl_2 (30 cm^3), triphenylphosphine (8.50 g, 32.4 mmol) and tetrabromomethane (5.28 g, 16.0 mmol), purified with 7:3 petroleum ether(40-60):DCM as eluent. 4.90 g. (89%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49 (2H, AA'XX'), 7.40 (1H, s), 6.87 (2H, AA'XX'), 3.96 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (12H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-(2,2-Dibromovinyl)-1-(tetradecyloxy)benzene: As above, with 4-tetradecyloxybenzaldehyde (4.81 g, 15.2 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (10.3 g, 39.3 mmol) and tetrabromomethane (6.58 g, 20.0 mmol), purified with 7:3 petroleum ether(40-60):DCM as eluent. 5.39 g. (76%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49 (2H, AA'XX'), 7.40 (1H, s), 6.87 (2H, AA'XX'), 3.96 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.81 (2H, m), 1.46 (2H, m), 1.24 (14H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-(2,2-Dibromovinyl)-1,2-bis(octyloxy)benzene:



4-(2,2-Dibromovinyl)-1,2-bis(octyloxy)benzene: As above, with 3,4-bis(octyloxy)benzaldehyde (3.40 g, 9.39 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (6.51 g, 24.8 mmol) and carbon tetrabromide (4.09 g, 12.4 mmol), purified using petroleum ether:CH_2Cl_2 (1:1) as the eluent. Yield: 4.28 g (88%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38 (1H, s), 7.19 (1H, d, $^4J_{HH}$ = 2.0 Hz), 7.06 (1H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.0 Hz), 6.84 (1H, d, $^3J_{HH}$ = 8.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.6 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (16H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-(2,2-Dibromovinyl)-1,2-bis(decyloxy)benzene: As above, with 3,4-bis(decyloxy)benzaldehyde (6.01 g, 14.3 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (9.79 g, 37.4 mmol) and carbon tetrabromide (6.21 g, 18.7 mmol), purified using petroleum ether:CH_2Cl_2 (1:1) as the eluent. Yield: 6.34 g (77 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38 (1H, s), 7.18 (1H, d, $^4J_{HH}$ = 2.0 Hz), 7.05 (1H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.0 Hz), 6.84 (1H, d, $^3J_{HH}$ = 8.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.6 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (24H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

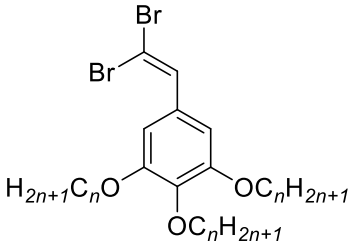
4-(2,2-Dibromovinyl)-1,2-bis(dodecyloxy)benzene: As above, with 3,4-bis(dodecyloxy)benzaldehyde (5.01 g, 10.5 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (7.17 g, 27.4 mmol) and carbon tetrabromide (4.50 g, 13.7 mmol), purified using petroleum ether:CH_2Cl_2 (1:1) as the eluent. Yield: 5.46 g (82 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38 (1H, s), 7.18 (1H, d, $^4J_{HH}$ = 2.0 Hz), 7.05 (1H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.0 Hz), 6.84 (1H, d, $^3J_{HH}$ = 8.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.6 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (32H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-(2,2-Dibromovinyl)-1,2-bis(tetradecyloxy)benzene: As above, with 3,4-bis(decyloxy)benzaldehyde (5.01 g, 9.42 mmol) in CH_2Cl_2 (40 cm^3), triphenylphosphine (6.42 g, 24.5 mmol) and carbon tetrabromide (4.06 g, 12.2 mmol), purified using petroleum ether:CH_2Cl_2 (1:1) as the eluent. The residue was crystallised from ethyl acetate to give a colourless solid. Yield: 4.04 g (24 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38 (1H, s), 7.18 (1H, d, $^4J_{HH}$ = 2.0 Hz), 7.05 (1H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.0 Hz), 6.84 (1H, d, $^3J_{HH}$ = 8.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.6 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (4H, m), 1.46 (4H, m), 1.28 (40H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

5-(2,2-Dibromovinyl)-1,2,3-tris(alkyloxy)benzene:



5-(2,2-Dibromovinyl)-1,2,3-tris(octyloxy)benzene: As above, using tetrabromomethane (527 mg, 1.60 mmol), triphenylphosphine (837 mg, 3.21 mmol) and 3,4,5-tris(octyloxy)benzaldehyde (602 mg, 1.21 mmol) in CH_2Cl_2 (25 cm^3). The residue was purified by column chromatography on silica gel using CH_2Cl_2/ petroleum ether (40-60) (1:1) to give a colourless solid. 650 mg (82 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37 (1H, s), 6.76 (2H, s), 3.96 (2H, t, $^3J_{HH}$ = 6.6 Hz), 3.96 (4H, t, $^3J_{HH}$ = 6.6 Hz), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (24H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm.

5-(2,2-Dibromovinyl)-1,2,3-tris(decyloxy)benzene: As above, using tetrabromomethane (1.65 g, 5.01 mmol), triphenylphosphine (2.61 g, 10.0 mmol) and 3,4,5-tris(decyloxy)benzaldehyde (2.21 g, 3.19 mmol) in CH_2Cl_2 (30 cm^3). The residue was purified by column chromatography on silica gel using petroleum ether (40-60)/ethyl acetate (9:1) to give a colourless solid. 2.28 g (82 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37 (1H, s), 6.76 (2H, s), 3.97 (2H, t, $^3J_{HH}$ = 6.6 Hz), 3.96 (4H, t, $^3J_{HH}$ = 6.6 Hz), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (36H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm.

5-(2,2-Dibromovinyl)-1,2,3-tris(dodecyloxy)benzene: As above, using tetrabromomethane (3.21 g, 9.59 mmol), triphenylphosphine (5.09 g, 19.4 mmol) and 3,4,5-tris(dodecyloxy)benzaldehyde (2.00 g, 4.20 mmol) in CH_2Cl_2 (30 cm^3). The residue was purified by column chromatography on silica gel using CH_2Cl_2/ petroleum ether (40-60) (1:1) to give a colourless solid. 1.19 g (48 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37 (1H, s), 6.76 (2H, s), 3.96 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (4H, t, $^3J_{HH}$ = 6.5 Hz), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (48H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz). CHN elemental analysis: observed (calculated) ppm: %C 64.7 (64.9), %H 9.7 (9.7).

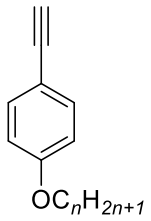
5-(2,2-Dibromovinyl)-1,2,3-tris(tetradecyloxy)benzene: As above, using tetrabromomethane (506 mg, 1.50 mmol), triphenylphosphine (809 mg, 3.12 mmol) and 3,4,5-tris(tetradecyloxy)benzaldehyde (882 mg, 1.22 mmol) in CH_2Cl_2 (25 cm^3). The residue was purified by column chromatography on silica gel using CH_2Cl_2/ petroleum ether (40-60) (1:1) to give a colourless solid. 854 mg (81 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37 (1H, s), 6.76 (2H, s), 3.96 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (4H, t, $^3J_{HH}$ = 6.5 Hz), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (60H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm.

General Procedure for Synthesis of 1-alkoxy-4-ethynylbenzene, 1,2,-bis(alkoxy)-4-ethynylbenzene and 1,2,3-tris(alkoxy)-5-ethynylbenzene:

Under an atmosphere of nitrogen, ethylmagnesium bromide (3M solution in THF) was added dropwise to a solution of the appropriate 2,2-dibromovinyl(alkoxy)benzene in dry THF (60 cm^3). The mixture was stirred for 30 minutes at room temperature, followed by addition of solid ammonium chloride (excess). The solution was poured into hexane (50 cm^3) and filtered through a pad of Celite®. The solvent was removed from the filtrate *in vacuo* and the residue purified by column chromatography on silica gel.

1-Alkoxy-4-ethynylbenzene:



4-Ethynyl-1-(octyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1-(octyloxy)benzene (3.21 g, 8.21 mmol) and ethylmagnesium bromide (3M solution in THF) (5.3 cm^3, 15.9 mmol), purified using 1:1 petroleum ether(40-60):CH_2Cl_2. 1.62 g. (86%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41 (4H, AA'XX'), 6.82 (4H, AA'XX'), 3.95 (2H, t, $^3J_{HH}$ = 6.4 Hz), 2.99 (1H, s), 1.81 (2H, m), 1.46 (2H, m), 1.24 (8H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz); CHN elemental analysis: observed (calculated): %C 83.5 (83.4), %H 9.7 (9.6) ppm.

4-Ethynyl-1-(decyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1-(decyloxy)benzene (5.61 g, 13.4 mmol) and ethylmagnesium bromide (3M solution in THF) (8.9 cm^3, 26.7 mmol), purified using 1:1 petroleum ether(40-60):CH_2Cl_2. 2.71 g. (62%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41 (4H, AA'XX'), 6.82 (4H, AA'XX'), 3.95 (2H, t, $^3J_{HH}$ = 6.4 Hz), 2.99 (1H, s), 1.81 (2H, m), 1.46 (2H, m), 1.24 (10H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz); CHN elemental analysis: observed (calculated) ppm: %C 83.3 (83.7), %H 10.1 (10.1)

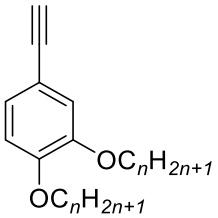
4-Ethynyl-1-(dodecyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1-(dodecyloxy)benzene (4.09 g, 9.20 mmol) and ethylmagnesium bromide (3M solution in THF) (6.2 cm^3, 18.6 mmol), purified using 1:1 petroleum ether(40-60):CH_2Cl_2. 2.52 g. (96%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41 (4H, AA'XX'), 6.82 (4H, AA'XX'), 3.95 (2H, t, $^3J_{HH}$ = 6.4 Hz), 2.99 (1H, s), 1.81 (2H, m), 1.46 (2H, m), 1.24 (12H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm; CHN elemental analysis: observed (calculated): %C 83.6 (83.9), %H 10.4 (10.6).

4-Ethynyl-1-(tetradecyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1-(tetradecyloxy)benzene (4.90 g, 10.4 mmol) and ethylmagnesium bromide (3M solution in THF) (6.9 cm^3, 20.7 mmol), purified using 1:1 petroleum ether(40-60):CH_2Cl_2. 2.91 g. (89%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41 (4H, AA'XX'), 6.82 (4H, AA'XX'), 3.95 (2H, t, $^3J_{HH}$ = 6.4 Hz), 2.99 (1H, s), 1.81 (2H, m), 1.46 (2H, m), 1.24 (14H, m), 0.89 (3H, t, $^3J_{HH}$ = 6.8 Hz) ppm; CHN elemental analysis: observed (calculated): %C 84.1 (84.0), %H 11.2 (10.9).

4-Ethynyl-1,2-bis(alkyloxy)benzene:



4-Ethynyl-1,2-bis(octyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1,2-bis(octyloxy)benzene (3.01 g, 5.82 mmol) and EtMgBr (3 M solution in ether) (3.9 cm^3, 11.7 mmol), purified using CH_2Cl_2 as eluent. 1.50 g (72%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.05 (1H, dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 2.0 Hz), 6.99 (1H, d, $^4J_{HH}$ = 2.0 Hz), 6.79 (1H, d, $^3J_{HH}$ = 8.2 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.7 Hz), 2.98 (1H, s), 1.81 (4H, m), 1.46 (4H, m), 1.28 (16H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-Ethynyl-1,2-bis(decyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1,2-bis(decyloxy)benzene (5.99 g, 10.4 mmol) and EtMgBr (3 M solution in ether) (7.0 cm^3, 20.9 mmol), purified using 7:3 petroleum ether (40-60):CH_2Cl_2 as eluent. 3.61 g (83%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.05 (1H, dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 2.0 Hz), 6.99 (1H, d, $^4J_{HH}$ = 2.0 Hz), 6.79 (1H, d, $^3J_{HH}$ = 8.2 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.7 Hz), 2.98 (1H, s), 1.81 (4H, m), 1.46 (4H, m), 1.28 (24H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

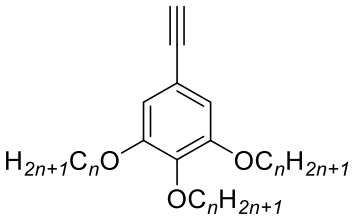
4-Ethynyl-1,2-bis(dodecyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1,2-bis(dodecyloxy)benzene (4.51 g, 7.12 mmol) and EtMgBr (3 M solution in ether) (4.8 cm^3, 14.4 mmol), purified using CH_2Cl_2 as eluent. 3.10 g (93%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.05 (1H, dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 2.0 Hz), 6.99 (1H, d, $^4J_{HH}$ = 2.0 Hz), 6.79 (1H, d, $^3J_{HH}$ = 8.2 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.7 Hz), 2.98 (1H, s), 1.81 (4H, m), 1.46 (4H, m), 1.28 (32H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

4-Ethynyl-1,2-bis(tetradecyloxy)benzene: As above, using 4-(2,2-dibromovinyl)-1,2-bis(tetradecyloxy)benzene (3.00 g, 4.37 mmol) and EtMgBr (3 M solution in ether) (2.9 cm^3, 8.69 mmol), purified using CH_2Cl_2 as eluent. 2.21 g (93%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.05 (1H, dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 2.0 Hz), 6.99 (1H, d, $^4J_{HH}$ = 2.0 Hz), 6.79 (1H, d, $^3J_{HH}$ = 8.2 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.7 Hz), 2.98 (1H, s), 1.81 (4H, m), 1.46 (4H, m), 1.28 (40H, m), 0.89 (6H, t, $^3J_{HH}$ = 6.8 Hz) ppm.

5-Ethynyl-1,2,3-tris(alkyloxy)benzene:



5-Ethynyl-1,2,3-tris(octyloxy)benzene: As above, using 5-(2,2-dibromovinyl)-1,2,3-tris(octyloxy)benzene (452 mg, 703 μmol) and ethylmagnesium bromide (3M solution in ether) (0.6 cm^3, 1.80 mmol), purified using petroleum ether(40-60)/CH_2Cl_2 (7:3) as eluent to give a light yellow oil. 254 mg (75 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.69 (2H, s), 3.95 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.94 (4H, t, $^3J_{HH}$ = 6.5 Hz), 2.99 (1H, s), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (24H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm.

5-Ethynyl-1,2,3-tris(decyloxy)benzene: As above, using 5-(2,2-dibromovinyl)-1,2,3-tris(decyloxy)benzene (1.89 g, 2.61 mmol) and ethylmagnesium bromide (3M solution in ether) (0.86 cm^3, 2.60 mmol), purified using petroleum ether(40-60)/CH_2Cl_2 (9:1) as eluent to give a colourless solid. 1.10 g (76 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.69 (2H, s), 3.95 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.94 (4H, t, $^3J_{HH}$ = 6.5 Hz), 2.99 (1H, s), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (36H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm.

5-Ethynyl-1,2,3-tris(dodecyloxy)benzene: As above, using 5-(2,2-dibromovinyl)-1,2,3-tris(dodecyloxy)benzene (1.32 g, 2.11 mmol) and ethylmagnesium bromide (3M solution in

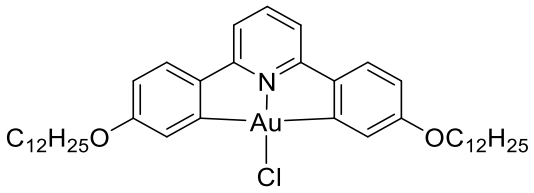
ether) (0.8 cm^3, 2.40 mmol), purified using petroleum ether(40-60)/CH_2Cl_2 (7:3) as eluent to give a colourless solid. 292 mg (34 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.69 (2H, s), 3.95 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.94 (4H, t, $^3J_{HH}$ = 6.5 Hz), 2.99 (1H, s), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (48H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm. CHN elemental analysis: observed (calculated): %C 80.5 (80.7), %H 12.1 (12.0)

5-Ethynyl-1,2,3-tris(tetradecyloxy)benzene: As above, using 5-(2,2-dibromovinyl)-1,2,3-tris(tetradecyloxy)benzene (893 mg, 1.02 mmol) and ethylmagnesium bromide (3M solution in ether) (0.66 cm^3, 2.02 mmol), purified using petroleum ether(40-60)/CH_2Cl_2 (7:3) as eluent to give a colourless solid. 411 mg (57 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.69 (2H, s), 3.95 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.94 (4H, t, $^3J_{HH}$ = 6.5 Hz), 2.99 (1H, s), 1.79 (4H, m), 1.73 (2H, m), 1.46 (6H, m), 1.26 (60H, broad m), 0.88 (9H, t, $^3J_{HH}$ = 7.0 Hz) ppm.

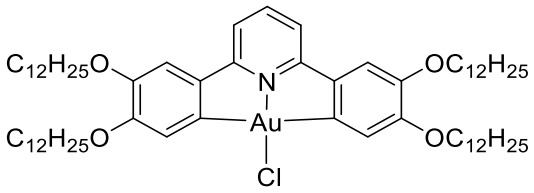
Chlorogold(III) Complexes



5: $Hg(OAc)_2$ (5.02 g, 15.7 mmol) and 2,6-bis(4-(dodecyloxy)phenyl)pyridine (1.88 g, 3.31 mmol) were heated under vigorous reflux in ethanol (500 cm^3) for 24 hours. The solution was cooled to 50 ^oC and a solution of LiCl (265 mg, 6.20 mmol) in methanol (50 cm^3) was added. The resulting mixture was allowed to stir for 15 min. The reaction mixture cooled to room temperature and was then added to distilled water (200 cm^3) and filtered. The precipitate was washed with copious amounts of water and air-dried. The dried precipitate was dissolved in the minimum amount of boiling $CHCl_3$ and filtered through Celite®, after which the solvent was removed from the filtrate under reduced pressure. The residue was crystallised from $CHCl_3$ and acetone, the resulting precipitate removed *via* filtration and the filtrate concentrated *in vacuo*. The residue used without further purification. $K[AuCl_4]$ (800 mg, 2.12 mmol) and the mixed product (2.81 g, 73.5% estimated **4**) were heated in acetonitrile (400 cm^3) under reflux for 24 hours. The reaction mixture was then cooled and added to distilled water (150 cm^3) and isolated by filtration. The solid was washed with acetone (50 cm^3) and air-dried. The product was further purified by flash chromatography on silica gel using petroleum ether/chloroform as eluent (3:2), and crystallised from CH_2Cl_2/ethyl acetate. 674 mg (26%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.69 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.43 (2H, d, $^4J_{HH}$ = 2.8 Hz), 7.42 (2H, d, $^3J_{HH}$ = 8.4 Hz), 7.16 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.7 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.4 Hz), 4.05 (4H, t, $^3J_{HH}$

= 6.4 Hz), 1.79 (4H, m), 1.47 (4H, m), 1.21 (32H, broad m), 0.87 (6H, t, $^3J_{HH}$ = 7.2 Hz) ppm; CHN elemental analysis: observed (calculated): %C 59.0 (59.3), %H 7.1 (7.2), %N 1.5 (1.7).

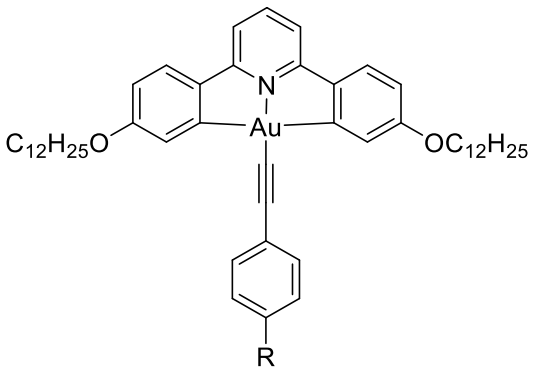


14: $Hg(OAc)_2$ (10.5 g, 32.9 mmol) and 2,6-bis(3,4-bis(dodecyloxy)phenylpyridine (8.02 g, 8.19 mmol) were heated under vigorous reflux in ethanol (500 cm^3) for 24 hours. The solution was cooled to 50 °C and a solution of LiCl (265 mg, 6.21 mmol) in methanol (50 cm^3) was added. The resulting mixture was allowed to stir for 15 min. The reaction mixture was then cooled to room temperature and added to distilled water (200 cm^3) and filtered. The precipitate was washed with copious amounts of water and air-dried. The mercurated complex, **4**, was used without further purification. $K[AuCl_4]$ (720 mg, 2.11 mmol) and the mixed product (2.40 g) were heated in an acetonitrile/chloroform (1:1) mixture (400 cm^3) under reflux for 24 hours. The reaction mixture was cooled and concentrated *in vacuo*. The residue was treated with acetonitrile and the insoluble material isolated *via* filtration. The solid was crystallised from CH_2Cl_2 and the resulting solid isolated by filtration, then further crystallised from CH_2Cl_2 and hexane resulting in the pure product as a vibrantly yellow solid. 1.29 g (13%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.65 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.38 (2H, s), 7.06 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.99 (2H, s), 4.13 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.98 (4H, t, $^3J_{HH}$ = 6.8 Hz), 1.79 (8H, m), 1.47 (8H, m), 1.21 (64H, broad m), 0.87 (12H, t, $^3J_{HH}$ = 7.2 Hz) ppm; CHN elemental analysis: observed (calculated): %C 65.1 (64.8), %H 9.2 (9.0), %N 1.1 (1.2).

General Procedure for Gold(III) Alkynyl Complexes

The [Au(C^N^C)Cl] precursor (5 or 16) and CuI (10 mol%) were added to a 3-necked flask which was placed under N_2. Dry, degassed dichloromethane (40 cm^3) was added, followed by the appropriate acetylene (2.5 eq.) and triethylamine (45 mol%). The reaction mixture was stirred at room temperature for 5 h under a N_2 atmosphere, after which the reaction mixture was filtered through a pad of Celite and the solvent was removed *in vacuo*. The residue was purified by flash chromatography on silica gel and subsequently crystallised from acetone or $CHCl_3$/acetonitrile.



R = H or C_nH_{2n+1}

6a: As above, using **5** (302 mg, 63 μmol) and phenylacetylene (0.06 cm^3, 542 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), crystallised from $CHCl_3$/acetonitrile. 247 mg (77%).

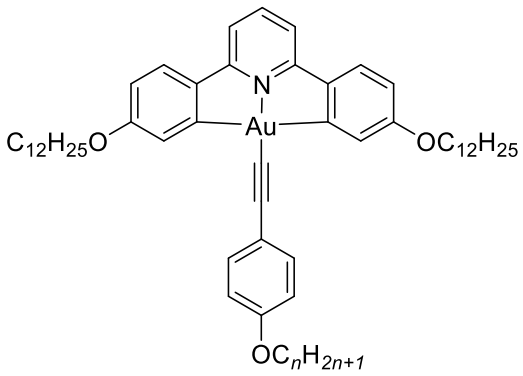
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.66 (2H, d, $^4J_{HH}$ = 2.8 Hz), 7.60 (2H, m), 7.48 (2H, d, $^3J_{HH}$ = 8.4 Hz), 7.31 (3H, m), 7.21 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.71 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.4 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz), 1.79 (4H, m), 1.47 (4H, m), 1.21 (32H, broad m), 0.87 (6H, t, $^3J_{HH}$ = 7.2 Hz) ppm. MS m/z (APCI+): 896.47 (calculated 896.0). CHN elemental analysis: observed (calculated): %C 65.2 (65.7), %H 7.0 (7.2), %N 1.6 (1.6)

6b: As above, using **5** (201 mg, 263 μmol) and 1-ethynyl-4-pentylbenzene (0.07 cm^3, 362 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), crystallised from $CHCl_3$/acetonitrile. 154 mg (66%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.67 (2H, d, $^4J_{HH}$ = 2.8 Hz), 7.51 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.48 (2H, d, $^3J_{HH}$ = 8.4 Hz), 7.21 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.14 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.71 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.4 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz), 2.61 (2H, t, $^3J_{HH}$ = 8.0 Hz) 1.80 (4H, m), 1.63 (2H, m), 1.47 (4H, m), 1.33 (4H, m), 1.21 (32H, broad m), 0.87 (6H, t, $^3J_{HH}$ = 7.2 Hz), 0.87 (3H, m) ppm. MS m/z (APCI+): 966.54 (calc. 966.14); CHN elemental analysis: observed (calculated): %C 67.1 (67.1), %H 7.8 (7.7), %N 1.4 (1.5).

6c: As above, using **5** (203 mg, 264 μmol) and 1-ethynyl-4-octylbenzene (0.09 cm^3, 362 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), crystallised from $CHCl_3$/acetonitrile. 172 mg (71%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.67 (2H, d, $^4J_{HH}$ = 2.8 Hz), 7.51 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.48 (2H, d, $^3J_{HH}$ = 8.4 Hz), 7.21 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.14 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.71 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.4 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz), 2.61 (2H, t, $^3J_{HH}$ = 8.0 Hz), 1.80 (4H, m), 1.63 (2H, m), 1.47 (4H, m), 1.31 (10H, m), 1.21 (32H, broad m), 0.87 (6H, t, $^3J_{HH}$ = 7.2 Hz), 0.87 (3H, m) ppm. MS m/z (APCI+): 1008.59 (Calc. 1008.22). CHN elemental analysis: observed (calculated): %C 67.5 (67.90), %H 7.9 (8.0), %N 1.3 (1.4).



7a: Synthesised as above using **5**, (79.1 mg, 102 μmol) and 4-ethynyl-1-(octyloxy)benzene (44.1 mg, 192 μmol), purified using petroleum ether/CH_2Cl_2 (initially 7:3, followed by 1:1) as eluent, crystallised from $CHCl_3$/acetonitrile. 64.2 mg (66 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.63 (2H, d, $^4J_{HH}$ = 2.7 Hz), 7.52 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 7.45 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.18 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.85 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 6.68 (2H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.6 Hz), 4.04 (4H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.80 (6H, m), 1.46 (6H, m), 1.27 (40H, broad m), 0.88 (9H, m) ppm; MS m/z (APCI+): 1024.58 (calc. 1024.22); CHN elemental analysis: observed (calculated): %C 66.6 (66.8), %H 7.7 (7.9), %N 1.2 (1.4).

7b: Synthesised as above using **5**, (69.4 mg, 82.1 μmol) and 4-ethynyl-1-(decyloxy)benzene (44.1 mg, 152 μmol), purified using petroleum ether/CH_2Cl_2 (initially 7:3, followed by 1:1) as eluent, crystallised from $CHCl_3$/acetonitrile. 84.2 mg (95 %).

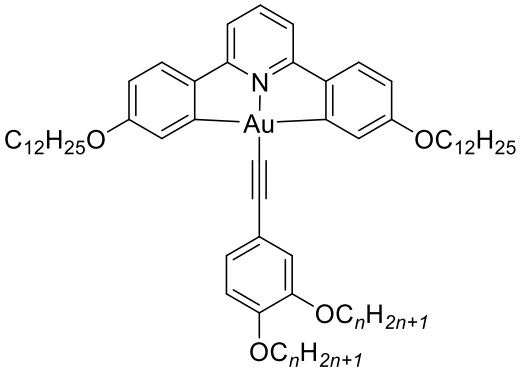
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.7 Hz), 7.52 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 7.46 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.19 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.86 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 6.69 (2H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.6 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.80 (6H, m), 1.46 (6H, m), 1.27 (44H, broad m), 0.88 (9H, m) ppm; MS m/z (APCI+): 1052.62 (calc. 1052.27); CHN elemental analysis: observed (calculated): %C 67.5 (67.3), %H 7.6 (8.0), %N 1.5 (1.3).

7c: Synthesised as above using **5**, (62.5 mg, 803 μmol) and 4-ethynyl-1-(dodecyloxy)benzene (41.9 mg, 132 μmol), purified using petroleum ether/CH_2Cl_2 (initially 7:3, followed by 1:1) as eluent, crystallised from $CHCl_3$/acetonitrile. 79.1 mg (97 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.7 Hz), 7.52 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 7.46 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.19 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.85 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 6.70 (2H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.6 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.80 (6H, m), 1.46 (6H, m), 1.27 (48H, broad m), 0.88 (9H, m) ppm; MS m/z (APCI+): 1080.65 (calc. 1080.32); CHN elemental analysis: observed (calculated): %C 67.8 (67.4), %H 8.1 (8.2), %N 1.4 (1.3).

7d: Synthesised as above using **5**, (80.2 mg, 105 μmol) and 4-ethynyl-1-(tetradecyloxy)benzene (60.1 mg, 183 μmol), purified using petroleum ether/CH_2Cl_2 (initially 7:3, followed by 1:1) as eluent, crystallised from $CHCl_3$/acetonitrile. 83.2 mg (78 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.7 Hz), 7.52 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 7.46 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.19 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.85 (2H, AA'XX', $^3J_{HH}$ = 8.6 Hz), 6.70 (2H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.6 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.7 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.80 (6H, m), 1.46 (6H, m), 1.27 (52H, broad m), 0.88 (9H, m) ppm; MS m/z (APCI+): 1108.68 (calc. 1108.38); CHN elemental analysis: observed (calculated): %C 67.9 (68.3), %H 8.3 (8.4), %N 1.2 (1.3).



8a: Synthesised as above using **5** (118 mg, 142 μmol) and 4-ethynyl-1,2-bisoctyloxybenzene (132 mg, 368 μmol), purified using petroleum ether/CH_2Cl_2 as eluent (1:1), crystallised from acetone. 128 mg (75%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.64 (2H, d, $^4J_{HH}$ = 2.2 Hz), 7.45 (2H, d, $^3J_{HH}$ = 8.6 Hz), 7.18 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.15 (2H, m), 6.83 (1H, d, $^3J_{HH}$ = 8.0 Hz), 6.69 (2H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.6 Hz), 4.04 (4H, t, $^3J_{HH}$ = 6.6 Hz), 4.02 (2H, t, $^3J_{HH}$ = 6.7 Hz), 4.01 (2H, t, $^3J_{HH}$ = 6.7 Hz), 1.81 (8H, m), 1.46 (8H, m), 1.25 (48H, broad m), 0.88 (12H, m) ppm. MS m/z (APCI+): 1152.71 (calc. 1152.43). CHN elemental analysis: observed (calculated): %C 67.4 (67.7), %H 8.7 (8.4), %N 1.4 (1.2).

8b: Synthesised as above using **5** (117 mg, 141 μmol) and 4-ethynyl-1,2-bisdecyloxybenzene (151 mg, 362 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), followed by a second column with CH_2Cl_2 as the eluent, crystallised from acetone. 103 mg (61%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.5 Hz), 7.46 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.19 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.15 (2H, m), 6.82 (1H, d, $^3J_{HH}$ = 8.0 Hz), 6.70 (2H, dd, $^3J_{HH}$ = 8.5 Hz, $^4J_{HH}$ = 2.6 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.6 Hz), 4.02 (2H, t, $^3J_{HH}$ = 6.7 Hz), 4.01 (2H, t, $^3J_{HH}$ = 6.7 Hz), 1.81 (8H, m), 1.46 (8H, m), 1.25 (56H, broad m), 0.88 (12H, m) ppm; MS m/z (APCI+): 1208.77 (calc. 1208.53); CHN elemental analysis: observed (calculated): %C 67.7 (68.6), %H 8.6 (8.7), %N 1.0 (1.2). The CHN data for this complex are outside of the bounds required to confirm purity. However, the 1H NMR spectrum was clean and fully assigned and the LC

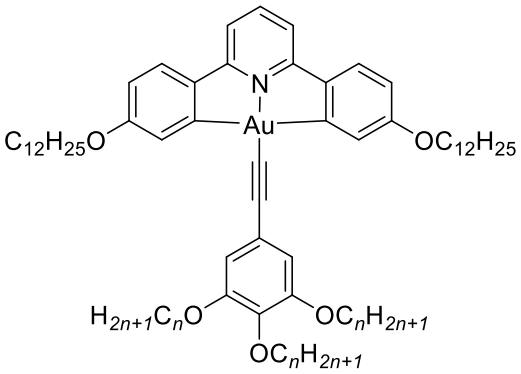
properties do not deviate from that which might be expected. We also note that melting and clearing points were not unduly broad and also that this complex was not studied in detail for its photophysical properties. As such, we do not believe that the small margin of error for this one complex is significant.

8c: Synthesised as above using **5** (98.1 mg, 110 μmol) and 4-ethynyl-1,2-bisdodecyloxybenzene (141 mg, 303 μmol), purified using petroleum ether/CH_2Cl_2 as eluent (1:1), crystallised from acetone. 93.1 mg (66 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.67 (2H, d, $^4J_{HH}$ = 2.6 Hz), 7.48 (2H, d, $^3J_{HH}$ = 8.6 Hz), 7.21 (2H, d, $^3J_{HH}$ = 8.1 Hz), 7.15 (2H, m), 6.82 (1H, d, $^3J_{HH}$ = 8.2 Hz), 6.72 (2H, dd, $^3J_{HH}$ = 8.6 Hz, $^4J_{HH}$ = 2.7 Hz), 4.06 (4H, t, $^3J_{HH}$ = 6.6 Hz), 4.02 (2H, t, $^3J_{HH}$ = 6.6 Hz), 4.01 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (8H, m), 1.46 (8H, m), 1.25 (64H, broad m), 0.88 (12H, m) ppm. MS m/z (APCI+): 1264.83 (calc. 1264.64); CHN elemental analysis: observed (calculated): %C 69.2 (69.3), %H 9.1 (8.9), %N 1.0 (1.1).

8d: Synthesised as above using **5** (97.2 mg, 113 μmol) and 4-ethynyl-1,2-bistetradecyloxybenzene (158 mg, 302 μmol), purified using petroleum ether/CH_2Cl_2 as eluent (1:1), crystallised from acetone. 99.1 mg (65 %)**.**

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (1H, t, $^3J_{HH}$ = 8.1 Hz), 7.67 (2H, d, $^4J_{HH}$ = 2.5 Hz), 7.48 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.22 (2H, d, $^3J_{HH}$ = 8.1 Hz), 7.15 (2H, m), 6.82 (1H, d, $^3J_{HH}$ = 8.1 Hz), 6.72 (2H, dd, $^3J_{HH}$ = 8.6 Hz, $^4J_{HH}$ = 2.7 Hz), 4.06 (4H, t, $^3J_{HH}$ = 6.6 Hz), 4.02 (2H, t, $^3J_{HH}$ = 6.6 Hz), 4.01 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (8H, m), 1.46 (8H, m), 1.25 (72H, broad m), 0.88 (12H, m) ppm. MS m/z (APCI+): 1320.90 (calc. 1320.75); CHN elemental analysis: observed (calculated): %C 69.5 (70.0), %H 9.2 (9.2), %N 1.0 (1.1)



9a: Synthesised as above using **5** (113 mg, 142 μmol) and 5-ethynyl-1,2,3-trisoctyloxybenzene (98.2 mg, 201 μmol), purified using petroleum ether/ethyl acetate as eluent (7:3), crystallised from acetone. 110 mg (64%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.72 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.3 Hz), 7.49 (2H, d, $^3J_{HH}$ = 8.7 Hz), 7.22 (2H, d, $^3J_{HH}$ = 7.8 Hz), 6.81 (2H, s, $^3J_{HH}$ = 8.0 Hz), 6.72 (2H, dd, $^3J_{HH}$ = 8.7 Hz, $^4J_{HH}$ = 2.6 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.79

(10H, m), 1.47 (10H, m), 1.25 (56H, broad m), 0.87 (15H, m) ppm. MS m/z (APCI+): 1280.83 (calc. 1280.64). CHN elemental analysis: observed (calculated): %C 68.1 (68.5), %H 8.7 (8.8), %N 1.0 (1.1).

9b: Synthesised as above using **5** (132 mg, 159 μmol) and 5-ethynyl-1,2,3-trisdecyloxybenzene (225 mg, 389 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), crystallised from acetone. 156 mg (72 %).

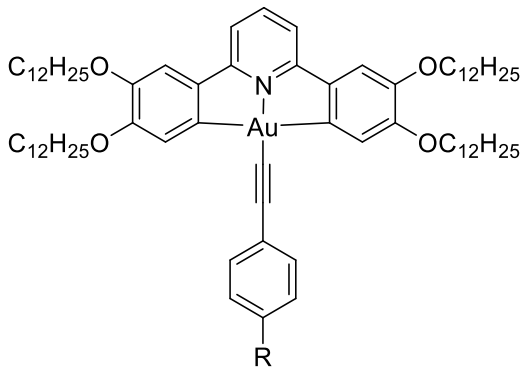
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.7 Hz), 7.49 (2H, d, $^3J_{HH}$ = 8.5 Hz), 7.22 (2H, d, $^3J_{HH}$ = 7.9 Hz), 6.81 (2H, s, $^3J_{HH}$ = 8.0 Hz), 6.72 (2H, dd, $^3J_{HH}$ = 8.6 Hz, $^4J_{HH}$ = 2.7 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.79 (10H, m), 1.47 (10H, m), 1.25 (68H, broad m), 0.87 (15H, m) ppm; MS m/z (APCI+): 1364.92 (calc. 1364.80); CHN elemental analysis: observed (calculated): %C 69.1 (69.5), %H 9.3 (9.2), %N 1.2 (1.0).

9c: Synthesised as above using **5** (85.2 mg, 100 μmol) and 5-ethynyl-1,2,3-tris(dodecyloxy)benzene (102 mg, 152 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), crystallised from acetone. 92.4 mg (62%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.72 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.65 (2H, d, $^4J_{HH}$ = 2.3 Hz), 7.49 (2H, d, $^3J_{HH}$ = 8.7 Hz), 7.22 (2H, d, $^3J_{HH}$ = 7.8 Hz), 6.81 (2H, s), 6.72 (2H, dd, $^3J_{HH}$ = 8.7 Hz, $^4J_{HH}$ = 2.6 Hz), 4.05 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.80 (10H, m), 1.47 (10H, m), 1.25 (80H, broad m), 0.87 (15H, m) ppm. MS m/z (APCI+): 1449.01 (calc. 1448.96). CHN elemental analysis: observed (calculated): %C 70.4 (70.5), %H 9.4 (9.5), %N 0.9 (1.0)

9d: Synthesised as above using **5** (102 mg, 121 μmol) and 5-ethynyl-1,2,3-tris(tetradecyloxy)benzene (222 mg, 299 μmol), purified using petroleum ether/ethyl acetate as eluent (4:1), crystallised from acetone. 165 mg (89 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.64 (2H, d, $^4J_{HH}$ = 2.5 Hz), 7.48 (2H, d, $^3J_{HH}$ = 8.6 Hz), 7.21 (2H, d, $^3J_{HH}$ = 8.0 Hz), 6.81 (2H, s), 6.71 (2H, dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.6 Hz), 4.04 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.97 (2H, t, $^3J_{HH}$ = 6.4 Hz), 1.80 (10H, m), 1.47 (10H, m), 1.25 (92H, broad m), 0.87 (15H, m) ppm.; MS m/z (APCI+): 1533.10 (calc. 1533.12); CHN elemental analysis: observed (calculated): %C 70.8 (71.3), %H 9.5 (9.7), %N 0.7 (0.9).



R = H or C_nH_{2n+1}

10a: Synthesised as above using **14** (201 mg, 161 μmol) and phenylacetylene (0.03 cm^3, 273 μmol), purified using petroleum ether/ethyl acetate as eluent (1:4), crystallised from $CHCl_3$/acetonitrile. 169 mg (80%).

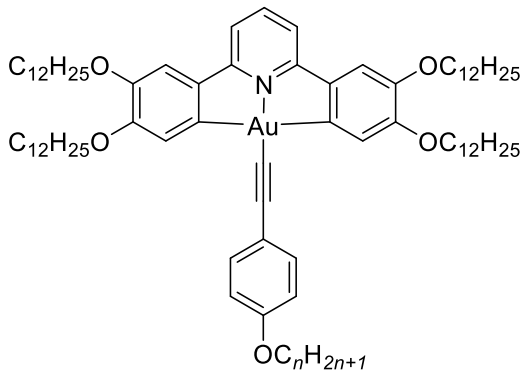
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.61 (2H, s), 7.57 (2H, m), 7.31 (3H, m), 7.14 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.06 (2H, s), 4.14 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.8 Hz), 1.79 (8H, m), 1.47 (8H, m), 1.21 (64H, broad m), 0.87 (12H, t, $^3J_{HH}$ = 7.2 Hz) ppm. MS m/z (APCI+): 1264.84 (calc. 1264.64). CHN elemental analysis: observed (calculated): %C 68.9 (69.3), %H 8.8 (8.9), %N 1.1 (1.1).

10b: Synthesised as above using **14** (150 mg, 132 μmol) and 1-ethynyl-4-pentylbenzene (0.04 cm^3, 203 μmol), purified using petroleum ether/ethyl acetate as eluent (1:4), crystallised from $CHCl_3$/acetonitrile. 135 mg (81%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.66 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.61 (2H, s), 7.48 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.13 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.12 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.05 (2H, s), 4.14 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.8 Hz), 2.60 (2H, t, $^3J_{HH}$ = 7.6 Hz), 1.79 (8H, m), 1.47 (8H, m), 1.61 (2H, m), 1.31 (4H, m), 1.21 (64H, broad m), 0.87 (15H, t, $^3J_{HH}$ = 7.2 Hz), ppm. MS m/z (APCI+): 1334.91 (calc. 1334.91). CHN elemental analysis: observed (calculated): %C 70.1 (70.2), %H 9.4 (9.2), %N 0.9 (1.1)

10c: Synthesised as above using **14** (198 mg, 164 μmol) and 1-ethynyl-4-octylbenzene (0.06 cm^3, 242 μmol), purified using petroleum ether/ethyl acetate as eluent (1:4), crystallised from $CHCl_3$/acetonitrile. 198 mg (86%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.62 (2H, s), 7.48 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.13 (2H, d, $^3J_{HH}$ = 8.4 Hz), 7.12 (2H, d, $^3J_{HH}$ = 8.4 Hz), 7.06 (2H, s), 4.14 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.8 Hz), 2.60 (2H, t, $^3J_{HH}$ = 7.6 Hz), 1.79 (8H, m), 1.47 (8H, m), 1.61 (2H, m), 1.31 (10H, m), 1.21 (64H, broad m), 0.87 (15H, t, $^3J_{HH}$ = 7.2 Hz) ppm; MS m/z (APCI+): 1376.96 (calc. 1376.85); CHN elemental analysis: observed (calculated): %C 70.26 (70.66), %H 9.25 (9.37), %N 0.91 (1.02).



11a: Synthesised as above using **14** (130 mg, 124 μmol) and 4-ethynyl-1-(octyloxy)benzene (63.0 mg, 272 μmol), purified using petroleum ether/ethyl acetate as eluent (9:1) and crystallised from acetone. 121 mg (80 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.6 (2H, s), 7.49 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 7.13 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.06 (2H, s), 6.84 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 4.15 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (2H, t, $^3J_{HH}$ = 6.7 Hz), 1.82 (10H, m), 1.46 (10H, m), 1.25 (72H, broad m), 0.87 (15H, m) ppm. MS m/z (APCI+): 1392.95 (calc. 1392.85). CHN elemental analysis: observed (calculated): %C 69.6 (69.9), %H 9.6 (9.3), %N 1.0 (0.9).

11b: Synthesised as above using **14** (131 mg, 121 μmol) and 4-ethynyl-1-(decyloxy)benzene (70.0 mg, 271 μmol), purified using petroleum ether/ethyl acetate as eluent (9:1) and crystallised from acetone. 135 mg (87 %).

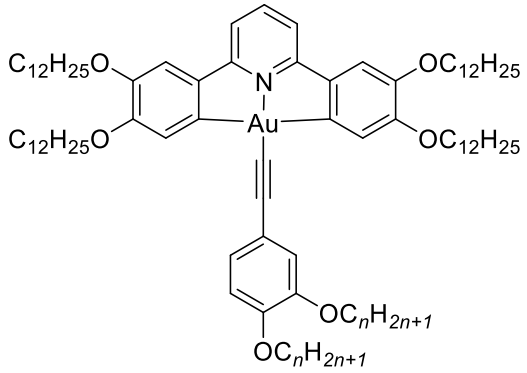
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.62 (2H, s), 7.49 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 7.13 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.06 (2H, s), 6.84 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 4.15 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (2H, t, $^3J_{HH}$ = 6.7 Hz), 1.82 (10H, m), 1.46 (10H, m), 1.25 (78H, broad m), 0.87 (15H, m) ppm; MS m/z (APCI+): 1420.98 (calc. 1420.91). CHN elemental analysis: observed (calculated): %C 70.0 (70.2), %H 9.8 (9.4), %N 0.9 (1.0).

11c: Synthesised as above using **14** (129 mg, 121 μmol) and 4-ethynyl-1-(dodecyloxy)benzene (78.0 mg, 271 μmol), purified using petroleum ether/ethyl acetate as eluent (9:1) and crystallised from acetone. 135 mg (87 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.63 (2H, s), 7.49 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 7.14 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.07 (2H, s), 6.84 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 4.15 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (2H, t, $^3J_{HH}$ = 6.7 Hz), 1.83 (10H, m), 1.46 (10H, m), 1.25 (82H, broad m), 0.88 (15H, m) ppm. MS m/z (APCI+): 1449.02 (calc. 1448.96). CHN elemental analysis: observed (calculated): %C 70.3 (70.5), %H 9.6 (9.5), %N 1.0 (1.0).

11d: Synthesised as above using **14** (131 mg, 110 μmol) and 4-ethynyl-1-(tetradecyloxy)benzene (85.1 mg, 272 μmol), purified using petroleum ether/ethyl acetate as eluent (9:1) and crystallised from acetone. 141 mg (88 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.62 (2H, s), 7.49 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 7.13 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.06 (2H, s), 6.84 (2H, AA'XX', $^3J_{HH}$ = 8.7 Hz), 4.15 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (2H, t, $^3J_{HH}$ = 6.7 Hz), 1.83 (10H, m), 1.46 (10H, m), 1.25 (86H, broad m), 0.88 (15H, m) ppm. MS m/z (APCI+): 1477.05 (calc. 1477.01); CHN elemental analysis: observed (calculated): %C 70.51 (70.75), %H 9.14 (9.55), %N 0.86 (0.95).



12a: Synthesised as above using **14** (118 mg, 101 μmol) and 4-ethynyl-1,2-bis(octyloxy)benzene (92.1 mg, 262 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 87.0 mg (59 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.65 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.60 (2H, s), 7.11 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.11 (1H, m), 7.04 (2H, s), 6.81 (2H, d, $^3J_{HH}$ = 8.2Hz), 4.14 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (12H, m), 1.46 (12H, m), 1.25 (80H, broad m), 0.87 (18H, m) ppm. MS m/z (APCI+): 1521.07 (calc. 1521.07). CHN elemental analysis: observed (calculated): %C 70.0 (70.3), %H 9.7 (9.5), %N 0.9 (0.9).

12b: Synthesised as above using **14** (117 mg, 102 μmol) and 4-ethynyl-1,2-bis(decyloxy)benzene (102 mg, 250 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 104 mg (67%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.61 (2H, s), 7.13 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.12 (1H, m), 7.07 (2H, s), 6.81 (2H, d, $^3J_{HH}$ = 8.2Hz), 4.14 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (6H, t, $^3J_{HH}$ = 6.5 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (12H, m), 1.46 (12H, m), 1.25 (88H, broad m), 0.87 (18H, m). MS m/z (APCI+): 1577.13 (calc. 1577.17)**.** CHN elemental analysis: observed (calculated): %C 70.4 (70.8), %H 9.9 (9.7), %N 0.8 (0.9)**.**

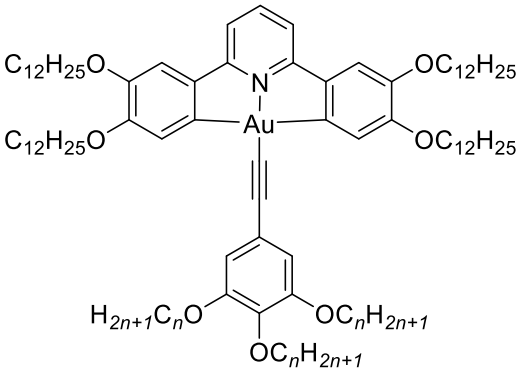
12c: Synthesised as above using **14** (117 mg, 101 μmol) and 4-ethynyl-1,2-bis(dodecyloxy)benzene (72.1 mg, 150 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 133 mg (84%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.66 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.60 (2H, s), 7.12 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.10 (1H, m), 7.05 (2H, s), 6.81 (2H, d, $^3J_{HH}$ = 8.2Hz), 4.14 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (2H, t, $^3J_{HH}$ = 6.5 Hz), 3.99 (6H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (12H, m), 1.46 (12H, m), 1.25 (96H, broad m), 0.87 (18H,

m) ppm. MS m/z (APCI+): 1633.20 (calc. 1633.28). CHN elemental analysis: observed (calculated): %C 71.2 (71.3), %H 10.1 (9.8), %N 0.8 (0.9).

12d: Synthesised as above using **14** (118 mg, 102 μmol) and 4-ethynyl-1,2-bis(tetradecyloxy)benzene (82.1 mg, 162 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 128 mg (78%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.61 (2H, s), 7.13 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.12 (1H, m), 7.06 (2H, s), 6.81 (2H, d, $^3J_{HH}$ = 8.2Hz), 4.14 (4H, t, $^3J_{HH}$ = 6.5 Hz), 4.0 (6H, t, $^3J_{HH}$ = 6.6 Hz), 3.99 (2H, t, $^3J_{HH}$ = 6.6 Hz), 1.81 (12H, m), 1.46 (12H, m), 1.25 (104H, broad m), 0.87 (18H, m) ppm. MS m/z (APCI+): 1689.26 (calc. 1689.38)**.** CHN elemental analysis: observed (calculated): %C 71.6 (71.8), %H 10.4 (10.0), %N 0.9 (0.8)**.**



13a: Synthesised as above using **14** (98.2 mg, 80.3 μmol) and 5-ethynyl-1,2,3-tris(octyloxy)benzene (61.1 mg, 130 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 110 mg (82 %)**.**

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.69 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.60 (2H, s), 7.14 (2H, d, $^3J_{HH}$ = 8.0 Hz), 7.07 (2H, s), 6.78 (2H, s), 4.13 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (4H, t, $^3J_{HH}$ = 6.5 Hz), 3.96 (6H, t, $^3J_{HH}$ = 6.5 Hz), 1.81 (14H, m), 1.46 (14H, m), 1.25 (88H, broad m), 0.87 (21H, m) ppm. MS m/z (APCI+): 1649.19 (calc. 1649.28)**.** CHN elemental analysis: observed (calculated): %C 70.4 (70.6), %H 9.6 (9.9), %N 0.8 (0.9)

13b: Synthesised as above using **14** (131 mg, 111 μmol) and 5-ethynyl-1,2,3-tris(decyloxy)benzene (156 mg, 270 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 159 mg (84 %)**.**

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.59 (2H, s), 7.13 (2H, d, $^3J_{HH}$ = 8.1 Hz), 7.06 (2H, s), 6.78 (2H, s), 4.13 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.99 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.96 (6H, t, $^3J_{HH}$ = 6.8 Hz), 1.81 (14H, m), 1.46 (14H, m), 1.25 (100H, broad m), 0.87 (21H, m) ppm. MS m/z (APCI+): 1733.29 (calc. 1733.44)**.** CHN elemental analysis: observed (calculated): %C 71.3 (71.4), %H 10.0 (10.0), %N 0.8 (0.8).

13c: Synthesised as above using **14** (94.1 mg, 80.2 μmol) and 5-ethynyl-1,2,3-tris(dodecyloxy)benzene (77.0 mg, 120 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 81.1 mg (58 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.69 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.60 (2H, s), 7.14 (2H, d, $^3J_{HH}$ = 8.1 Hz), 7.07 (2H, s), 6.78 (2H, s), 4.13 (4H, t, $^3J_{HH}$ = 6.1 Hz), 4.00 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.96 (6H, t, $^3J_{HH}$ = 6.8 Hz), 1.81 (14H, m), 1.46 (14H, m), 1.25 (112H, broad m), 0.87 (21H, m) ppm. MS m/z (APCI+): 1817.38 (calc. 1817.60). CHN elemental analysis: observed (calculated): %C 71.8 (72.0), %H 10.2 (10.2), %N 0.8 (0.8).

13d: Synthesised as above using **14** (129 mg, 113 μmol) and 5-ethynyl-1,2,3-tris(tetradecyloxy)benzene (205 mg, 280 μmol), purified using petroleum ether/ethyl acetate as eluent (95:5) and crystallised from acetone. 138 mg (71 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (1H, t, $^3J_{HH}$ = 8.0 Hz), 7.60 (2H, s), 7.14 (2H, d, $^3J_{HH}$ = 8.1 Hz), 7.07 (2H, s), 6.78 (2H, s), 4.13 (4H, t, $^3J_{HH}$ = 6.4 Hz), 4.00 (4H, t, $^3J_{HH}$ = 6.4 Hz), 3.96 (6H, t, $^3J_{HH}$ = 6.8 Hz), 1.81 (14H, m), 1.46 (14H, m), 1.25 (124H, broad m), 0.87 (21H, m) ppm. MS m/z (APCI+): 1901.48 (calc. 1901.76). CHN elemental analysis: observed (calculated): %C 72.4 (72.6), %H 10.3 (10.4), %N 0.9 (0.7).

Single Crystal X-ray Structures of Complex 5

The complex shares broadly similar structural parameters with those described in the main manuscript and all may be interrogated using the deposited cif file. The packing motif for these complexes is directly analogous to that illustrated in Chart 2c for complex **6c**.

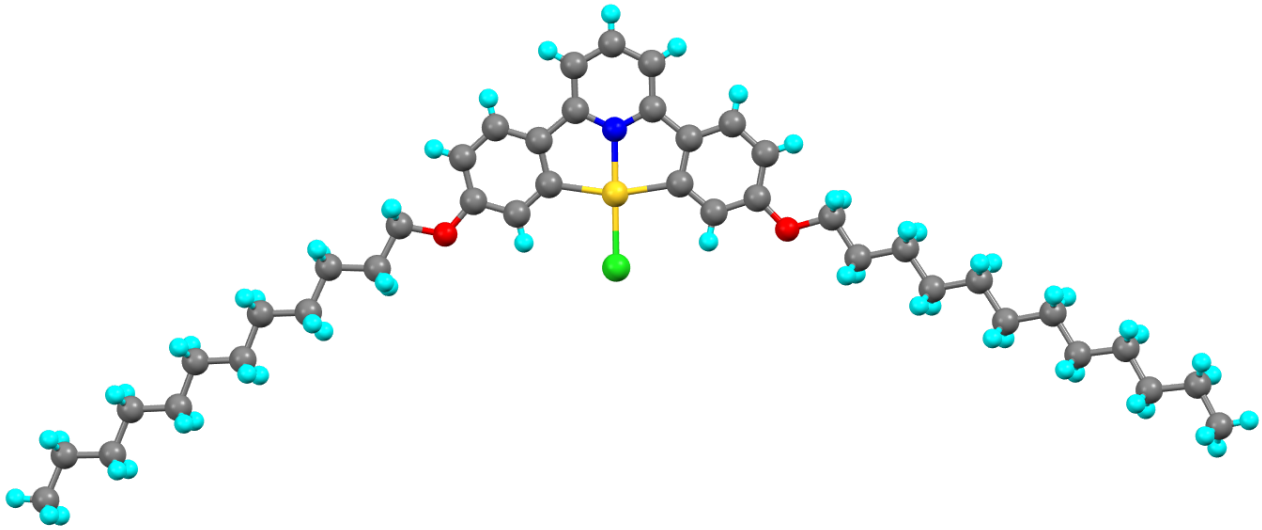


Figure S1 Molecular structure of complex **5**.

Table S1: Summary of X-ray diffraction data for 5, 6a and 6b.

Complex (CCDC No.)	**5** (1991483)	**6a** (1991485)	**6b** (1991484)
Empirical formula	$C_{41}H_{59}AuClNO_2$	$C_{49}H_{63}AuNO_2$	$C_{54}H_{74}AuNO_2$
Formula weight	830.30	894.97	966.10
Temperature/K	110.05(10)	110.05(10)	109.95(10)
Crystal system	triclinic	triclinic	triclinic
Space group	*P*–1	*P*–1	*P*–1
a/Å	10.0951(4)	12.7876(5)	13.7316(4)
b/Å	19.5688(6)	14.4385(7)	13.9293(4)
c/Å	29.1623(8)	23.1895(10)	26.4188(6)
α/°	97.315(2)	87.661(4)	86.646(2)
β/°	95.911(3)	77.162(4)	86.841(2)
γ/°	99.572(3)	86.370(4)	66.516(3)
Volume/Å^3	5589.0(3)	4164.6(3)	4623.9(2)
Z	6	4	4
ρ_{calc} g/cm^3	1.480	1.427	1.388
μ/mm^{-1}	8.336	6.928	6.279
F(000)	2544.0	1836.0	2000.0
Crystal size/mm^3	0.467 × 0.059 × 0.053	0.288 × 0.062 × 0.045	0.214 × 0.079 × 0.058
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θrange for data collection/°	7.142 to 134.154	7.1 to 134.16	6.924 to 134.136
Index ranges	-11 ≤ *h* ≤ 11, -23 ≤ *k* ≤ 23, -23 ≤ *l* ≤ 34	-15 ≤ *h* ≤ 15, -17 ≤ *k* ≤ 17, -19 ≤ *l* ≤ 27	-16 ≤ *h* ≤ 16, -16 ≤ *k* ≤ 16, -24 ≤ *l* ≤ 31
Reflections collected	20716	29085	48560
Independent reflections	15577 [R_{int} = 0.0523, R_{sigma} = 0.0939]	14876 [R_{int} = 0.0451, R_{sigma} = 0.0595]	16525 [R_{int} = 0.0402, R_{sigma} = 0.0427]
Data/ restraints/ parameters	15577/0/1231	14876/0/953	16525/0/1051
Goodness-of-fit on F^2	1.050	1.032	1.044
Final *R* indexes [$I \geq 2\sigma$(I)]	R_1 = 0.0606, wR_2 = 0.1413	R_1 = 0.0599, wR_2 = 0.1516	R_1 = 0.0492, wR_2 = 0.1159
Final *R* indexes [all data]	R_1 = 0.0831, wR_2 = 0.1598	R_1 = 0.0805, wR_2 = 0.1740	R_1 = 0.0663, wR_2 = 0.1301
Largest diff. peak/hole / e Å^{-3}	4.70/-1.87	8.73/-2.46	4.98/-2.33

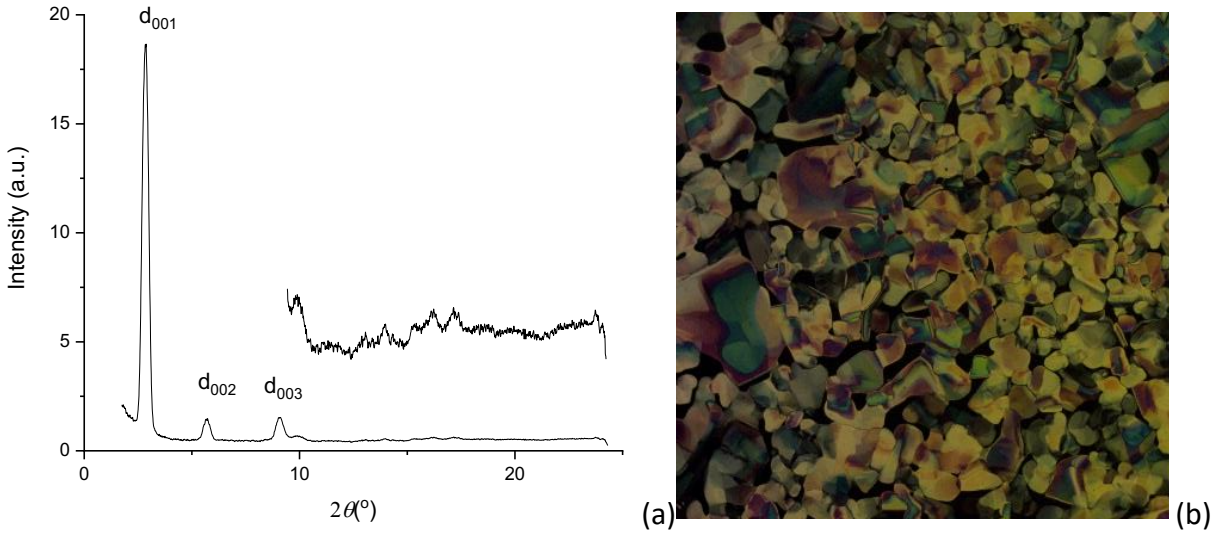


Figure S2a) SAXS pattern for **5** (R = H) at 155.0 °C on cooling from the isotropic liquid and b) optical texture at 158.2 °C on cooling from the isotropic liquid.

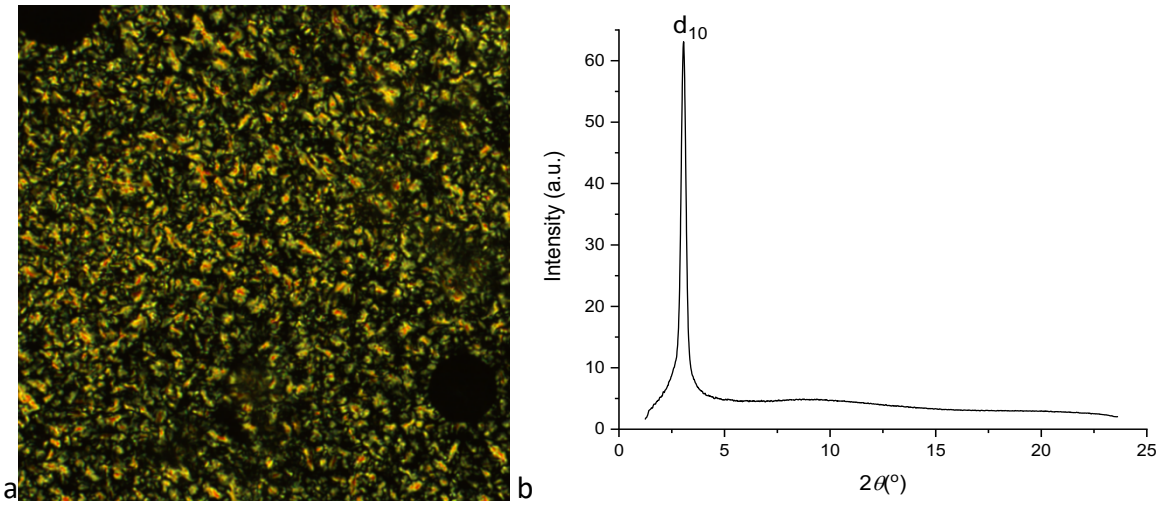


Figure S3a) photomicrograph of Col_h phase of **6c** at 70.7 °C on cooling from the isotropic liquid and b) corresponding SAXS pattern at 66.0 °C on cooling from the isotropic liquid.

Table S2: X-ray diffraction data for complexes **5 to 9**, presenting the measured and calculated spacing, Miller indices and calculated parameters (where applicable).

Complex	Phase	2θ/ °	d_{obs} /Å	d_{calc}/ Å	*hkl*	*a*/ Å
5	Lam	2.87	30.7	30.7	001	-
	T = 155.0 °C cooling	5.73	15.4	15.4	002	
		9.14	9.7	10.2	003	
		9.92	8.9			
		13.95	6.3			
		16.13	5.5			
		17.26	5.1			
6c	Col_h	3.04	29.0	29.0	10	33.5
	T = 60.4 °C cooling					
7a	Col_h	3.01	29.3	29.3	10	33.8
	T = 80.0 °C cooling					
8a	Col_h	2.83	31.2	31.2	10	36.0
	T = 51.1 °C cooling	4.90	18.0	18.0	11	
8b	Col_h^1	2.82	31.3	31.3	10	36.1
	T = 80 °C cooling	4.88	18.1	18.1	11	
	Col_h^2	2.65	33.3	33.3	10	38.5
	T = 30 °C cooling	4.62	19.1	19.2	11	
	Col_h^3	2.74	32.2	32.2	10	37.2
	T = 60 °C 2nd heating	4.78	18.5	18.6	11	
8c	Col_h	2.64	33.4	33.4	10	38.6
	T = 80.0 °C cooling	4.57	19.3	19.3	11	
		5.24	16.8	16.7	20	
8d	Col_h	2.68	32.9	32.9	10	38.0
	T = 95 °C heating	4.61	19.1	19.0	11	
9a	Col_r	2.46	35.9	35.9	11	*a* = 59.8
	T = 60.4 °C cooling	2.95	29.9	29.9	20	
		4.82	18.3	18.2	31	*b* = 44.9
		7.27	12.1	11.9	33	
		9.45	9.3	9.3	53	
9b	Col_h	2.84	31.1	31.1	10	*a* = 35.9
	T = 75 °C cooling	4.91	18.0	18.0	11	

	Col_r	2.30	38.4	38.4	11	*a* = 63.2 *b* = 48.3
	T = 50 °C cooling	2.79	31.6	31.6	20	
		4.54	19.4	19.3	31	
		6.78	13.0	12.8	33	
		8.97	9.8	9.7	05	
		12.55	7.0	7.1	65	
		11.2	7.9	7.8	55	
		12.6	7.0	7.0	46	
9c	Col_r	2.19	40.3	40.3	11	*a* = 65.6 *b* = 51.1
	T = 83.8 °C cooling	2.69	32.8	32.8	20	
		3.46	25.4	25.5	02	
		4.34	20.3	20.1	31	
		6.48	13.6	13.8	42	
		7.50	11.8	11.8	43	
		8.67	10.2	10.2	05	
		9.59	9.2	9.2	63	
		10.64	8.3	8.2	26	
	Col_h	2.78	31.7	31.7	10	*a* = 36.6
	T = 86.1 °C cooling	4.81	18.3	18.3	11	
		5.67	15.6	15.8	20	
9d	Col_h	2.65	33.3	33.3	10	*a* = 38.5
	T = 79.0 °C cooling	4.58	19.3	19.2	11	
		5.28	16.7	16.7	20	
	Col_r	2.12	41.6	41.6	11	*a* = 67.2 *b* = 53.0
	T = 60 °C cooling	2.63	33.6	33.6	20	
		4.56	19.4			
		5.27	16.7	16.8	40	
		6.29	14.0	13.9	33	
		8.33	10.6	10.7	53	
		10.32	8.6	8.6	46	

Table S3. X-ray diffraction data for complexes **10 to 13**, presenting the measured and calculated spacing, Miller indices and calculated parameters (where applicable).

Complex	Phase	2θ/ °	d_{obs} /Å	d_{calc}/ Å	*hk*	*a*/ Å
10a	Col_h	3.95	22.3	22.3	10	25.7
	T = 105.0 °C cooling	6.88	12.8	12.9	11	
		7.88	11.2	11.2	20	
10b	Col_h	3.74	23.6	23.6	10	27.3
	T = 110 °C cooling	6.44	13.7	13.6	11	
		7.46	11.8	11.8	20	
10c	Col_h	3.69	23.9	23.9	10	27.6
	T = 82.7 °C heating	6.38	13.8	13.8	11	
		7.39	11.9	12.0	20	
11a	Col_h	3.63	24.3	24.3	10	28.1
	T = 107.3 °C heating	6.29	14.0	14.0	11	
		7.21	12.2	12.2	20	
11b	Col_h	3.55	24.9	24.9	10	28.8
	T = 90.5 °C heating	6.16	14.3	14.3	11	
		7.12	12.4	12.5	20	
11c	Col_h	3.49	25.3	25.3	10	29.2
	T = 97.2 °C heating	6.10	14.5	14.6	11	
		6.92	12.8	12.7	20	
11d	Col_h	3.46	25.5	25.5	10	29.4
	T = 110.0 °C cooling	6.02	14.7	14.7	11	
		6.97	12.7	12.8	20	
12a	Col_h	3.46	25.5	25.5	10	29.4
	T = 160.9 °C heating	5.97	14.8	14.7	11	
		6.96	12.7	12.8	20	
12b	Col_h	3.35	26.3	26.3	10	30.4
	T = 120.7 °C cooling	5.82	15.2	15.2	11	
		6.75	13.1	13.2	20	
		8.95	9.9	9.9	21	

12c	Col_h *T* = 109.5 °C cooling	3.24	27.2	27.2	10	31.4
		5.66	15.6	15.7	11	
		6.52	13.5	13.6	20	
		8.65	10.2	10.3	21	
12d	Col_h *T* = 109.5 °C cooling	3.22	27.4	27.4	10	31.6
		5.56	15.9	15.8	11	
		6.43	13.7	13.7	20	
13a	Col_h *T* = 80.5 °C heating	3.31	26.7	26.7	10	30.8
		5.77	15.3	15.3	11	
		6.64	13.3	13.3	20	
		8.72	10.1	10.1	21	
13b	Col_h *T* = 100.6 °C heat	3.25	27.2	27.2	10	31.4
		5.64	15.7	15.7	11	
		6.54	13.5	13.6	20	
		8.65	10.2	10.2	21	
13c	Col_h *T* = 160.9 °C cool	3.22	27.4	27.4	10	31.6
		5.58	15.8	15.8	11	
		6.44	13.7	13.7	20	
		8.52	10.4	10.3	21	
	Lam *T* = 26.9 °C cool	2.41	36.6	36.6	001	-
		4.88	18.1	18.3	002	
		5.39	16.4			
		7.27	12.1	12.2	003	
		20.86	4.3		broad	
13d	Col_h *T* = 100.6 °C heat	3.08	28.7	28.7	10	33.1
		5.34	16.5	16.5	11	
		6.14	14.4	14.4	20	
		8.14	10.8	10.8	21	

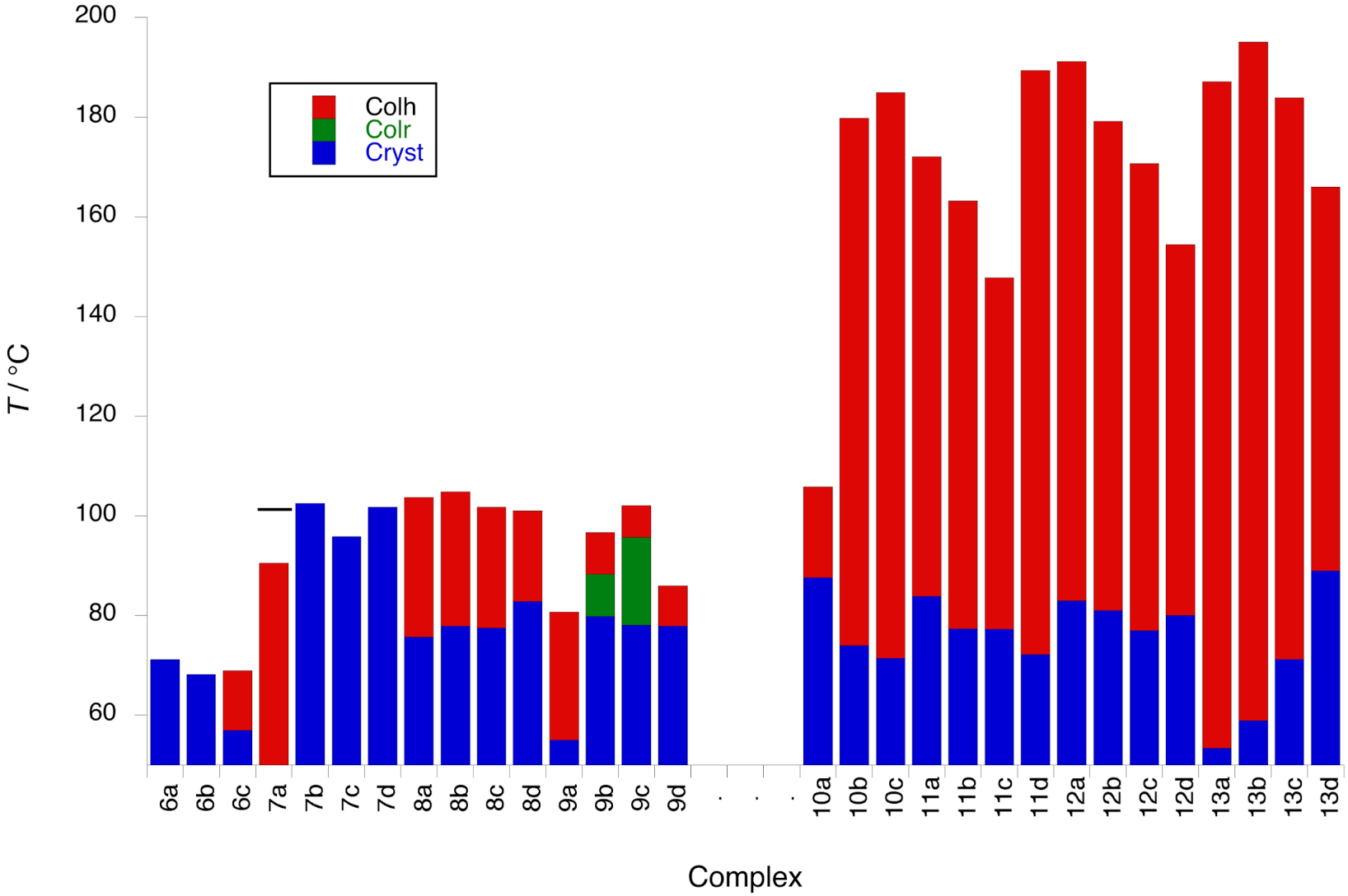


Figure S4: Transition temperatures and phases for complexes **6** to **13**. The melting point of **7a** is shown as a black bar (phase is monotropic).

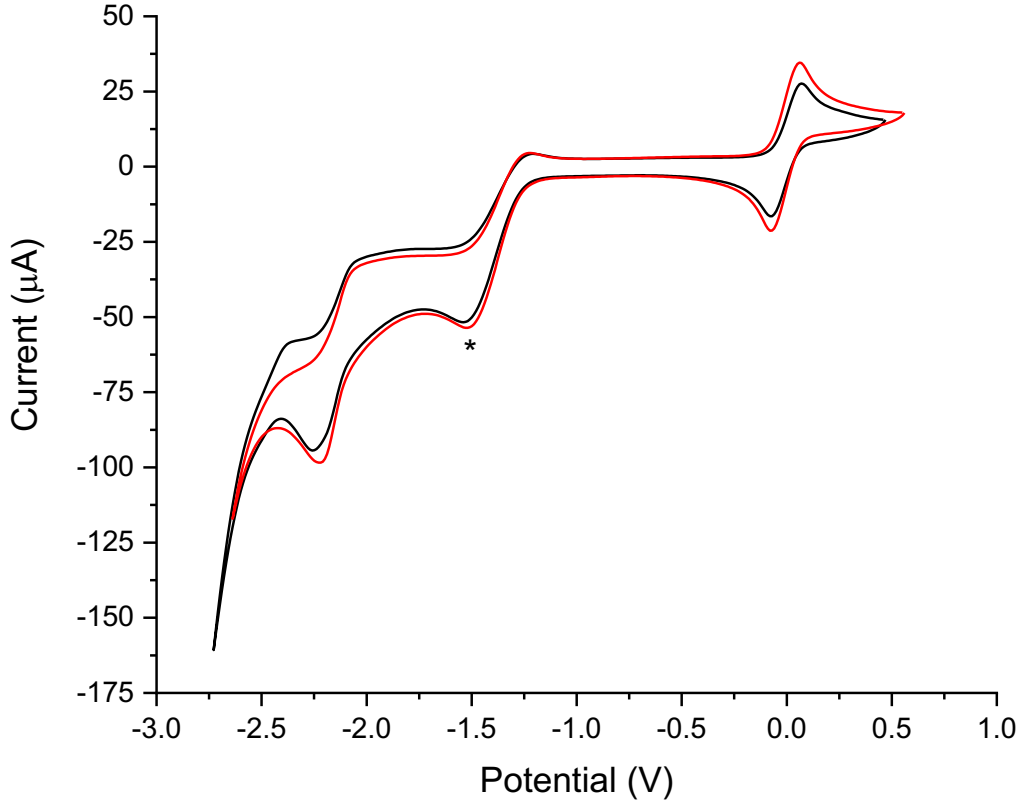


Figure S5. Cyclic voltammograms of **6a** (black) and **10a** (red), referenced against the ferrocene/ferrocenium couple. The presence of water is marked by an * and should be ignored.

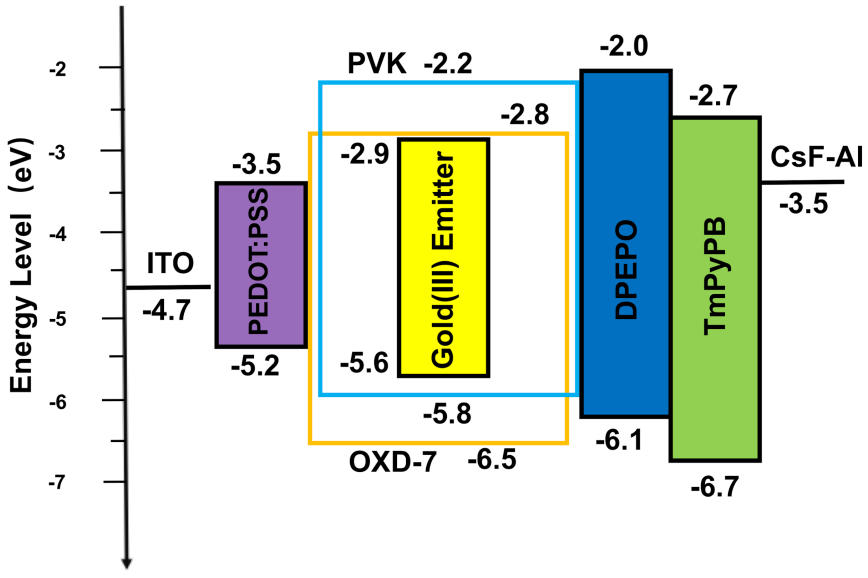


Figure S6. General schematic for the structure of doped-devices with gold(III) emitters (emitter energy levels shown are those calculated for **6a**).

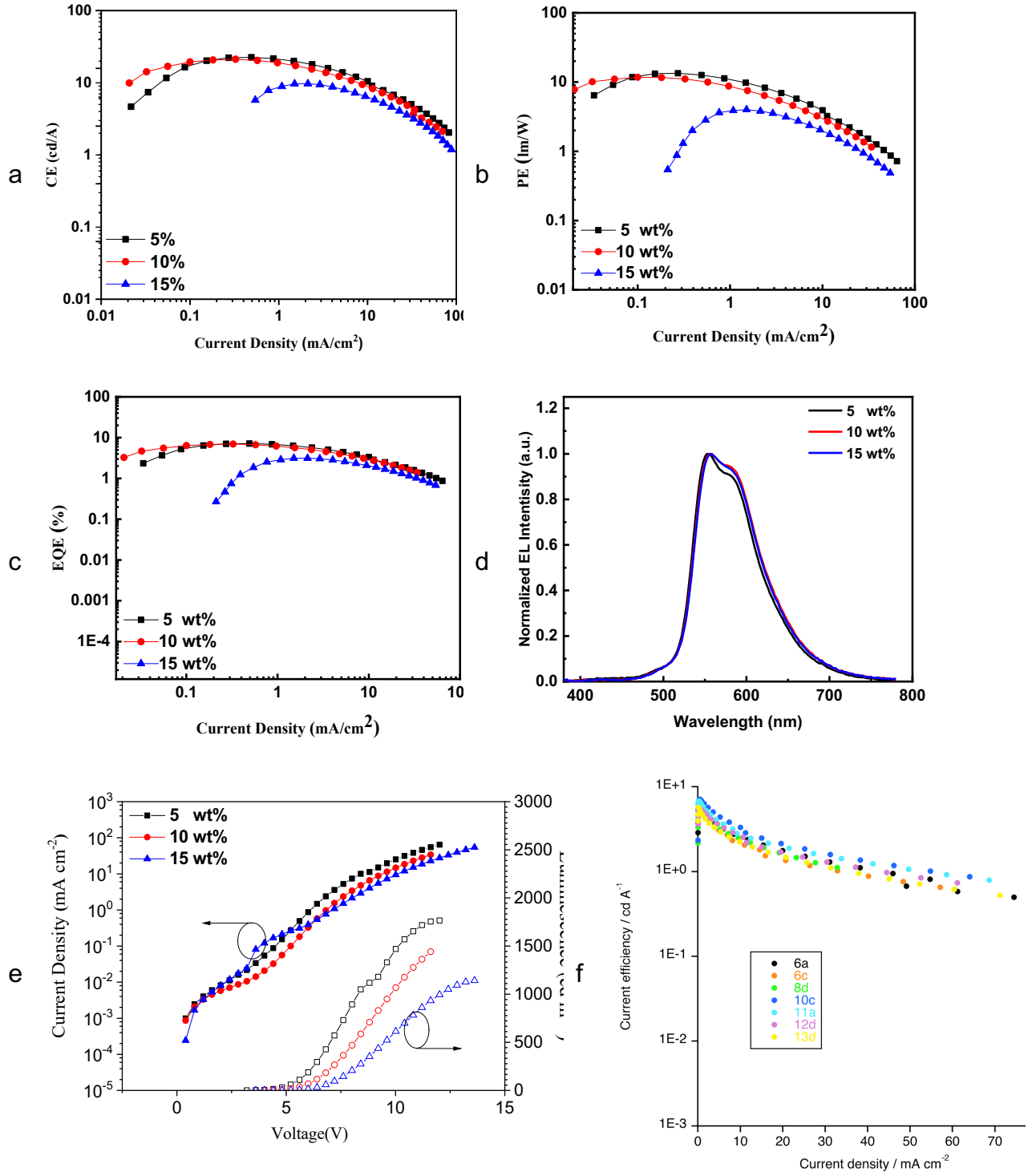


Figure S7. Device performance comparison of **6a** at 5 (black), 10 (red) and 15 (blue) wt% in PVK:OXD-7 (7:3) showing a) current efficiency as a function of current density; b) power efficiency as a function of current density; c) external quantum efficiency as a function of current density; d) electroluminescence emission profile; e) current density and luminescence as a function of voltage; f) Current efficiency as a function of current density.

Electron Mobility

For the devices, SCLC is described by the formula $J = (9/8)\varepsilon_0\varepsilon_r\mu(V\ d^{-3})$, where J is the current density, ε_0 is the permittivity under vacuum ($\varepsilon_0 = 8.85 \times 10^{-12}$ F m^{-1}), ε_r is the dielectric constant ($\varepsilon_r = 3$), μ is the hole/electron mobility, and d is the sample thickness.

Device fabrication and Measurements: The patterned ITO substrates (0.06 cm^2) were rinsed with acetone and isopropyl alcohol using sonication for 15 min, followed by 15 min UV-ozone-treatment. After surface treatment, the PEDOT:PSS layer was spin-coated onto the ITO substrate as the hole-injecting layer with a rate of 3200 rpm, and then annealed at 150 °C for 15 min. The ZnO was prepared by spin-coating onto the PEDOT:PSS and then annealed at 200 °C for 15 min. The Au complexes in chloroform (15 mg cm^{-3}) were spin-coated with the rate of 1000 rpm, then annealing (**8d**: 90 °C; **12d**: 120 °C;**13d**: 120 °C) or not. The cathode materials were thermally evaporated onto the emitter layer in a vacuum chamber. The thermally evaporated deposition rate is 1.5-1.8 Å s^{-1} for Al electrode.

Computational Chemistry

All calculations were performed using the TURBOMOLE V6.4 package using the resolution of identity (RI) approximation.[9-16] Initial optimisations were performed at the (RI-)BP86/SV(P) level with an m5 grid, followed by frequency calculations at the same level. All minima were confirmed as such by the absence of imaginary frequencies. Single-point and TD-DFT calculations on the (RI-)BP86/SV(P) optimised geometries were performed using the hybrid PBE0 functional and the flexible def2-TZVPP basis set with a 60-electron effective core potential. Energies, xyz coordinates and the first 50 lines of the vibrational spectra are presented.

6-H

SCF Energy (au) BP86/SV(P)	-1381.0627125650
SCF Energy (au) PBE0/def2-TZVPP	-1380.764732503
Zero Point Energy (au)	0.3838163
Chemical potential (kJ mol^{-1})	846.35

xyz coordinates
51

Au	0.02583	-0.04773	-0.58212
C	-0.08134	0.09423	1.38095
N	0.14062	-0.19299	-2.63061
C	-1.52483	1.28051	-1.11435
C	-0.74082	0.55170	-3.35961
C	3.69483	-3.23297	-1.43588
H	4.49706	-3.93081	-1.71591
C	1.61616	-1.42462	-0.74651
C	-1.65908	1.36330	-2.54586
C	-2.37139	2.03338	-0.30475
H	-2.29205	1.99282	0.79333
C	-3.36171	2.87691	-0.87268
C	2.36166	-2.04920	0.25003
H	2.16025	-1.85604	1.31581
C	-0.66921	0.45907	-4.76659
H	-1.35742	1.03909	-5.39808
C	2.94687	-2.60785	-2.44367
H	3.18875	-2.83769	-3.49511
C	3.40354	-2.95497	-0.07992
C	0.29400	-0.38395	-5.34430
H	0.35605	-0.46125	-6.44243
C	1.17994	-1.13015	-4.55025
H	1.93027	-1.78692	-5.01338
C	1.90884	-1.70605	-2.12824
C	1.09294	-1.02451	-3.14505
C	-2.64712	2.20512	-3.09851
H	-2.76796	2.28369	-4.19219
C	-3.49715	2.96034	-2.27819
H	-4.25670	3.60672	-2.74109
O	4.06444	-3.50514	0.97259
O	-4.13123	3.56439	0.01187
C	-0.14488	0.18728	2.61287
C	-0.21700	0.29519	4.03806
C	-0.35908	0.50978	6.86665
C	0.88783	0.53416	6.21588
C	0.96237	0.42619	4.82026
C	-1.46937	0.27427	4.70960
C	-1.53505	0.37805	6.10602
H	-0.41429	0.59359	7.96481
H	1.81529	0.63701	6.80417
H	1.93909	0.44375	4.31095
H	-2.39062	0.17225	4.11414
H	-2.51719	0.35731	6.60780
C	5.11876	-4.42049	0.72481
C	-5.14107	4.43106	-0.47797
H	-4.71398	5.24984	-1.10408
H	-5.62592	4.87343	0.41544
H	-5.90660	3.87836	-1.07243
H	5.94857	-3.94776	0.14791
H	4.76075	-5.32349	0.17592
H	5.49837	-4.72822	1.71987

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.48	0.03981	YES	YES
8	a	16.95	0.11771	YES	YES
9	a	18.45	0.03222	YES	YES
10	a	29.37	3.41086	YES	YES
11	a	56.17	0.00224	YES	YES
12	a	77.37	0.35631	YES	YES
13	a	81.83	0.92929	YES	YES
14	a	85.97	0.00073	YES	YES
15	a	89.66	0.23850	YES	YES
16	a	94.31	0.47962	YES	YES
17	a	100.43	3.55880	YES	YES
18	a	141.33	0.02554	YES	YES
19	a	150.93	0.75501	YES	YES
20	a	179.59	0.01847	YES	YES
21	a	185.46	1.23813	YES	YES
22	a	186.90	0.00839	YES	YES
23	a	221.04	0.40323	YES	YES
24	a	225.17	0.16702	YES	YES
25	a	225.65	1.15690	YES	YES
26	a	240.12	3.91463	YES	YES
27	a	242.74	0.00028	YES	YES
28	a	247.02	0.00659	YES	YES
29	a	270.16	3.38208	YES	YES
30	a	286.85	0.43979	YES	YES
31	a	300.60	9.61786	YES	YES
32	a	320.69	1.01800	YES	YES
33	a	320.73	1.27441	YES	YES
34	a	336.06	0.26671	YES	YES
35	a	368.80	0.10147	YES	YES
36	a	394.38	0.71396	YES	YES
37	a	401.68	0.10086	YES	YES
38	a	408.35	1.97915	YES	YES
39	a	426.22	0.08401	YES	YES
40	a	435.77	3.12034	YES	YES
41	a	475.59	2.16310	YES	YES
42	a	486.89	7.14000	YES	YES
43	a	507.70	0.55743	YES	YES
44	a	526.49	0.92302	YES	YES
45	a	531.23	14.98263	YES	YES
46	a	543.03	3.82574	YES	YES
47	a	547.35	0.05585	YES	YES
48	a	565.03	1.10414	YES	YES
49	a	585.61	18.17709	YES	YES
50	a	592.80	1.31267	YES	YES

^{3}[6-H]

SCF Energy (au) BP86/SV(P)	-1380.9779862660
SCF Energy (au) PBE0/def2-TZVPP	-1380.668581507
Zero Point Energy (au)	0.379264
Chemical potential (kJ mol^{-1})	833.36

xyz coordinates
51

Au	0.04678	-0.03601	-0.57899
C	-0.06254	0.12278	1.38484
N	0.17991	-0.16055	-2.59879
C	-1.51475	1.26406	-1.11697
C	-0.71468	0.60650	-3.36152
C	3.67803	-3.26446	-1.44976
H	4.47873	-3.96589	-1.72550
C	1.60610	-1.44187	-0.75331
C	-1.61506	1.39532	-2.57304
C	-2.41604	1.94155	-0.30766
H	-2.36453	1.86585	0.79018
C	-3.41172	2.78885	-0.86921
C	2.30499	-2.12259	0.24291
H	2.08562	-1.95653	1.30949
C	-0.61686	0.51087	-4.77536
H	-1.30689	1.09502	-5.40422
C	2.97443	-2.59708	-2.45523
H	3.23778	-2.79826	-3.50711
C	3.34166	-3.03071	-0.08854
C	0.34082	-0.31931	-5.36834
H	0.41132	-0.39380	-6.46400
C	1.22360	-1.08397	-4.54137
H	1.97360	-1.74745	-4.99695
C	1.93066	-1.69242	-2.14198
C	1.12734	-0.99093	-3.14187
C	-2.61112	2.27615	-3.11359
H	-2.69941	2.40367	-4.20508
C	-3.49540	2.95529	-2.28628
H	-4.25671	3.61118	-2.73361
O	3.96953	-3.62283	0.96083
O	-4.22454	3.41816	0.01943
C	-0.12668	0.22516	2.62130
C	-0.19454	0.34569	4.03966
C	-0.32747	0.58808	6.86615
C	0.91394	0.66562	6.20648
C	0.98445	0.54734	4.81304
C	-1.44198	0.26873	4.72274
C	-1.50256	0.38974	6.11648
H	-0.37903	0.68196	7.96358
H	1.83820	0.82117	6.78792
H	1.95442	0.60935	4.29467
H	-2.36000	0.11142	4.13464
H	-2.47820	0.32820	6.62720
C	5.05226	-4.50738	0.71839
C	-5.19262	4.34569	-0.44658
H	-4.71845	5.19260	-0.99544
H	-5.70187	4.73632	0.45700
H	-5.94610	3.85582	-1.10693
H	5.89016	-3.99665	0.18819
H	4.73245	-5.39729	0.12687
H	5.40295	-4.84216	1.71524

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.38	0.67792	YES	YES
8	a	16.72	0.10479	YES	YES
9	a	18.64	0.00766	YES	YES
10	a	27.35	3.49486	YES	YES
11	a	53.43	0.08662	YES	YES
12	a	74.51	0.03787	YES	YES
13	a	79.23	8.25369	YES	YES
14	a	83.16	0.45350	YES	YES
15	a	84.55	0.33578	YES	YES
16	a	88.13	2.70953	YES	YES
17	a	91.78	0.48841	YES	YES
18	a	148.11	0.02668	YES	YES
19	a	150.32	0.79323	YES	YES
20	a	169.92	2.42181	YES	YES
21	a	178.61	2.80908	YES	YES
22	a	185.14	0.11620	YES	YES
23	a	201.61	3.24570	YES	YES
24	a	224.07	3.44004	YES	YES
25	a	224.31	3.54249	YES	YES
26	a	229.22	0.78598	YES	YES
27	a	237.24	4.64925	YES	YES
28	a	239.86	0.37322	YES	YES
29	a	258.15	1.69966	YES	YES
30	a	281.06	9.11118	YES	YES
31	a	294.83	7.86739	YES	YES
32	a	300.86	7.26716	YES	YES
33	a	318.96	1.46196	YES	YES
34	a	322.30	1.50193	YES	YES
35	a	335.79	10.94679	YES	YES
36	a	390.06	4.77392	YES	YES
37	a	398.25	5.27201	YES	YES
38	a	400.25	0.44543	YES	YES
39	a	404.44	5.71587	YES	YES
40	a	419.14	3.01368	YES	YES
41	a	447.27	8.07839	YES	YES
42	a	477.38	36.37047	YES	YES
43	a	503.35	0.47286	YES	YES
44	a	514.44	7.97084	YES	YES
45	a	520.84	13.67183	YES	YES
46	a	528.09	34.43783	YES	YES
47	a	541.39	2.46744	YES	YES
48	a	560.75	30.04266	YES	YES
49	a	564.37	3.26396	YES	YES
50	a	577.27	35.25224	YES	YES

6-Et

SCF Energy (au) BP86/SV(P)	-1459.6278575420
SCF Energy (au) PBE0/def2-TZVPP	-1459.324239818
Zero Point Energy (au)	0.438186
Chemical potential (kJ mol^{-1})	976.92

xyz coordinates
57

Au	0.08295	-0.01131	-1.54335
C	-0.02855	0.13347	0.41923
N	0.19953	-0.16153	-3.59155
C	-1.46494	1.31807	-2.08029
C	-0.68018	0.58261	-4.32314
C	3.74650	-3.20567	-2.38619
H	4.54742	-3.90599	-2.66383
C	1.67073	-1.39154	-1.70302
C	-1.59792	1.39759	-3.51211
C	-2.31125	2.07403	-1.27324
H	-2.23264	2.03584	-0.17498
C	-3.30012	2.91723	-1.84405
C	2.41479	-2.01448	-0.70433
H	2.21299	-1.81776	0.36073
C	-0.60775	0.48619	-5.72983
H	-1.29466	1.06558	-6.36330
C	3.00000	-2.58228	-3.39615
H	3.24145	-2.81614	-4.44683
C	3.45548	-2.92264	-1.03120
C	0.35434	-0.36010	-6.30465
H	0.41703	-0.44041	-7.40253
C	1.23822	-1.10595	-5.50797
H	1.98754	-1.76548	-5.96881
C	1.96392	-1.67716	-3.08381
C	1.15032	-0.99648	-4.10311
C	-2.58428	2.23944	-4.06767
H	-2.70390	2.31578	-5.16164
C	-3.43423	2.99752	-3.24988
H	-4.19274	3.64355	-3.71500
O	4.11621	-3.46977	0.02321
O	-4.06999	3.60757	-0.96178
C	-0.09864	0.22544	1.65101
C	-0.18010	0.33150	3.07542
C	-0.34423	0.55167	5.92855
C	0.90163	0.57343	5.26400
C	0.98942	0.46443	3.87040
C	-1.43401	0.31334	3.74275
C	-1.50661	0.41890	5.13733
C	-0.42896	0.62034	7.44147
H	1.82789	0.68285	5.85529
H	1.97226	0.48778	3.37316
H	-2.35452	0.21686	3.14515
H	-2.49600	0.40513	5.62782
C	5.16859	-4.38797	-0.22169
C	-5.07883	4.47349	-1.45478
H	-4.65078	5.29048	-2.08262
H	-5.56433	4.91841	-0.56297
H	-5.84413	3.91972	-2.04860
H	5.99946	-3.91883	-0.80007
H	4.80883	-5.29197	-0.76779
H	5.54767	-4.69336	0.77432
H	-1.36341	1.14965	7.73691
H	0.41537	1.23223	7.83273
C	-0.40119	-0.76741	8.11393

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H   -0.46538   -0.67679    9.22156
H    0.53628   -1.31321    7.86720
H   -1.25257   -1.39587    7.77059

$vibrational spectrum (first 50 lines)
```

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.49	0.06170	YES	YES
8	a	13.41	0.19012	YES	YES
9	a	16.73	0.23745	YES	YES
10	a	27.34	3.04765	YES	YES
11	a	38.01	0.10535	YES	YES
12	a	54.10	0.15333	YES	YES
13	a	56.18	0.00327	YES	YES
14	a	75.04	0.25149	YES	YES
15	a	80.88	0.91581	YES	YES
16	a	85.95	0.00399	YES	YES
17	a	86.34	0.59495	YES	YES
18	a	100.34	3.66109	YES	YES
19	a	129.00	0.11926	YES	YES
20	a	141.32	0.03620	YES	YES
21	a	150.96	0.54455	YES	YES
22	a	166.16	0.14037	YES	YES
23	a	186.90	0.01021	YES	YES
24	a	189.80	0.77115	YES	YES
25	a	219.54	0.28770	YES	YES
26	a	221.04	0.42736	YES	YES
27	a	225.07	0.06444	YES	YES
28	a	226.32	1.01438	YES	YES
29	a	233.18	2.88600	YES	YES
30	a	242.92	0.00376	YES	YES
31	a	247.58	0.26144	YES	YES
32	a	265.23	3.24604	YES	YES
33	a	286.79	0.38949	YES	YES
34	a	298.81	7.49395	YES	YES
35	a	309.83	5.02214	YES	YES
36	a	320.77	0.04074	YES	YES
37	a	335.61	0.26568	YES	YES
38	a	345.03	0.36204	YES	YES
39	a	359.29	0.05517	YES	YES
40	a	372.51	0.01226	YES	YES
41	a	402.63	0.16427	YES	YES
42	a	408.34	2.09091	YES	YES
43	a	426.25	0.10971	YES	YES
44	a	435.65	2.81989	YES	YES
45	a	453.43	2.76278	YES	YES
46	a	475.84	1.93348	YES	YES
47	a	486.89	7.02271	YES	YES
48	a	508.91	0.58930	YES	YES
49	a	513.47	0.28362	YES	YES
50	a	526.97	0.78825	YES	YES

7-OMe

SCF Energy (au) BP86/SV(P)	-1495.5055220410
SCF Energy (au) PBE0/def2-TZVPP	-1495.208858234
Zero Point Energy (au)	0.4153144
Chemical potential (kJ mol^{-1})	920.81

xyz coordinates

55

Au	-0.02432	-0.13864	-1.25600
C	-0.12416	0.06445	0.70204
N	0.07876	-0.35148	-3.29957
C	-1.65672	1.07421	-1.81682
C	-0.85339	0.31158	-4.04411
C	3.81588	-3.13459	-2.03918
C	1.64345	-1.42367	-1.39023
C	-1.81004	1.09685	-3.24878
C	-2.53783	1.80606	-1.02471
H	-2.44427	1.81028	0.07305
C	-3.58141	2.56908	-1.61046
C	2.43427	-1.96738	-0.38108
H	2.23193	-1.74681	0.67921
C	-0.79112	0.17112	-5.44762
H	-1.51956	0.68515	-6.09108
C	3.02271	-2.59112	-3.05970
H	3.26613	-2.84614	-4.10502
C	3.52315	-2.82326	-0.69081
C	0.21461	-0.63422	-6.00638
H	0.26951	-0.74872	-7.10164
C	1.15166	-1.29669	-5.19676
H	1.93473	-1.92498	-5.64503
C	1.93798	-1.73882	-2.76438
C	1.07306	-1.14417	-3.79538
C	-2.85106	1.85921	-3.81930
H	-2.98689	1.89106	-4.91360
C	-3.73564	2.59313	-3.01635
C	-0.18776	0.19091	1.93133
C	-0.26510	0.33709	3.35201
C	-0.42056	0.62997	6.18436
C	0.82986	0.68292	5.53119
C	0.89822	0.53477	4.13721
C	-1.51544	0.29004	4.03152
C	-1.59192	0.43032	5.41748
O	-0.60065	0.75882	7.53217
H	1.87854	0.57590	3.63625
H	-2.43520	0.13661	3.44505
C	0.53507	0.96365	8.35130
H	1.07148	1.90733	8.08988
H	1.25324	0.11116	8.28735
H	0.15676	1.03960	9.39109
O	4.22656	-3.29511	0.37280
O	-4.38142	3.24265	-0.74192
H	1.76036	0.83761	6.09753
H	-2.55963	0.39100	5.94245
C	5.32611	-4.16053	0.14458
C	-5.44465	4.03062	-1.25069
H	-5.07236	4.84912	-1.91130
H	-5.94575	4.47690	-0.36822
H	-6.18263	3.41314	-1.81562
H	6.12287	-3.66560	-0.45980
H	5.01195	-5.10116	-0.36675
H	5.73304	-4.41069	1.14503
H	-4.53626	3.17701	-3.49291

H 4.65385 -3.79556 -2.30363

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.01	0.64504	YES	YES
8	a	13.46	0.20879	YES	YES
9	a	16.76	0.25982	YES	YES
10	a	27.73	3.26871	YES	YES
11	a	56.23	0.00532	YES	YES
12	a	57.19	0.20097	YES	YES
13	a	70.23	0.28364	YES	YES
14	a	80.81	0.93994	YES	YES
15	a	85.05	0.92267	YES	YES
16	a	86.31	0.00235	YES	YES
17	a	100.61	3.59573	YES	YES
18	a	109.48	2.15390	YES	YES
19	a	141.35	0.05996	YES	YES
20	a	148.84	0.38029	YES	YES
21	a	157.13	0.03938	YES	YES
22	a	172.42	0.42730	YES	YES
23	a	186.97	0.01420	YES	YES
24	a	208.51	2.31768	YES	YES
25	a	221.12	0.30973	YES	YES
26	a	225.11	0.06791	YES	YES
27	a	227.14	1.17706	YES	YES
28	a	230.73	1.77566	YES	YES
29	a	243.10	0.01095	YES	YES
30	a	246.35	2.04375	YES	YES
31	a	253.87	3.47767	YES	YES
32	a	262.41	3.09068	YES	YES
33	a	286.86	0.40351	YES	YES
34	a	301.38	9.64901	YES	YES
35	a	309.32	3.69703	YES	YES
36	a	320.94	0.06636	YES	YES
37	a	335.61	0.21584	YES	YES
38	a	339.97	0.44807	YES	YES
39	a	370.79	0.11401	YES	YES
40	a	408.28	1.83432	YES	YES
41	a	411.77	0.34673	YES	YES
42	a	426.25	0.16471	YES	YES
43	a	435.34	3.03745	YES	YES
44	a	439.75	0.57440	YES	YES
45	a	451.71	0.86192	YES	YES
46	a	476.01	2.14127	YES	YES
47	a	486.83	6.94192	YES	YES
48	a	503.59	4.44609	YES	YES
49	a	526.43	1.55431	YES	YES
50	a	531.08	14.94124	YES	YES

8-OMe

SCF Energy (au) BP86/SV(P) -1609.9391332850
SCF Energy (au) PBE0/def2-TZVPP -1609.644128610
Zero Point Energy (au) 0.4463643
Chemical potential (kJ mol^{-1}) 991.40

xyz coordinates
59

Au	0.19681	-0.26470	-1.71879
C	0.11592	-0.03784	0.23739
N	0.27982	-0.50215	-3.76059
C	-1.41110	0.97967	-2.28129
C	-0.64232	0.17411	-4.50566
C	3.96166	-3.35620	-2.49632
C	1.83312	-1.58979	-1.85071
C	-1.57468	0.98988	-3.71219
C	-2.27019	1.73895	-1.49086
H	-2.16894	1.75234	-0.39387
C	-3.30140	2.51791	-2.07748
C	2.61886	-2.14028	-0.84126
H	2.42917	-1.90399	0.21800
C	-0.59386	0.01683	-5.90792
H	-1.31506	0.54048	-6.55177
C	3.17328	-2.80620	-3.51706
H	3.40306	-3.07807	-4.56121
C	3.68603	-3.02370	-1.14938
C	0.38879	-0.81768	-6.46492
H	0.43304	-0.94516	-7.55924
C	1.31620	-1.49292	-5.65478
H	2.08086	-2.14445	-6.10164
C	2.11034	-1.92635	-3.22338
C	1.25171	-1.32315	-4.25466
C	-2.60285	1.76876	-4.28363
H	-2.74593	1.79191	-5.37722
C	-3.46536	2.53034	-3.48241
C	0.06387	0.10325	1.46543
C	0.00295	0.26859	2.88514
C	-0.12987	0.58706	5.72051
C	1.10852	0.61991	5.04837
C	1.17573	0.45972	3.65556
C	-1.24230	0.25518	3.57032
C	-1.32357	0.40873	4.95882
O	-0.28319	0.69496	7.07497
H	2.15417	0.48035	3.15101
H	-2.18080	0.11150	3.01415
O	-2.55627	0.31413	5.55735
C	0.87516	0.82927	7.87794
H	1.44169	1.76121	7.63935
H	1.55722	-0.04705	7.76703
H	0.51899	0.88062	8.92689
C	-3.03637	1.47660	6.22799
H	-3.10581	2.34391	5.52776
H	-2.39461	1.75404	7.09352
H	-4.05454	1.22570	6.59184
O	4.38656	-3.49964	-0.08569
O	-4.08076	3.21761	-1.21065
H	2.04256	0.75886	5.61300
H	-4.25665	3.12629	-3.95962
H	4.78254	-4.03879	-2.75949
C	-5.13260	4.01995	-1.72045
C	5.46548	-4.39102	-0.31224
H	-4.75001	4.82359	-2.39335

```
H   -5.61826    4.48586   -0.83947
H   -5.88665    3.41032   -2.27249
H    5.87417   -4.63915    0.68800
H    6.26820   -3.91993   -0.92770
H    5.12745   -5.33016   -0.81095

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               4.23         0.34438       YES     YES
     8        a              12.32         0.37091       YES     YES
     9        a              16.33         0.49738       YES     YES
    10        a              27.35         3.54917       YES     YES
    11        a              51.35         1.09582       YES     YES
    12        a              56.22         0.00553       YES     YES
    13        a              60.93         0.07340       YES     YES
    14        a              75.33         2.35840       YES     YES
    15        a              80.29         1.67624       YES     YES
    16        a              84.57         1.25263       YES     YES
    17        a              86.12         0.00373       YES     YES
    18        a             100.41         3.44766       YES     YES
    19        a             107.26         2.52585       YES     YES
    20        a             129.95         1.55896       YES     YES
    21        a             141.32         0.06228       YES     YES
    22        a             144.50         0.14428       YES     YES
    23        a             149.19         0.44294       YES     YES
    24        a             163.14         1.33556       YES     YES
    25        a             179.28         0.90430       YES     YES
    26        a             186.97         0.01452       YES     YES
    27        a             205.73         0.45447       YES     YES
    28        a             220.87         0.46631       YES     YES
    29        a             224.99         0.03440       YES     YES
    30        a             226.27         0.92602       YES     YES
    31        a             229.83         1.70481       YES     YES
    32        a             237.67         3.04050       YES     YES
    33        a             243.12         0.00296       YES     YES
    34        a             250.71         0.21557       YES     YES
    35        a             265.57         2.56245       YES     YES
    36        a             286.54         0.32607       YES     YES
    37        a             293.96         3.40462       YES     YES
    38        a             301.78        10.55502       YES     YES
    39        a             307.57         7.47002       YES     YES
    40        a             320.95         0.06407       YES     YES
    41        a             335.31         0.40748       YES     YES
    42        a             343.99         2.04535       YES     YES
    43        a             356.13         0.84016       YES     YES
    44        a             371.98         0.18664       YES     YES
    45        a             408.35         1.81681       YES     YES
    46        a             426.25         0.17362       YES     YES
    47        a             435.48         3.07160       YES     YES
    48        a             448.25         2.23724       YES     YES
    49        a             459.19         3.04382       YES     YES
    50        a             473.14         2.87337       YES     YES
```

9-OMe

SCF Energy (au) BP86/SV(P) -1724.3771649480
SCF Energy (au) PBE0/def2-TZVPP -1724.084343638
Zero Point Energy (au) 0.4776731
Chemical potential (kJ mol^{-1}) 1064.93

xyz coordinates
63

Au	0.04497	-0.28914	-1.93615
C	-0.00621	-0.07876	0.02296
N	0.09856	-0.50979	-3.98074
C	-1.53030	1.00893	-2.46948
C	-0.81023	0.20140	-4.70946
C	3.70353	-3.48788	-2.78245
C	1.63853	-1.66193	-2.09803
C	-1.70875	1.03774	-3.89832
C	-2.35640	1.78756	-1.66281
H	-2.24203	1.78848	-0.56699
C	-3.36886	2.60396	-2.23095
C	2.41714	-2.24595	-1.10205
H	2.24594	-2.01392	-0.03869
C	-0.78153	0.05610	-6.11351
H	-1.49310	0.60761	-6.74469
C	2.92213	-2.90397	-3.78962
H	3.13232	-3.17307	-4.83859
C	3.45269	-3.15966	-1.42961
C	0.16915	-0.80275	-6.68882
H	0.19773	-0.92127	-7.78465
C	1.08407	-1.51353	-5.89511
H	1.82399	-2.18337	-6.35631
C	1.89023	-1.99429	-3.47661
C	1.03963	-1.35535	-4.49284
C	-2.71837	1.85331	-4.45125
H	-2.87276	1.89081	-5.54290
C	-3.54778	2.63416	-3.63374
C	-0.03834	0.05134	1.25284
C	-0.07541	0.20143	2.67590
C	-0.14720	0.48719	5.49876
C	1.08275	0.58867	4.79742
C	1.12109	0.44046	3.39849
C	-1.30810	0.11117	3.37048
C	-1.34441	0.26054	4.77013
O	-0.19041	0.56063	6.86598
O	2.17913	0.82169	5.58001
H	2.06559	0.50785	2.84258
H	-2.22369	-0.06940	2.79193
O	-2.48021	0.19954	5.52405
C	-0.12578	1.87524	7.41068
H	-0.98244	2.50092	7.06370
H	0.83147	2.38225	7.14788
H	-0.18539	1.76210	8.51355
C	-3.70717	-0.05864	4.86864
H	-3.69869	-1.04401	4.34439
H	-3.96234	0.73897	4.13006
H	-4.48154	-0.07781	5.66262
C	3.44746	0.89462	4.95580
H	3.50435	1.73540	4.22366
H	3.70601	-0.05644	4.43239
H	4.18070	1.07174	5.76893
O	4.14888	-3.66703	-0.37795
O	-4.11594	3.32031	-1.34934
H	-4.32510	3.25895	-4.09678

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H    4.49994   -4.19317   -3.06049
C   -5.14478    4.16315   -1.84088
C    5.19283   -4.59474   -0.62331
H   -4.74138    4.95984   -2.50978
H   -5.60555    4.63669   -0.95066
H   -5.92450    3.58509   -2.39123
H    6.00602   -4.14715   -1.24252
H    4.81591   -5.51615   -1.12701
H    5.60190   -4.86664    0.37054

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol          IR     RAMAN
     1                        0.00       0.00000         -       -
     2                        0.00       0.00000         -       -
     3                        0.00       0.00000         -       -
     4                        0.00       0.00000         -       -
     5                        0.00       0.00000         -       -
     6                        0.00       0.00000         -       -
     7        a               5.35       0.05642       YES     YES
     8        a              11.86       0.09718       YES     YES
     9        a              16.11       0.21335       YES     YES
    10        a              26.71       2.33852       YES     YES
    11        a              36.30       3.30537       YES     YES
    12        a              52.48       1.39913       YES     YES
    13        a              56.22       0.07064       YES     YES
    14        a              56.25       0.99352       YES     YES
    15        a              71.66       2.79872       YES     YES
    16        a              78.56       0.77588       YES     YES
    17        a              84.38       1.16515       YES     YES
    18        a              86.14       0.00207       YES     YES
    19        a             100.39       3.57485       YES     YES
    20        a             108.66       0.00265       YES     YES
    21        a             119.80       2.47917       YES     YES
    22        a             133.84       0.42700       YES     YES
    23        a             141.34       0.05991       YES     YES
    24        a             150.17       0.17286       YES     YES
    25        a             150.56       0.39372       YES     YES
    26        a             179.50       0.26465       YES     YES
    27        a             186.97       0.01600       YES     YES
    28        a             190.29       0.82657       YES     YES
    29        a             200.62       0.23183       YES     YES
    30        a             216.36       1.43844       YES     YES
    31        a             221.00       0.46868       YES     YES
    32        a             224.18       0.67599       YES     YES
    33        a             225.50       0.15358       YES     YES
    34        a             236.83       4.29294       YES     YES
    35        a             239.11       4.74695       YES     YES
    36        a             243.09       0.00269       YES     YES
    37        a             254.17       1.11939       YES     YES
    38        a             259.29       3.52165       YES     YES
    39        a             279.72       3.87806       YES     YES
    40        a             286.92       0.83323       YES     YES
    41        a             292.17       0.18119       YES     YES
    42        a             297.43       4.04039       YES     YES
    43        a             308.35      13.43631       YES     YES
    44        a             320.93       0.06007       YES     YES
    45        a             335.64       0.16267       YES     YES
    46        a             345.96       3.53939       YES     YES
    47        a             360.11       0.05491       YES     YES
    48        a             370.94       0.87531       YES     YES
    49        a             394.42       2.56373       YES     YES
    50        a             408.36       1.75714       YES     YES
```

10-Et

SCF Energy (au) BP86/SV(P)	-1688.4974938730
SCF Energy (au) PBE0/def2-TZVPP	-1688.195495855
Zero Point Energy (au)	0.5008318
Chemical potential (kJ mol^{-1})	1123.19

xyz coordinates
65

Au	-0.10346	-0.11064	-1.09574
C	-0.21631	0.08315	0.86317
N	0.00465	-0.30736	-3.13947
C	-1.74035	1.09294	-1.65722
C	-0.93325	0.35532	-3.87750
C	3.76653	-3.08126	-1.91446
O	4.80085	-3.94942	-2.14851
C	1.57289	-1.38146	-1.24288
C	-1.89390	1.12685	-3.07626
C	-2.63343	1.82178	-0.85747
H	-2.50805	1.79326	0.23526
C	-3.67388	2.58106	-1.42957
C	2.38995	-1.92396	-0.24732
H	2.20230	-1.71102	0.81715
C	-0.86879	0.22527	-5.28332
H	-1.60008	0.73834	-5.92420
C	2.96299	-2.52881	-2.92455
H	3.17391	-2.77630	-3.97516
C	3.49095	-2.75621	-0.54780
C	0.14326	-0.56809	-5.84709
H	0.19952	-0.67348	-6.94331
C	1.08584	-1.22962	-5.04276
H	1.87409	-1.84709	-5.49684
C	1.87217	-1.68242	-2.60994
C	1.00491	-1.08827	-3.63958
C	-2.94236	1.88862	-3.65875
H	-3.05921	1.91245	-4.75209
C	-3.83043	2.61242	-2.85564
O	-4.86528	3.37186	-3.31299
O	4.18210	-3.24165	0.51849
O	-4.57643	3.31427	-0.73301
C	-0.29487	0.20679	2.09201
C	-0.38272	0.34770	3.51297
C	-0.55976	0.63217	6.36471
C	0.65924	0.83162	5.68422
C	0.75172	0.69156	4.29113
C	-1.61256	0.14753	4.19829
C	-1.69017	0.28609	5.58745
C	-0.70463	0.77210	7.87382
H	1.56676	1.10172	6.24761
H	1.71693	0.85120	3.78452
H	-2.50810	-0.12599	3.61747
H	-2.65944	0.12081	6.09096
C	5.59388	-3.44527	0.46983
C	-4.48254	3.33858	0.68364
H	-4.61149	2.32119	1.12106
H	-5.30591	3.99429	1.03163
H	-3.50736	3.75841	1.02371
H	5.92428	-3.48146	1.52910
H	6.10787	-2.60053	-0.04268
H	5.86204	-4.39567	-0.03721
C	-5.07570	3.44697	-4.70871
C	5.11215	-4.29205	-3.48512
H	-5.95513	4.10672	-4.85361

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H   -5.29581    2.44491   -5.15041
H   -4.19752    3.88971   -5.23827
H    5.40371   -3.39773   -4.08675
H    4.25949   -4.80627   -3.98992
H    5.97323   -4.98885   -3.43265
C    0.56239    1.13569    8.65581
H    0.97898    2.11622    8.33519
H    1.36015    0.37081    8.52820
H    0.33953    1.20737    9.74281
H   -1.49152    1.53572    8.08184
H   -1.11882   -0.18254    8.27676

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               7.44         0.04939      YES     YES
     8        a              12.69         0.12094      YES     YES
     9        a              15.99         0.47999      YES     YES
    10        a              22.79         1.46875      YES     YES
    11        a              33.53         0.12791      YES     YES
    12        a              34.68         0.38400      YES     YES
    13        a              45.53         2.34280      YES     YES
    14        a              57.19         3.65914      YES     YES
    15        a              64.51         0.40769      YES     YES
    16        a              67.68         0.48998      YES     YES
    17        a              69.66         0.48464      YES     YES
    18        a              77.73         4.01859      YES     YES
    19        a              93.88         7.00341      YES     YES
    20        a             111.48         0.14594      YES     YES
    21        a             132.43         0.03969      YES     YES
    22        a             137.04         0.63129      YES     YES
    23        a             146.26         0.40090      YES     YES
    24        a             154.35         0.47141      YES     YES
    25        a             155.68         0.18398      YES     YES
    26        a             164.10         2.04307      YES     YES
    27        a             173.24         0.31845      YES     YES
    28        a             176.49         0.13745      YES     YES
    29        a             189.74         0.27048      YES     YES
    30        a             200.28         0.42432      YES     YES
    31        a             209.04         2.59093      YES     YES
    32        a             214.64         3.13758      YES     YES
    33        a             221.12         0.54975      YES     YES
    34        a             229.49         1.36391      YES     YES
    35        a             238.49         0.34579      YES     YES
    36        a             240.78         0.97671      YES     YES
    37        a             259.88         0.36864      YES     YES
    38        a             275.75         0.75457      YES     YES
    39        a             282.71        11.94828      YES     YES
    40        a             287.03         0.24883      YES     YES
    41        a             294.58         0.08474      YES     YES
    42        a             317.60         4.06318      YES     YES
    43        a             323.13         4.94366      YES     YES
    44        a             327.39         2.67527      YES     YES
    45        a             336.05         3.94460      YES     YES
    46        a             354.29         0.96290      YES     YES
    47        a             378.21         2.67423      YES     YES
    48        a             391.26        13.66244      YES     YES
```

49	a	402.78	0.08502	YES	YES
50	a	403.00	0.92220	YES	YES

10-H

SCF Energy (au) BP86/SV(P)	-1609.9281049430
SCF Energy (au) PBE0/def2-TZVPP	-1609.630666720
Zero Point Energy (au)	0.4458342
Chemical potential (kJ mol^{-1})	988.03

xyz coordinates
59

Au	-0.06037	-0.09264	-0.08518
C	-0.12574	0.07520	1.87721
N	0.01148	-0.25932	-2.13419
C	-1.65960	1.17997	-0.60189
C	-0.90713	0.45187	-2.84983
C	3.67808	-3.19848	-1.00658
O	4.67459	-4.10179	-1.26947
C	1.56160	-1.42594	-0.27709
C	-1.82853	1.24505	-2.02175
C	-2.51294	1.93610	0.20595
H	-2.41006	1.92586	1.30275
C	-3.53218	2.75192	-0.33306
C	2.36891	-2.01740	0.69805
H	2.20318	-1.81535	1.76829
C	-0.86474	0.34509	-4.25789
H	-1.58171	0.89878	-4.88095
C	2.88406	-2.59766	-1.99622
H	3.07174	-2.83539	-3.05346
C	3.43254	-2.88690	0.36919
C	0.10848	-0.47755	-4.84810
H	0.14773	-0.56585	-5.94652
C	1.03357	-1.18876	-4.06678
H	1.79220	-1.82769	-4.54122
C	1.83132	-1.71461	-1.65302
C	0.97526	-1.06945	-2.66025
C	-2.85651	2.04695	-2.57505
H	-2.99764	2.07473	-3.66539
C	-3.71889	2.78855	-1.75215
O	-4.76553	3.53946	-2.21966
O	4.11613	-3.41579	1.41886
O	-4.31231	3.40804	0.56722
C	-0.16662	0.18853	3.10849
C	-0.21490	0.32016	4.53252
C	-0.31097	0.58415	7.35916
C	0.92128	0.64405	6.68322
C	0.97315	0.51182	5.28866
C	-1.45234	0.26355	5.22935
C	-1.49519	0.39195	6.62459
H	-0.34834	0.68694	8.45648
H	1.85519	0.79397	7.25091
H	1.93847	0.55693	4.75970
H	-2.38014	0.11451	4.65435
H	-2.46602	0.34279	7.14608
C	5.51447	-3.69262	1.34723
C	-4.82996	4.71206	0.30377
H	-4.06481	5.36169	-0.17873
H	-5.08887	5.13393	1.29746
H	-5.73654	4.68018	-0.33608
H	5.85672	-3.75839	2.40125
H	6.06507	-2.87036	0.83649
H	5.72480	-4.64999	0.82635
C	-4.98107	3.61114	-3.61586
C	4.95633	-4.43152	-2.61580
H	-5.86156	4.26993	-3.75891

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H   -5.20374    2.60801   -4.05227
H   -4.10541    4.05269   -4.14972
H    5.27462   -3.53804   -3.20502
H    4.07862   -4.90370   -3.11874
H    5.79073   -5.16135   -2.58679

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               6.81         0.03841       YES     YES
     8        a              15.81         0.11429       YES     YES
     9        a              18.08         0.19353       YES     YES
    10        a              23.16         2.60763       YES     YES
    11        a              34.60         1.10529       YES     YES
    12        a              44.05         1.01804       YES     YES
    13        a              53.08         8.54710       YES     YES
    14        a              61.92         2.33438       YES     YES
    15        a              71.71         2.85497       YES     YES
    16        a              80.28         2.89913       YES     YES
    17        a              82.07         0.36617       YES     YES
    18        a              91.13         0.06788       YES     YES
    19        a             100.30         3.99418       YES     YES
    20        a             113.59         0.65384       YES     YES
    21        a             144.94         1.67792       YES     YES
    22        a             148.94         1.68379       YES     YES
    23        a             152.09         0.21050       YES     YES
    24        a             159.78         0.04367       YES     YES
    25        a             172.75         0.27678       YES     YES
    26        a             180.65         0.04331       YES     YES
    27        a             182.51         3.19505       YES     YES
    28        a             196.14         0.88967       YES     YES
    29        a             212.32         1.54262       YES     YES
    30        a             212.87         1.65610       YES     YES
    31        a             225.86         0.84112       YES     YES
    32        a             230.07         0.68442       YES     YES
    33        a             238.78         0.46750       YES     YES
    34        a             243.83         2.96936       YES     YES
    35        a             267.51         0.97199       YES     YES
    36        a             279.95         2.39770       YES     YES
    37        a             286.55         5.63960       YES     YES
    38        a             299.76         0.75961       YES     YES
    39        a             317.34        13.64811       YES     YES
    40        a             328.61         3.92641       YES     YES
    41        a             331.33         2.46314       YES     YES
    42        a             345.05         5.63141       YES     YES
    43        a             354.67         4.29477       YES     YES
    44        a             384.44         3.67916       YES     YES
    45        a             392.47         0.58071       YES     YES
    46        a             401.75         0.12201       YES     YES
    47        a             416.99         1.91854       YES     YES
    48        a             428.82         1.45852       YES     YES
    49        a             457.15         0.57279       YES     YES
    50        a             458.97         0.79762       YES     YES
```

11-OMe

SCF Energy (au) BP86/SV(P)	-1724.3764529870
SCF Energy (au) PBE0/def2-TZVPP	-1724.081207337
Zero Point Energy (au)	0.4778749
Chemical potential (kJ mol^{-1})	1066.09

xyz coordinates

63

Au	-0.13333	-0.09332	-0.82366
C	-0.23728	0.10269	1.13567
N	-0.03323	-0.28855	-2.86810
C	-1.77242	1.11012	-1.37773
C	-0.97342	0.37550	-3.60196
C	3.73116	-3.06633	-1.65995
O	4.76365	-3.93560	-1.89890
C	1.54226	-1.36412	-0.97838
C	-1.93105	1.14608	-2.79622
C	-2.66312	1.83724	-0.57373
H	-2.53331	1.80698	0.51846
C	-3.70604	2.59672	-1.14095
C	2.36203	-1.90952	0.01349
H	2.17791	-1.69774	1.07883
C	-0.91344	0.24798	-5.00825
H	-1.64683	0.76214	-5.64586
C	2.92495	-2.51134	-2.66650
H	3.13176	-2.75776	-3.71820
C	3.46055	-2.74304	-0.29195
C	0.09678	-0.54437	-5.57670
H	0.14947	-0.64788	-6.67328
C	1.04195	-1.20734	-4.77651
H	1.82852	-1.82434	-5.23421
C	1.83629	-1.66402	-2.34686
C	0.96554	-1.06828	-3.37285
C	-2.98125	1.90919	-3.37389
H	-3.10152	1.93531	-4.46680
C	-3.86679	2.63126	-2.56649
O	-4.90308	3.39182	-3.01913
O	4.15455	-3.23182	0.77132
O	-4.60753	3.32719	-0.43998
C	-0.30943	0.23267	2.36439
C	-0.39096	0.38247	3.78466
C	-0.55499	0.68790	6.61629
C	0.67522	0.87632	5.94997
C	0.74827	0.72174	4.55687
C	-1.62095	0.19757	4.47784
C	-1.70168	0.34485	5.86303
O	-0.73745	0.81162	7.96431
H	1.58691	1.14221	6.50556
H	1.71300	0.86974	4.04596
H	-2.52105	-0.07256	3.90285
H	-2.65338	0.19802	6.39820
C	5.56586	-3.43613	0.71754
C	-4.51054	3.34662	0.97654
H	-4.63713	2.32749	1.41060
H	-5.33402	3.99997	1.32871
H	-3.53517	3.76650	1.31603
H	5.89972	-3.47629	1.77563
H	6.07895	-2.58993	0.20639
H	5.83210	-4.38482	0.20627
C	-5.11725	3.47028	-4.41400
C	5.06987	-4.27636	-3.23709
H	-5.99714	4.13031	-4.55498

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H   -5.33844    2.46931   -4.85765
H   -4.24054    3.91435   -4.94492
H    5.36043   -3.38140   -3.83829
H    4.21485   -4.78864   -3.73992
H    5.93024   -4.97438   -3.18881
C    0.37566    1.14894    8.77072
H    0.80212    2.14355    8.49593
H    1.18305    0.38043    8.70730
H    0.00015    1.19280    9.81336

$vibrational spectrum (first 50 lines)
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol          IR     RAMAN
     1                        0.00       0.00000         -       -
     2                        0.00       0.00000         -       -
     3                        0.00       0.00000         -       -
     4                        0.00       0.00000         -       -
     5                        0.00       0.00000         -       -
     6                        0.00       0.00000         -       -
     7        a               8.49       0.66683       YES     YES
     8        a              12.89       0.08484       YES     YES
     9        a              16.15       0.42660       YES     YES
    10        a              22.92       1.60903       YES     YES
    11        a              34.63       0.38838       YES     YES
    12        a              45.22       2.30127       YES     YES
    13        a              55.61       1.09769       YES     YES
    14        a              58.52       3.10654       YES     YES
    15        a              68.32       0.57488       YES     YES
    16        a              70.11       0.50804       YES     YES
    17        a              77.69       3.94555       YES     YES
    18        a              93.56       7.33400       YES     YES
    19        a             107.63       1.53879       YES     YES
    20        a             111.83       0.08373       YES     YES
    21        a             133.45       0.29710       YES     YES
    22        a             138.55       0.23761       YES     YES
    23        a             148.70       0.43955       YES     YES
    24        a             154.79       0.76613       YES     YES
    25        a             156.79       0.30980       YES     YES
    26        a             164.17       1.89976       YES     YES
    27        a             175.92       0.18654       YES     YES
    28        a             180.94       0.06158       YES     YES
    29        a             197.40       0.30711       YES     YES
    30        a             204.31       0.91940       YES     YES
    31        a             211.26       2.00417       YES     YES
    32        a             215.37       5.37429       YES     YES
    33        a             228.83       1.01303       YES     YES
    34        a             233.12       0.49241       YES     YES
    35        a             240.03       0.75276       YES     YES
    36        a             251.49       3.21836       YES     YES
    37        a             259.65       0.03294       YES     YES
    38        a             261.23       1.70606       YES     YES
    39        a             282.88      12.42439       YES     YES
    40        a             286.90       0.26937       YES     YES
    41        a             292.90       0.55797       YES     YES
    42        a             317.83       4.84545       YES     YES
    43        a             324.71       3.49407       YES     YES
    44        a             330.42       6.94122       YES     YES
    45        a             340.07       0.52020       YES     YES
    46        a             354.56       0.69884       YES     YES
    47        a             378.27       2.83487       YES     YES
    48        a             391.34      13.07460       YES     YES
    49        a             411.87       0.26202       YES     YES
    50        a             416.94       3.25319       YES     YES
```

12-OMe

SCF Energy (au) BP86/SV(P)	-1838.8100353840
SCF Energy (au) PBE0/def2-TZVPP	-1838.516408622
Zero Point Energy (au)	0.5089504
Chemical potential (kJ mol^{-1})	1137.59

xyz coordinates
67

Au	0.06969	-0.18089	-1.26098
C	-0.02027	0.04788	0.69538
N	0.15782	-0.41085	-3.30231
C	-1.56901	1.01793	-1.82622
C	-0.78378	0.24442	-4.04220
C	3.91625	-3.18503	-2.06757
O	4.94300	-4.06360	-2.29724
C	1.73905	-1.46120	-1.40330
C	-1.73485	1.03114	-3.24431
C	-2.45471	1.75924	-1.02970
H	-2.32009	1.74569	0.06224
C	-3.49931	2.51103	-1.60398
C	2.56179	-1.99338	-0.40674
H	2.38423	-1.76287	0.65583
C	-0.73201	0.09300	-5.44644
H	-1.46669	0.59950	-6.08869
C	3.10721	-2.64333	-3.07908
H	3.30677	-2.90907	-4.12746
C	3.65487	-2.83696	-0.70389
C	0.27190	-0.71297	-6.00691
H	0.31785	-0.83560	-7.10182
C	1.21903	-1.36585	-5.20078
H	2.00124	-1.99284	-5.65229
C	2.02446	-1.78527	-2.76810
C	1.15077	-1.20298	-3.79926
C	-2.78652	1.78678	-3.82905
H	-2.91259	1.79488	-4.92159
C	-3.66667	2.52352	-3.02906
O	-4.70363	3.27895	-3.48882
O	4.35274	-3.31030	0.36386
O	-4.39694	3.25334	-0.91033
C	-0.08074	0.19447	1.92274
C	-0.14272	0.36284	3.34213
C	-0.27398	0.68172	6.17875
C	0.95369	0.79433	5.49559
C	1.02061	0.63471	4.10279
C	-1.37840	0.27035	4.03836
C	-1.45965	0.42432	5.42719
O	-0.42108	0.78036	7.53479
H	1.88121	0.99486	6.05237
H	1.99156	0.71804	3.59040
H	-2.30946	0.05816	3.49152
O	-2.68079	0.25043	6.03154
C	5.76255	-3.52323	0.30544
C	-4.29560	3.29141	0.50539
H	-4.42158	2.27825	0.95335
H	-5.11759	3.95004	0.85130
H	-3.31887	3.71514	0.83625
H	6.10245	-3.54655	1.36212
H	6.27717	-2.68905	-0.22361
H	6.02066	-4.48227	-0.19046
C	-4.92525	3.33424	-4.88362
C	5.23959	-4.42926	-3.63099
H	-5.80465	3.99354	-5.03100

H	-5.15076	2.32634	-5.30904
H	-4.05063	3.76752	-5.42679
H	5.53140	-3.54651	-4.24941
H	4.37896	-4.94560	-4.11989
H	6.09652	-5.13096	-3.57549
C	0.73397	0.98763	8.32720
H	1.23730	1.95425	8.08502
H	1.46948	0.15684	8.20827
H	0.38510	1.01480	9.37948
C	-3.22213	1.36727	6.73200
H	-3.33803	2.24818	6.05494
H	-2.59639	1.65652	7.60502
H	-4.22552	1.05256	7.08716

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.66	0.36450	YES	YES
8	a	11.39	0.25481	YES	YES
9	a	15.57	0.66711	YES	YES
10	a	22.80	1.72667	YES	YES
11	a	34.63	0.38922	YES	YES
12	a	45.07	2.51820	YES	YES
13	a	51.16	0.79043	YES	YES
14	a	55.70	3.01332	YES	YES
15	a	62.65	0.98156	YES	YES
16	a	68.46	0.88908	YES	YES
17	a	73.43	3.16669	YES	YES
18	a	77.52	4.29492	YES	YES
19	a	93.48	7.68799	YES	YES
20	a	106.55	1.35786	YES	YES
21	a	111.84	0.11038	YES	YES
22	a	128.44	2.13065	YES	YES
23	a	133.90	0.13154	YES	YES
24	a	138.77	0.47678	YES	YES
25	a	143.28	0.50130	YES	YES
26	a	149.06	0.27752	YES	YES
27	a	156.42	0.30604	YES	YES
28	a	163.90	1.78647	YES	YES
29	a	165.13	1.56789	YES	YES
30	a	176.05	0.16843	YES	YES
31	a	184.42	0.11255	YES	YES
32	a	199.56	0.54251	YES	YES
33	a	203.98	1.04273	YES	YES
34	a	212.55	0.27487	YES	YES
35	a	216.31	6.32720	YES	YES
36	a	221.28	0.22142	YES	YES
37	a	229.85	1.32321	YES	YES
38	a	240.03	0.67649	YES	YES
39	a	244.52	1.17679	YES	YES
40	a	260.01	0.22571	YES	YES
41	a	264.74	1.26574	YES	YES
42	a	281.71	10.66279	YES	YES
43	a	287.07	0.19415	YES	YES
44	a	291.20	2.93743	YES	YES
45	a	299.81	2.44724	YES	YES
46	a	316.31	5.45711	YES	YES

47	a	319.83	5.72818	YES	YES
48	a	330.17	9.40594	YES	YES
49	a	345.69	1.47490	YES	YES
50	a	354.16	0.45436	YES	YES

13-OMe

SCF Energy (au) BP86/SV(P)	-1953.2481300990
SCF Energy (au) PBE0/def2-TZVPP	-1952.956669995
Zero Point Energy (au)	0.5402214
Chemical potential (kJ mol^{-1})	1210.42

xyz coordinates
71

Au	-0.01642	-0.21658	-1.47297
C	-0.04615	0.01365	0.48530
N	0.00695	-0.44528	-3.51664
C	-1.51170	1.17048	-2.00473
C	-0.86307	0.32111	-4.23699
C	3.43065	-3.65223	-2.35853
O	4.34228	-4.64434	-2.60910
C	1.48519	-1.68636	-1.64966
C	-1.70053	1.21026	-3.41929
C	-2.29152	2.00377	-1.18882
H	-2.14111	1.96724	-0.09945
C	-3.25236	2.87468	-1.74078
C	2.25627	-2.31708	-0.66949
H	2.12730	-2.07210	0.39685
C	-0.85458	0.17200	-5.64241
H	-1.53503	0.76552	-6.26967
C	2.67388	-3.01323	-3.35364
H	2.82265	-3.29467	-4.40634
C	3.23591	-3.28326	-0.98904
C	0.03629	-0.74473	-6.22342
H	0.04823	-0.86593	-7.31939
C	0.91296	-1.51003	-5.43683
H	1.60676	-2.22331	-5.90449
C	1.70576	-2.03487	-3.02043
C	0.88944	-1.34754	-4.03367
C	-2.66789	2.08599	-3.98158
H	-2.81187	2.11496	-5.07156
C	-3.44257	2.91479	-3.16259
O	-4.39369	3.78706	-3.60010
O	3.89023	-3.84214	0.06408
O	-4.04540	3.71111	-1.02752
C	-0.07257	0.16473	1.71307
C	-0.10179	0.33714	3.13419
C	-0.15203	0.67025	5.95323
C	0.75714	1.41495	5.15748
C	0.78621	1.24858	3.76011
C	-1.01827	-0.40267	3.92352
C	-1.04929	-0.22991	5.32084
O	-0.14526	0.77104	7.31982
O	1.57385	2.26456	5.85088
H	1.48993	1.81129	3.13253
H	-1.69933	-1.10136	3.41982
O	-1.90060	-0.88732	6.16082
C	5.26430	-4.21945	-0.01821
C	-3.91478	3.72856	0.38651
H	-4.14687	2.73363	0.83279
H	-4.64976	4.47448	0.75038
H	-2.89026	4.03609	0.70065
H	5.61600	-4.28664	1.03261
H	5.86458	-3.44942	-0.55404
H	5.39910	-5.20024	-0.52033
C	-4.63315	3.87549	-4.99036
C	4.57183	-5.03483	-3.94911
H	-5.43321	4.63253	-5.11865

H	-4.98115	2.90271	-5.41489
H	-3.72454	4.20824	-5.54837
H	4.95503	-4.18892	-4.56911
H	3.64855	-5.44392	-4.42501
H	5.34129	-5.83245	-3.91075
C	-0.79927	1.91846	7.85237
H	-1.87837	1.93990	7.56745
H	-0.31066	2.86274	7.51737
H	-0.72008	1.84156	8.95716
C	-2.79206	-1.83536	5.60589
H	-2.24968	-2.66403	5.09121
H	-3.50274	-1.36780	4.88250
H	-3.36633	-2.25291	6.45810
C	2.54152	3.00493	5.13073
H	2.07227	3.69704	4.39101
H	3.25790	2.33795	4.59482
H	3.09568	3.60147	5.88391

$vibrational spectrum (first 50 lines)

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.72	0.08890	YES	YES
8	a	10.65	0.07928	YES	YES
9	a	15.15	0.43269	YES	YES
10	a	22.13	1.09014	YES	YES
11	a	34.62	0.31682	YES	YES
12	a	36.95	3.14799	YES	YES
13	a	44.35	1.09899	YES	YES
14	a	52.09	0.45646	YES	YES
15	a	53.47	4.73243	YES	YES
16	a	60.48	1.70669	YES	YES
17	a	67.20	0.74623	YES	YES
18	a	72.65	3.52193	YES	YES
19	a	77.25	3.59673	YES	YES
20	a	93.65	6.40757	YES	YES
21	a	108.84	0.01587	YES	YES
22	a	111.25	0.27855	YES	YES
23	a	120.36	3.26435	YES	YES
24	a	129.34	0.11927	YES	YES
25	a	133.18	0.22934	YES	YES
26	a	143.09	0.03744	YES	YES
27	a	148.56	0.43859	YES	YES
28	a	151.05	0.28231	YES	YES
29	a	157.19	0.11219	YES	YES
30	a	163.83	2.14751	YES	YES
31	a	175.09	0.16664	YES	YES
32	a	183.46	0.24414	YES	YES
33	a	189.13	0.66368	YES	YES
34	a	199.38	0.01655	YES	YES
35	a	203.64	0.72198	YES	YES
36	a	208.18	4.21408	YES	YES
37	a	213.25	1.08904	YES	YES
38	a	217.24	1.87226	YES	YES
39	a	221.61	1.35533	YES	YES
40	a	235.14	2.91492	YES	YES
41	a	241.12	2.96090	YES	YES
42	a	249.15	0.34557	YES	YES

43	a	257.81	2.40126	YES	YES
44	a	259.65	0.92180	YES	YES
45	a	279.97	5.92303	YES	YES
46	a	283.97	1.38326	YES	YES
47	a	287.11	1.84585	YES	YES
48	a	289.15	5.02818	YES	YES
49	a	292.08	0.09672	YES	YES
50	a	313.65	8.81586	YES	YES

^{3}[**10-H**]

SCF Energy (au) BP86/SV(P)	-1609.8517974340
SCF Energy (au) PBE0/def2-TZVPP	-1609.541933548
Zero Point Energy (au)	0.4411995
Chemical potential (kJ mol^{-1})	974.87

xyz coordinates
59

Au	-0.01193	-0.04181	-0.11077
C	-0.07512	0.13946	1.85763
N	0.07241	-0.19403	-2.13195
C	-1.62879	1.18648	-0.62371
C	-0.87102	0.51341	-2.88013
C	3.66991	-3.20461	-1.01185
O	4.66704	-4.10662	-1.25479
C	1.56407	-1.41221	-0.30057
C	-1.78287	1.28987	-2.07496
C	-2.52886	1.86066	0.19861
H	-2.44197	1.80613	1.29540
C	-3.55409	2.68187	-0.32309
C	2.30961	-2.05984	0.68817
H	2.11175	-1.87801	1.75628
C	-0.82151	0.38433	-4.28548
H	-1.55108	0.92723	-4.90703
C	2.92752	-2.56757	-2.01364
H	3.15332	-2.77620	-3.06941
C	3.36944	-2.93588	0.37386
C	0.14452	-0.43757	-4.89270
H	0.17730	-0.53973	-5.98798
C	1.07061	-1.15387	-4.08080
H	1.81846	-1.81272	-4.54787
C	1.86679	-1.68472	-1.68990
C	1.02339	-1.02719	-2.68457
C	-2.81355	2.11925	-2.60440
H	-2.93017	2.20390	-3.69443
C	-3.69955	2.79441	-1.76298
O	-4.74087	3.55751	-2.20179
O	4.00601	-3.50449	1.42954
O	-4.36560	3.27491	0.58844
C	-0.11633	0.25360	3.09207
C	-0.16009	0.39113	4.51257
C	-0.24652	0.66973	7.33973
C	0.98117	0.75111	6.65652
C	1.02826	0.61487	5.26290
C	-1.39286	0.31018	5.21884
C	-1.43099	0.44884	6.61254
H	-0.28007	0.77796	8.43662
H	1.91448	0.92386	7.21871
H	1.98889	0.68029	4.72761
H	-2.31985	0.13552	4.64977
H	-2.39759	0.38315	7.14006
C	5.38833	-3.85957	1.39854
C	-5.00388	4.53186	0.36313
H	-4.32030	5.25043	-0.14098
H	-5.26333	4.91548	1.37176
H	-5.92763	4.42049	-0.24285
H	5.69688	-3.93469	2.46211
H	5.99792	-3.07752	0.89337
H	5.55325	-4.83389	0.89260
C	-4.96314	3.68076	-3.59741
C	4.98796	-4.42857	-2.59697
H	-5.85262	4.33247	-3.71036

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H   -5.16946    2.69005   -4.06559
H   -4.09223    4.15324   -4.10940
H    5.33500   -3.53201   -3.16321
H    4.11842   -4.88174   -3.12874
H    5.81118   -5.16941   -2.54708

$vibrational spectrum (first 50 lines)
```

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.31	1.09814	YES	YES
8	a	15.73	0.07671	YES	YES
9	a	18.13	0.11895	YES	YES
10	a	22.46	3.39703	YES	YES
11	a	31.85	6.14421	YES	YES
12	a	39.30	1.18654	YES	YES
13	a	49.70	9.24544	YES	YES
14	a	56.22	17.62587	YES	YES
15	a	71.13	1.00251	YES	YES
16	a	80.46	0.29835	YES	YES
17	a	85.99	2.90599	YES	YES
18	a	91.07	0.83044	YES	YES
19	a	103.42	7.12190	YES	YES
20	a	121.19	14.19310	YES	YES
21	a	138.94	29.32670	YES	YES
22	a	145.59	0.03422	YES	YES
23	a	155.47	41.22492	YES	YES
24	a	166.92	1.30878	YES	YES
25	a	170.37	1.57737	YES	YES
26	a	178.94	3.10812	YES	YES
27	a	183.55	0.03202	YES	YES
28	a	192.62	3.83979	YES	YES
29	a	200.59	4.15380	YES	YES
30	a	214.60	9.01672	YES	YES
31	a	217.22	11.57560	YES	YES
32	a	227.07	1.50105	YES	YES
33	a	233.49	10.54861	YES	YES
34	a	240.68	2.65784	YES	YES
35	a	259.06	0.43878	YES	YES
36	a	270.00	27.94506	YES	YES
37	a	276.70	15.40868	YES	YES
38	a	285.88	1.92262	YES	YES
39	a	311.16	6.05176	YES	YES
40	a	323.10	9.89410	YES	YES
41	a	328.50	17.53157	YES	YES
42	a	339.81	28.49956	YES	YES
43	a	351.45	52.61644	YES	YES
44	a	355.09	9.33560	YES	YES
45	a	380.03	131.73043	YES	YES
46	a	397.02	0.81214	YES	YES
47	a	400.39	16.66924	YES	YES
48	a	413.08	283.47386	YES	YES
49	a	435.56	205.14898	YES	YES
50	a	439.87	5.95888	YES	YES

References

1. K. Suzuki, A. Kobayashi, S. Kaneko, K. Takehira, T. Yoshihara, H. Ishida, Y. Shiina, S. Oishi and S. Tobita, *Phys. Chem. Chem. Phys.*, 2009, **11**, 9850–9860.
2. *CrysAlisPro, Oxford Diffraction Ltd. Version 1.171.34.41*.
3. *Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm within CrysAlisPro software, Oxford Diffraction Ltd. Version 1.171.34.40*.
4. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.
5. G. Sheldrick, *Acta Crystallogr. A*, 2015, **71**, 3-8.
6. G. Sheldrick, *Acta Crystallogr. A*, 2008, **64**, 112-122.
7. T. Cardinaels, J. Ramaekers, P. Nockemann, K. Driesen, K. Van Hecke, L. Van Meervelt, G. Wang, S. De Feyter, E. F. Iglesias, D. Guillon, B. Donnio, K. Binnemans and D. W. Bruce, *Soft Matter*, 2008, **4**, 2172-2185.
8. *US Pat.*, US20180237433A1, 2018
9. P. Császár and P. Pulay, *J. Mol. Struct.*, 1984, **114**, 31-34.
10. R. Ahlrichs, M. Bär, M. Häser, H. Horn and C. Kölmel, *Chem. Phys. Lett*, 1989, **162**, 165-169.
11. P. Deglmann, F. Furche and R. Ahlrichs, *Chem. Phys. Lett*, 2002, **362**, 511-518.
12. P. Deglmann, K. May, F. Furche and R. Ahlrichs, *Chem. Phys. Lett*, 2004, **384**, 103-107.
13. K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett*, 1995, **242**, 652-660.
14. K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theor. Chem. Acc.*, 1997, **97**, 119-124.
15. O. Treutler and R. Ahlrichs, *J. Chem. Phys.*, 1995, **102**, 346-354.
16. M. von Arnim and R. Ahlrichs, *J. Chem. Phys.*, 1999, **111**, 9183-9190.