# Supplemental Information

## Synthesis, structural characterization, electronic spectroscopy, and microfluidic detection of Cu$^{+2}$ and UO$_2$$^{+2}$ [di-tert-butyl-salphenazine] complexes

B. A. Maynard,[a] J. C. Brooks,[a] E. E. Hardy[a], C. J. Easley,[a] and A. E. V. Gorden[a*]

[a] Department of Chemistry and Biochemistry, Auburn University, 179 Chemistry Building, Auburn, Alabama 36849, USA.

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## Experimental

*Caution! The UO$_2$(NO$_3$)$_2$•6H$_2$O used in this study contained depleted uranium, standard precautions for handling radioactive materials or heavy metals, such as uranyl nitrate, were followed.*

Pyridine (99.8%, Sigma-Aldrich), 3,5-di-tert-butylsalicyaldehyde (98%, TCI), 2,3-diaminophenazine (98%, Aldrich), and Copper (II) acetyacetonate (98% STREM) were used as received without further purification. UO$_2$(NO$_3$)$_2$•6H$_2$O (98%, J. T. Baker) was recrystallized from a nitric acid solution and stored under hexanes until use.

## Synthesis

Complex **Cu[di-tert-butylsal-phenazine]**: 50 ml of pyridine was placed in a round bottom flask charged with a stir bar and heated at 80 ºC. A 0.2204 gram (0.9406 mmol) addition of 3,5-ditertbutyl salicyaldehyde was added to dissolve in the warmed solution. A 0.1253 gram (0.4787 mmol) addition of copper (II) acetylacetonate was dissolved in the warmed solution. In a separate beaker 0.0982 gram (0.4671 mmol) of 2,3-diaminophenazine was dissolved in about 25 ml of pyridine. The pyridine solution was added slowly with the aide of a syringe pump set to deliver 4ml/hr. The reaction was allowed to proceed for 24 hours, then the reaction mixture was allowed to come to room temperature and subsequently rotovapped to dryness. Column chromatography was performed with a mobile phase of 3:4 acetone to hexanes. This was set up in an attempt to isolate the red/maroon/violet spot seen on the TLC plate. Single crystals of X-ray diffraction quality were obtained after 2 days of slow evaporation. M+1 found 703.1739 and calculated 704.4018. A THF solution containing ~50 mg was placed in several test tubes and then put in secondary containers for slow diffusion crystallization containing secondary solvents. Crystals were observed in the MeOH and EtOH slow evaporation chambers. CCDC# 1019624

Complex **UO$_2$[di-tert-butylsal-phenazine]**: 50 ml of pyridine was placed in a round bottom flask charged with a stir bar and heated at 80 ºC.  A 0.2219 gram (0.9500 mmol) addition of 3,5-di-tert-butylsalicyaldehyde was added to dissolve in the warmed solution.  A 0.2381 gram (0.4740 mmol) addition of UO$_2$(NO$_3$)$_2$•6H$_2$O was then added to the flask and allowed to dissolve in the warmed solution.  Several increments totaling 0.0996 g (0.474 mmol) of 2,3 diaminophenazine was then added to the flask in equal increments over the course of 1 hour.  The reaction was then allowed to heat for 24 hours.   A mixture of products were obtained by mass spectroscopy analysis.   This mixture was purified by column chromatography using a 1:1 ratio of ethyl acetate to hexanes as the mobile phase.  LCMS: M+1  found 911.4117 and calculated 913.8996 calculated.  A THF solution containing ~50 mg was placed in several test tubes and then put in secondary containers for slow diffusion crystallization containing secondary solvents.  Crystals were observed in the MeOH and EtOH slow evaporation chambers. CCDC# 1019622

Ligand **L**: UO$_2$[di-tert-butylsalphenazine] (50 mg, 0.055 mmol) was dissolved in 15 mL of THF and 20 mL of Chloroform. Twice the molar equivalent of nitric acid (0.11 mmol) was added to the organic phase in a separatory funnel. Solution was shaken, vented and organic layer removed. The organic layer was then washed with ~30 mL of water three times. This process of alternating an acid wash with three aqueous washes was repeated until an orange color was obtained. Solvent was removed using a rotovap. Products were confirmed via mass spec analysis with peaks at 643.4036 m/z (**L** = di-tert-butylsalphenazine)

**Microfluidic Device Fabrication**

Microdevices were fabricated using polydimethylsiloxane (PDMS) and soft lithography techniques.[1,2]The silicon wafer master design (Figure 4a) was a previously established droplet generating chip designed in house.[1] Wafers were pre-treated with 1mL of chlorotrimethylsilane for 30 min. After mixing 10:1 base to curing agent of PDMS, the de-gassed mixture was cured on top of the wafer at 65˚C overnight. Once cured, the PDMS was carefully peeled off the wafer and designated inlet/outlets were punched for sample and outlet wells. The PDMS along with a glass microscope slide was then washed with methanol, dried with a nitrogen air gun, and cleaned with scotch tape. Once cleaned, both the PDMS chip and the microscope slide were placed in an air plasma cleaner for 45 sec (Harrick Plasma) and immediately placed on top of each other to bond together. 1.5cm OD Tygon tubing was inserted into the outlet well, and a blunt ended needle was inserted into the opposite end of the tubing. Aquapel (Pittsburgh Glass Works) was applied to each of the inlet channels of the chip and pulled through with a mild vacuum to surface treat the channels. Methanol was washed through as well to remove any excess Aquapel. Chips were then placed back into the 65 ˚C oven to dry for at least 4 hours. Solutions were flowed through the chips passively, via a handheld, 25mL syringe connected to the needle in the tubing. Chips were taped to the imaging stage to hold them in place. Vacuum was applied to the chip on the stage and the droplets were imaged directly on the chip. In order to form oil in organic droplets, 1.8% w/w Krytox 157 FSL surfactant (Dupont) in HFE-7500 oil (3M) droplet carrier fluid was applied to the oil well.[1]

# Electronic Spectroscopy
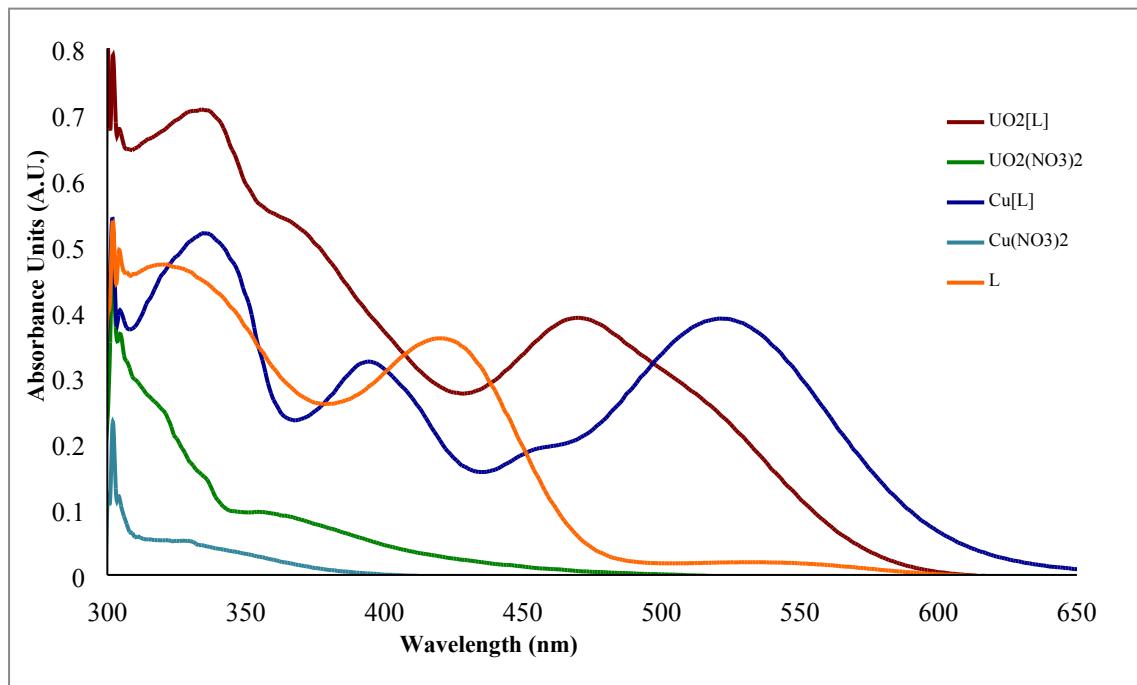


**Figure SI1** Electronic spectra in the UV-Vis energy range of L, Cu[L], $UO_2[L]$, $Cu(NO_3)_2$, and $UO_2(NO_3)_2$ starting materials. All samples were run at 20 μM.
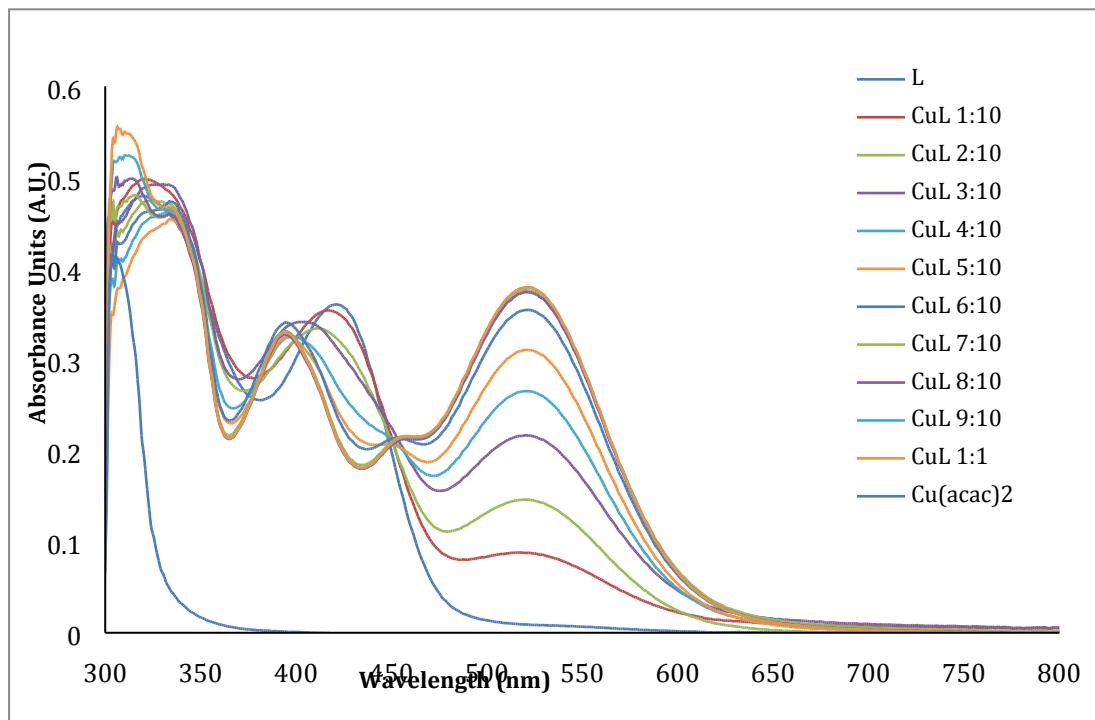


**Figure SI2** $Cu^{+2}$ titration of the ligand in pyridine indicates a 1:1 $Cu^{+2}$ to L complex. L concentration was kept at 20 μM. Spectra were obtained minutes after the solutions were made.
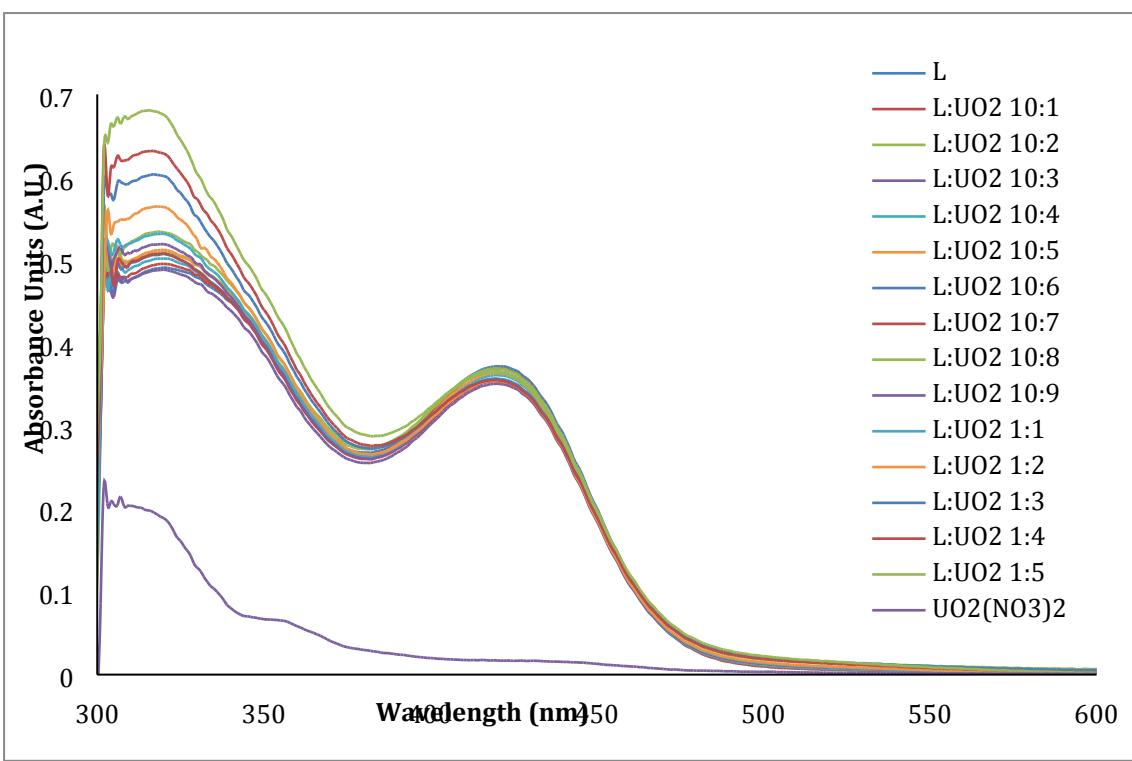
**Figure SI3** $UO_2^{+2}$ titration of the ligand in pyridine indicates a 1:1 $UO_2^{+2}$ to L complex. L concentration was kept at 20 μM. Spectra were obtained minutes after the solutions were made.
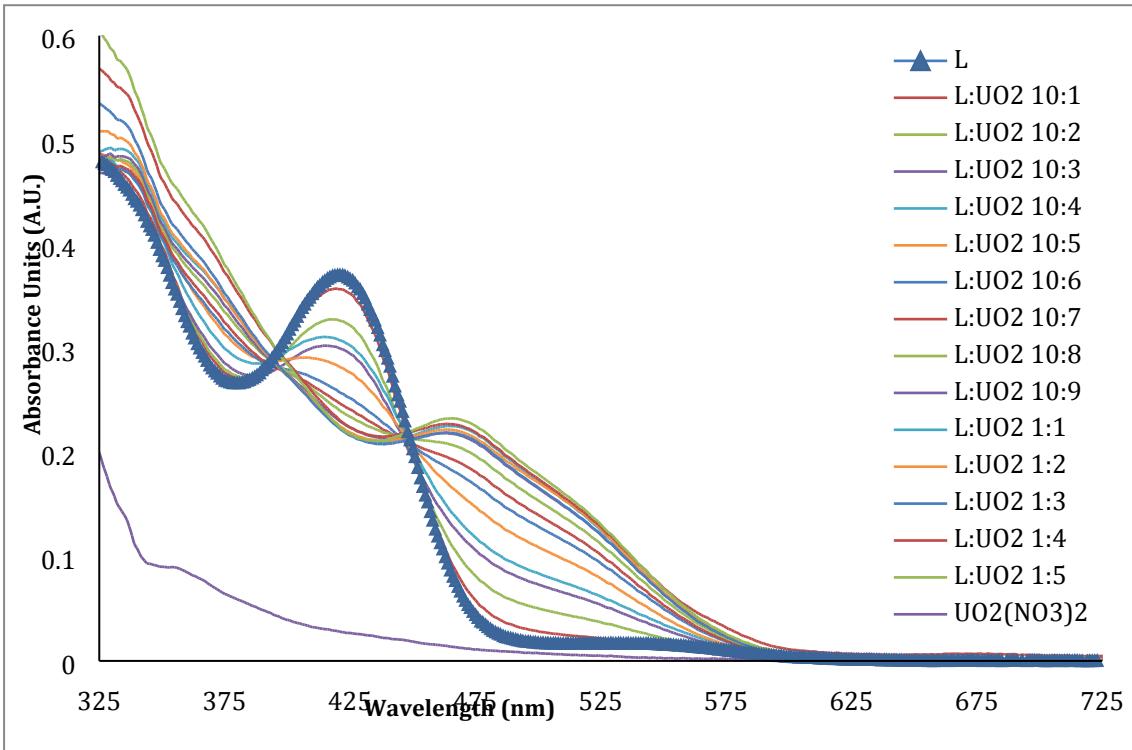


**Figure SI4** $UO_2^{+2}$ titration of the ligand in pyridine indicates a 1:1 $UO_2^{+2}$ to L complex. L concentration was kept at 20 μM. Spectra were obtained after 3days.

## Microspectophotometer Imaging

UV−Visible data were acquired from microfluidic droplets and microwells using a CRAIC Technologies 20/20 PV microspectrophotometer. 400 picoliter droplets were generated on the microfluidic chip and the data were collected from 200 to 800 nm. Microwell data was also measured using the same parameters and fixed pathlength. The exposure time was auto-optimized by the CRAIC Minerva 8.7.3.12 software.

## µWell Chips

2.5mm diameter holes were punched into flat pieces of PDMS. These portions of PDMS were made in a similar fashion as the droplet generating chip, but they were cured over a plain, untemplated wafer. Chips with up to 30 holes were then plasma oxidized, bonded, and treated as stated previously. Each well served as a micro sized cuvette (10 µL) for collecting spectral data on the CRAIC microspectrophotometer. Samples were pipetted into separate wells and the chip was placed onto the imaging stage. Spectral data was collected directly from the chip.
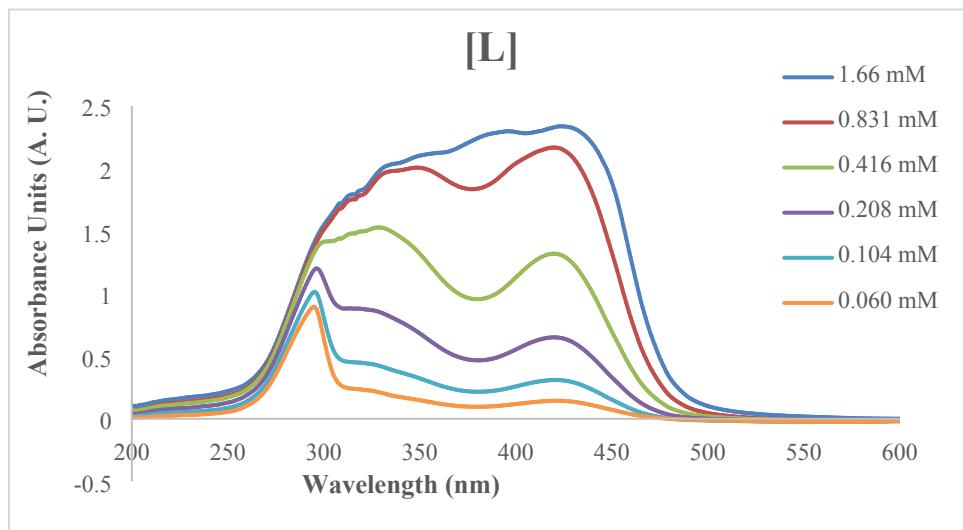


**Figure SI5** Electronic spectra in the UV-Vis energy range of L at various concentrations as collected on the chip using the microspectrophotometer
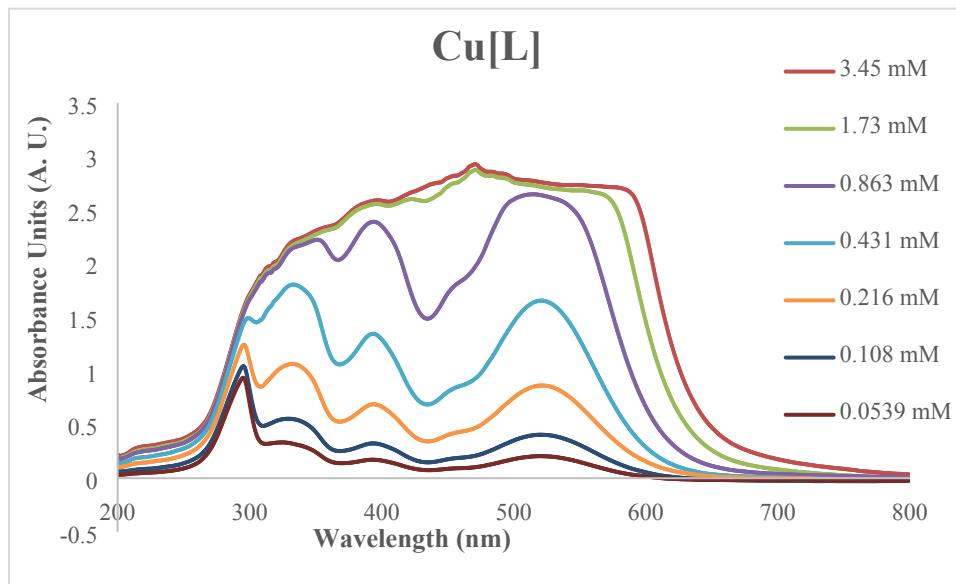


**Figure SI6** Electronic spectra in the UV-Vis energy range of Cu[L] at various concentrations as collected on the chip using the microspectrophotometer
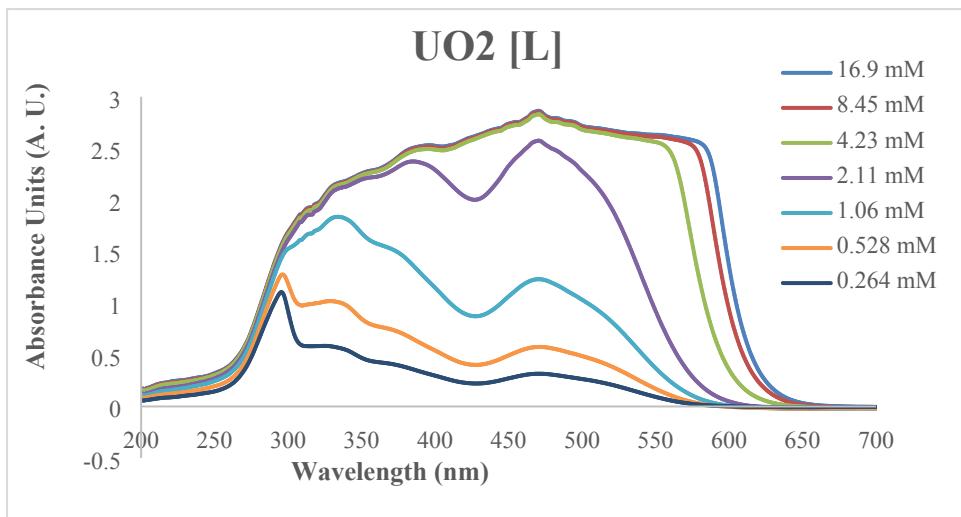
**Figure SI7** Electronic spectra in the UV-Vis energy range of $UO_2[L]$ at various concentrations as collected on the chip using the microspectrophotometer

## Single crystal X-ray diffraction

The X-ray diffraction datasets were collected at 183K, on a Bruker SMART APEX CCD X-ray diffractometer unit using Mo Kα radiation, from crystals mounted in Paratone-N oil on glass fibers. SMART (v 5.624) was used for preliminary determination of cell constants and data collection control. Determination of integrated intensities and global cell refinement were performed with the Bruker SAINT software package using a narrow-frame integration algorithm. The program suite ShelXTL (v 5.1) was used for space group determination, structure solution, and refinement.[3] Refinement was performed against $F^2$ by weighted full-matrix least squares, and empirical absorption correction (SADABS) was applied.[4] Projections were generated in the Olex2.1-1 graphics program.[5]

# Cu[di-tert-butyl-salphenazine]
## Crystal Data and Experimental
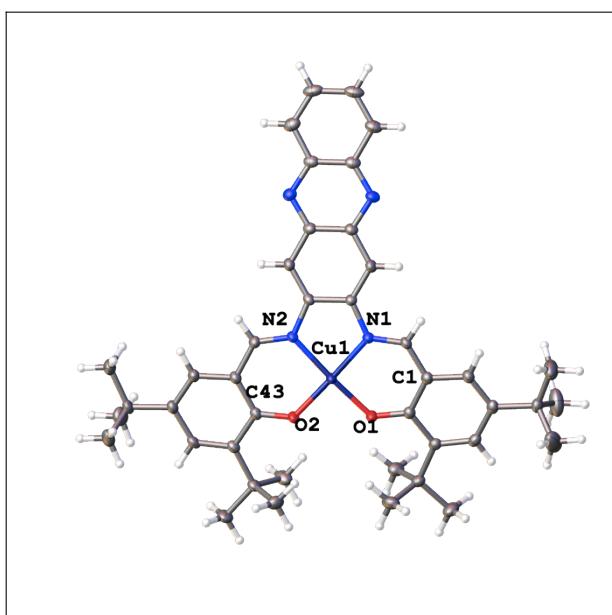


| | |
|---|---|
| CCDC | 1019624 |
| Formula | $C_{42}H_{48}CuN_4O_2$ |
| $D_{calc.}$/ g cm$^{-3}$ | 1.274 |
| $\mu$/ mm$^{-1}$ | 0.636 |
| Formula Weight | 704.39 |
| Colour | Red |
| Shape | Prism |
| Size/$mm^3$ | $0.48 \times 0.11 \times 0.05$ |
| T/K | 180(2) |
| Crystal System | Triclinic |
| Space Group | $P\bar{1}$ |
| a/ | 9.9751(2) |
| b/ | 12.6630(3) |
| c/ | 14.8623(3) |
| $\alpha$/° | 93.6100(10) |
| $\beta$/° | 96.8350(10) |
| $\gamma$/° | 98.7160(10) |
| $V$/$^3$ | 1836.17(7) |
| $Z$ | 2 |
| $\Theta_{min}$° | 1.38 |
| $\Theta_{max}$/° | 26.77 |
| Measured Refl. | 60413 |
| Independent Refl. | 7756 |
| Reflections Used | 6595 |
| $R_{int}$ | 0.0333 |
| Parameters | 454 |
| Restraints | 0 |
| Largest Peak | 0.925 |
| Deepest Hole | -0.422 |
| GooF | 1.062 |
| $wR_2$(all data) | 0.0966 |
| $wR_2$ | 0.0924 |
| $R_1$(all data) | 0.0465 |
| $R_1$ | 0.0365 |

**Crystal Data**. $C_{42}H_{48}CuN_4O_2$, M = 704.39, Tri- clinic, $P\bar{1}$ (No. 2, $a$ = 9.9751(2) A, $b$ = 12.6630(3) A, $c$ = 14.8623(3) A, $\alpha$ = 93.61°, $\beta$ = 96.835°, $\gamma$ = 98.716°, $V$ = 1836.17(7)$A^3$, $T$ = 180(2) K, $Z$ = 2, $\mu$(Mo K$\alpha$) = 0.636, 60413 reflections measured, 7756 unique ($R_{int}$ = 0.0333) which were used in all calculations. The final $wR_2$ was 0.0966 (all data) and $R_1$ was 0.0365 (> $2\sigma(I)$).

**Experimental**. Single crystals of $C_{42}H_{48}CuN_4O_2$ (**Cu[di-tert-butylsal-phenazine**) were obtained by recrystallization from slow evaporation from a concentrated THF solution at room temperature. A suitable crystal ($0.48 \times 0.11 \times 0.05 mm^3$) was selected and mounted on a glass fiber with paratone N cryoprotectant on a Bruker APEX diffractometer. The crystal was kept at 180(2) K during data collection. Using Bruker APEX2, the structure was solved with the ShelX structure solution program, using direct methods. The model was refined with the ShelXL refinement package using least squares minimization.

Table 1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{A}^2 \times 10^3$) for Cu[di-tert-butylsal-phenazine. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{IJ}$ tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| Cu1 | −34.8(2) | 9894.14(17) | 3409.36(14) | 17.76(8) |
| O2 | −646.1(13) | 10812.6(10) | 2549.2(9) | 22.9(3) |
| O1 | −1372.4(13) | 8750.6(10) | 2809.7(9) | 24.1(3) |
| N1 | 588.6(15) | 9024.8(12) | 4345(1) | 18.0(3) |
| C3 | −3235.1(19) | 7306.3(16) | 1497.6(13) | 24.2(4) |
| N4 | 5471.4(16) | 11198.0(13) | 6253.3(11) | 23.1(3) |
| N3 | 4452.3(16) | 9069.5(13) | 6656.1(11) | 23.7(3) |
| N2 | 1449.6(15) | 10983.9(12) | 4003.7(10) | 17.7(3) |
| C16 | 1790.7(18) | 9523.4(14) | 4912.7(12) | 17.7(4) |
| C27 | 2288.2(18) | 10608.6(14) | 4713.9(12) | 17.5(4) |
| C28 | 1706.0(19) | 11965.6(14) | 3766.8(12) | 19.8(4) |
| C29 | 998.2(19) | 12396.8(14) | 3027.6(12) | 20.1(4) |
| C43 | −122.2(18) | 11788.1(14) | 2426.6(12) | 19.0(4) |
| C37 | −663.1(19) | 12281.2(15) | 1643.1(12) | 20.1(4) |
| C36 | −99.0(19) | 13318.1(15) | 1536.1(13) | 22.1(4) |
| C31 | 988.2(19) | 13946.8(15) | 2130.2(13) | 21.9(4) |
| C30 | 1511.9(19) | 13475.5(15) | 2864.0(13) | 22.4(4) |
| C32 | 1516(2) | 15084.3(15) | 1897.2(14) | 25.9(4) |
| C35 | 352(2) | 15754.7(17) | 1855.0(18) | 38.1(5) |
| C34 | 2026(2) | 15012.7(19) | 961.7(16) | 39.2(5) |
| C33 | 2697(2) | 15652.5(17) | 2588.3(17) | 37.7(5) |
| C38 | −1808(2) | 11645.7(15) | 945.4(13) | 22.9(4) |
| C41 | −1302(2) | 10660.0(18) | 533.4(14) | 34.4(5) |
| C40 | −3098(2) | 11297.0(18) | 1389.9(15) | 32.8(5) |
| C39 | −2209(2) | 12309.9(18) | 157.7(15) | 34.5(5) |
| C26 | 3487.7(19) | 11152.2(15) | 5171.1(12) | 20.9(4) |
| C25 | 4265.3(19) | 10661.9(15) | 5844.6(12) | 19.9(4) |
| C18 | 3756.9(19) | 9592.4(15) | 6046.1(12) | 20.2(4) |
| C19 | 5648.7(19) | 9611.1(16) | 7076.5(12) | 22.7(4) |
| C20 | 6433(2) | 9106.4(18) | 7742.6(13) | 28.6(4) |
| C21 | 7645(2) | 9636.1(19) | 8175.4(14) | 31.3(5) |
| C22 | 8161(2) | 10687.6(19) | 7974.3(14) | 31.2(5) |
| C23 | 7451(2) | 11198.4(17) | 7336.8(14) | 28.4(4) |
| C24 | 6165.1(19) | 10677.2(16) | 6873.5(12) | 22.3(4) |
| C17 | 2502.2(19) | 9047.7(15) | 5569.3(13) | 21.8(4) |
| C14 | −1085.7(19) | 7423.9(15) | 3867.0(13) | 20.7(4) |
| C1 | −1681.0(18) | 7780.3(14) | 3036.6(13) | 19.8(4) |
| C2 | −2645.7(18) | 7006.0(15) | 2436.5(13) | 21.0(4) |
| C4 | −4160(2) | 6347.5(18) | 939.3(15) | 35.6(5) |
| C6 | −2070(2) | 7673.1(18) | 939.1(14) | 30.9(5) |
| C5 | −4094(2) | 8202.1(19) | 1618.6(16) | 35.2(5) |
| C7 | −3006.8(19) | 5999.8(15) | 2728.0(13) | 22.8(4) |
| C8 | −2483.1(19) | 5651.4(15) | 3570.4(13) | 21.5(4) |
| C13 | −1523.9(19) | 6368.2(15) | 4111.4(13) | 22.3(4) |
| C9 | −2928(2) | 4494.5(15) | 3793.5(14) | 25.1(4) |
| C10 | −4474(3) | 4182(2) | 3670(3) | 66.5(9) |
| C15 | 13.9(18) | 8047.6(14) | 4448.7(12) | 19.2(4) |
| C11 | −2341(4) | 3735(2) | 3154(2) | 60.1(8) |
| C12 | −2397(3) | 4299(2) | 4772.4(19) | 55.0(7) |

Table 2: Anisotropic Displacement Parameters ($\times 10^4$) **bam151_0m**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^* \times b \times U_{12}]$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Cu1 | 22.10(13) | 15.05(12) | 14.70(12) | 3.27(8) | −2.47(8) | 1.40(8) |
| O2 | 27.3(7) | 18.9(7) | 19.8(7) | 6.2(5) | −5.0(5) | 0.0(5) |
| O1 | 28.0(7) | 18.4(7) | 22.3(7) | 4.3(5) | −7.0(6) | −0.8(5) |
| N1 | 20.5(8) | 17.6(7) | 15.0(7) | 1.5(6) | −0.5(6) | 2.4(6) |
| C3 | 23(1) | 24.7(10) | 22.5(10) | 1.0(8) | −2.8(8) | 0.7(8) |
| N4 | 23.7(8) | 23.6(8) | 20.7(8) | −1.1(6) | −0.1(6) | 2.7(7) |
| N3 | 23.9(8) | 28.2(9) | 18.6(8) | 5.8(7) | −1.1(6) | 4.7(7) |
| N2 | 21.3(8) | 16.8(7) | 14.7(7) | 2.6(6) | −0.2(6) | 3.5(6) |
| C16 | 19.2(9) | 18.1(9) | 15.2(9) | 0.6(7) | 0.8(7) | 2.6(7) |
| C27 | 22.0(9) | 17.5(9) | 13.4(8) | 1.8(7) | 1.6(7) | 5.1(7) |
| C28 | 23.5(9) | 17.3(9) | 17.5(9) | 0.9(7) | 0.2(7) | 1.9(7) |
| C29 | 24.1(9) | 18.5(9) | 18.1(9) | 3.8(7) | 2.1(7) | 4.8(7) |
| C43 | 22.5(9) | 17.9(9) | 17.6(9) | 3.2(7) | 3.6(7) | 5.2(7) |
| C37 | 22.7(9) | 21.7(9) | 17.5(9) | 4.1(7) | 3.2(7) | 6.7(7) |
| C36 | 24.3(10) | 23.6(10) | 20.8(10) | 9.0(8) | 2.6(7) | 8.7(8) |
| C31 | 24(1) | 17.9(9) | 25.3(10) | 6.4(7) | 4.1(8) | 4.9(7) |
| C30 | 23.6(10) | 18.1(9) | 24.8(10) | 3.3(7) | 0.0(8) | 2.8(7) |
| C32 | 27.4(10) | 19.8(9) | 31.4(11) | 11.0(8) | 2.3(8) | 4.2(8) |
| C35 | 35.7(12) | 24.2(11) | 56.3(15) | 12.1(10) | 4.7(11) | 8.6(9) |
| C34 | 43.2(13) | 36.3(13) | 38.7(13) | 14.5(10) | 11.2(10) | −0.5(10) |
| C33 | 40.2(13) | 23.6(11) | 45.7(14) | 12.5(10) | −5.3(10) | −2.3(9) |
| C38 | 27.2(10) | 23.4(10) | 17.7(9) | 5.1(7) | −1.3(8) | 5.0(8) |
| C41 | 46.1(13) | 33.7(12) | 21.9(11) | −3.2(9) | −5.9(9) | 12(1) |
| C40 | 24.9(10) | 39.2(12) | 31.8(12) | 6.1(9) | −1.2(9) | −0.5(9) |
| C39 | 38.6(12) | 35.1(12) | 27.1(11) | 10.6(9) | −9.1(9) | 4(1) |
| C26 | 25.8(10) | 16.5(9) | 19.8(9) | 2.9(7) | 0.6(7) | 2.6(7) |
| C25 | 21.3(9) | 21.7(9) | 16.0(9) | −1.7(7) | 0.0(7) | 4.4(7) |
| C18 | 21.6(9) | 23.5(9) | 15.5(9) | 2.5(7) | 1.2(7) | 4.4(7) |
| C19 | 22.1(9) | 31.4(11) | 15.5(9) | 0.7(8) | 2.3(7) | 7.2(8) |
| C20 | 28.3(11) | 38.6(12) | 20(1) | 4.6(8) | 0.3(8) | 10.7(9) |
| C21 | 26.9(11) | 48.9(13) | 19.4(10) | −0.2(9) | −2.1(8) | 15.9(10) |
| C22 | 22.1(10) | 47.1(13) | 22.5(10) | −8.6(9) | −3.1(8) | 8.7(9) |
| C23 | 25.3(10) | 32.6(11) | 25.4(11) | −7.1(8) | 1.1(8) | 4.0(8) |
| C24 | 22.4(9) | 28.3(10) | 16.4(9) | −3.1(8) | 1.0(7) | 7.8(8) |
| C17 | 25.3(10) | 19.1(9) | 20.4(10) | 6.2(7) | 0.4(8) | 1.6(7) |
| C14 | 22.2(9) | 18.2(9) | 21.6(10) | 1.0(7) | 2.0(7) | 4.4(7) |
| C1 | 19.7(9) | 18.5(9) | 21.3(9) | 1.4(7) | 2.1(7) | 3.6(7) |
| C2 | 18.2(9) | 21.7(9) | 22.3(10) | 0.2(7) | 0.9(7) | 3.3(7) |
| C4 | 36.5(12) | 36.2(12) | 26.8(11) | 1.0(9) | −7.1(9) | −7.4(10) |
| C6 | 30.4(11) | 37.1(12) | 23.8(11) | 6.3(9) | 0.0(8) | 1.9(9) |
| C5 | 30.6(11) | 39.4(13) | 34.6(12) | 1.3(10) | −7.0(9) | 11.9(10) |
| C7 | 19.6(9) | 21.2(9) | 26.2(10) | −2.1(8) | 1.9(8) | 0.9(7) |
| C8 | 21.7(9) | 18.0(9) | 25.8(10) | 1.5(7) | 6.1(8) | 4.2(7) |
| C13 | 24.5(10) | 19.4(9) | 23.5(10) | 4.0(7) | 2.1(8) | 4.9(7) |
| C9 | 25.7(10) | 19.4(9) | 29.5(11) | 4.1(8) | 4.6(8) | 0.2(8) |
| C10 | 39.1(15) | 55.3(18) | 107(3) | 42.3(18) | 8.4(16) | −1.2(13) |
| C15 | 23.1(9) | 17.4(9) | 17.7(9) | 4.1(7) | 0.5(7) | 5.8(7) |
| C11 | 96(2) | 27.6(13) | 61.9(19) | 6.5(12) | 20.6(17) | 10.3(14) |
| C12 | 78(2) | 32.1(13) | 47.3(16) | 14.1(11) | −10.7(14) | −5.3(13) |

Table 3: Bond Lengths in Å for **Cu[L]**.

| Atom | Atom | Å | Atom | Atom | Å |
|------|------|------|------|------|------|
| Cu1 | O2 | 1.8909(12) | C31 | C30 | 1.364(3) |
| Cu1 | O1 | 1.9079(13) | C31 | C32 | 1.532(3) |
| Cu1 | N1 | 1.9305(15) | C32 | C33 | 1.524(3) |
| Cu1 | N2 | 1.9475(15) | C32 | C35 | 1.536(3) |
| O2 | C43 | 1.299(2) | C32 | C34 | 1.539(3) |
| O1 | C1 | 1.296(2) | C38 | C39 | 1.534(3) |
| N1 | C15 | 1.309(2) | C38 | C40 | 1.535(3) |
| N1 | C16 | 1.418(2) | C38 | C41 | 1.535(3) |
| C3 | C5 | 1.536(3) | C26 | C25 | 1.424(3) |
| C3 | C4 | 1.538(3) | C25 | C18 | 1.435(3) |
| C3 | C6 | 1.539(3) | C18 | C17 | 1.418(3) |
| C3 | C2 | 1.542(3) | C19 | C20 | 1.431(3) |
| N4 | C25 | 1.343(2) | C19 | C24 | 1.434(3) |
| N4 | C24 | 1.352(2) | C20 | C21 | 1.356(3) |
| N3 | C19 | 1.344(2) | C21 | C22 | 1.416(3) |
| N3 | C18 | 1.344(2) | C22 | C23 | 1.368(3) |
| N2 | C28 | 1.310(2) | C23 | C24 | 1.425(3) |
| N2 | C27 | 1.419(2) | C14 | C15 | 1.414(3) |
| C16 | C17 | 1.363(3) | C14 | C13 | 1.425(3) |
| C16 | C27 | 1.450(2) | C14 | C1 | 1.434(3) |
| C27 | C26 | 1.366(3) | C1 | C2 | 1.443(3) |
| C28 | C29 | 1.418(3) | C2 | C7 | 1.381(3) |
| C29 | C30 | 1.431(3) | C7 | C8 | 1.421(3) |
| C29 | C43 | 1.434(3) | C8 | C13 | 1.359(3) |
| C43 | C37 | 1.443(2) | C8 | C9 | 1.534(3) |
| C37 | C36 | 1.375(3) | C9 | C10 | 1.519(3) |
| C37 | C38 | 1.537(3) | C9 | C11 | 1.536(3) |
| C36 | C31 | 1.418(3) | C9 | C12 | 1.536(3) |

Table 4: Bond Angles in ° for **Cu[L]**.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|------|------|------|---------|------|------|------|---------|
| O2 | Cu1 | O1 | 89.19(5) | C31 | C32 | C34 | 108.48(17) |
| O2 | Cu1 | N1 | 176.50(6) | C35 | C32 | C34 | 109.18(18) |
| O1 | Cu1 | N1 | 93.26(6) | C39 | C38 | C40 | 107.49(17) |
| O2 | Cu1 | N2 | 93.50(6) | C39 | C38 | C41 | 107.14(17) |
| O1 | Cu1 | N2 | 175.04(6) | C40 | C38 | C41 | 110.14(17) |
| N1 | Cu1 | N2 | 84.24(6) | C39 | C38 | C37 | 111.88(16) |
| C43 | O2 | Cu1 | 129.18(12) | C40 | C38 | C37 | 110.92(16) |
| C1 | O1 | Cu1 | 128.99(12) | C41 | C38 | C37 | 109.19(16) |
| C15 | N1 | C16 | 121.28(15) | C27 | C26 | C25 | 120.61(17) |
| C15 | N1 | Cu1 | 124.84(12) | N4 | C25 | C26 | 119.25(17) |
| C16 | N1 | Cu1 | 113.84(11) | N4 | C25 | C18 | 121.80(17) |
| C5 | C3 | C4 | 107.91(17) | C26 | C25 | C18 | 118.92(16) |
| C5 | C3 | C6 | 110.12(17) | N3 | C18 | C17 | 118.30(17) |
| C4 | C3 | C6 | 106.81(17) | N3 | C18 | C25 | 122.19(17) |
| C5 | C3 | C2 | 109.76(16) | C17 | C18 | C25 | 119.47(16) |
| C4 | C3 | C2 | 111.93(16) | N3 | C19 | C20 | 119.00(18) |
| C6 | C3 | C2 | 110.26(15) | N3 | C19 | C24 | 121.92(17) |
| C25 | N4 | C24 | 116.07(16) | C20 | C19 | C24 | 119.08(18) |
| C19 | N3 | C18 | 116.09(17) | C21 | C20 | C19 | 120.1(2) |
| C28 | N2 | C27 | 121.75(16) | C20 | C21 | C22 | 120.96(19) |
| C28 | N2 | Cu1 | 124.57(12) | C23 | C22 | C21 | 120.98(19) |
| C27 | N2 | Cu1 | 113.63(11) | C22 | C23 | C24 | 120.0(2) |
| C17 | C16 | N1 | 125.35(17) | N4 | C24 | C23 | 119.18(18) |
| C17 | C16 | C27 | 120.23(17) | N4 | C24 | C19 | 121.92(17) |
| N1 | C16 | C27 | 114.35(15) | C23 | C24 | C19 | 118.91(17) |
| C26 | C27 | N2 | 126.27(16) | C16 | C17 | C18 | 120.60(17) |
| C26 | C27 | C16 | 120.14(16) | C15 | C14 | C13 | 116.33(16) |
| N2 | C27 | C16 | 113.53(15) | C15 | C14 | C1 | 123.08(17) |
| N2 | C28 | C29 | 126.28(17) | C13 | C14 | C1 | 120.43(17) |
| C28 | C29 | C30 | 116.47(17) | O1 | C1 | C14 | 122.68(17) |
| C28 | C29 | C43 | 123.27(17) | O1 | C1 | C2 | 119.92(16) |
| C30 | C29 | C43 | 120.15(16) | C14 | C1 | C2 | 117.39(16) |
| O2 | C43 | C29 | 122.89(16) | C7 | C2 | C1 | 118.03(17) |
| O2 | C43 | C37 | 119.10(16) | C7 | C2 | C3 | 121.79(17) |
| C29 | C43 | C37 | 117.99(16) | C1 | C2 | C3 | 120.18(16) |
| C36 | C37 | C43 | 117.83(17) | C2 | C7 | C8 | 125.23(18) |
| C36 | C37 | C38 | 121.80(16) | C13 | C8 | C7 | 116.32(17) |
| C43 | C37 | C38 | 120.36(16) | C13 | C8 | C9 | 123.62(17) |
| C37 | C36 | C31 | 125.35(17) | C7 | C8 | C9 | 119.89(17) |
| C30 | C31 | C36 | 116.81(17) | C8 | C13 | C14 | 122.40(17) |
| C30 | C31 | C32 | 124.63(18) | C10 | C9 | C8 | 112.12(18) |
| C36 | C31 | C32 | 118.54(16) | C10 | C9 | C11 | 108.3(2) |
| C31 | C30 | C29 | 121.82(18) | C8 | C9 | C11 | 108.79(17) |
| C33 | C32 | C31 | 112.48(16) | C10 | C9 | C12 | 107.4(2) |
| C33 | C32 | C35 | 108.61(18) | C8 | C9 | C12 | 112.64(17) |
| C31 | C32 | C35 | 109.85(16) | C11 | C9 | C12 | 107.3(2) |
| C33 | C32 | C34 | 108.18(18) | N1 | C15 | C14 | 126.45(17) |

# UO$_2$[di-tert-butylsal-phenazine]
## Crystal Data and Experimental
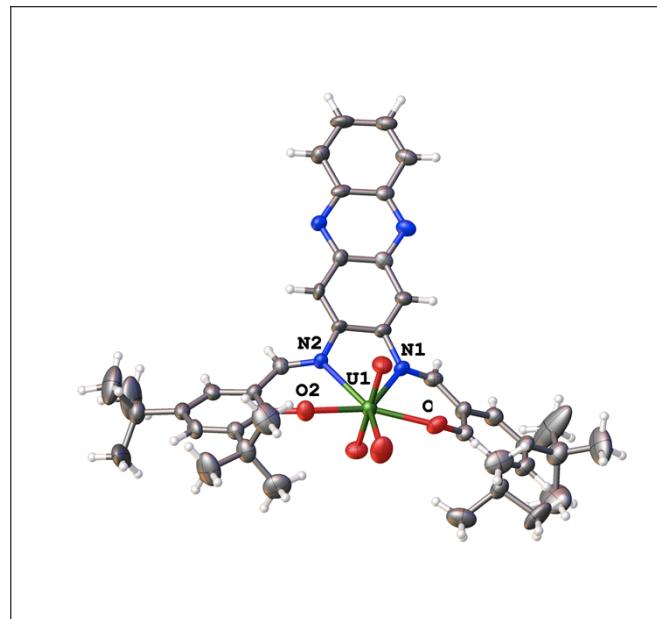


| Compound | UO$_2$[L] |
|---|---|
| CCDC | **1019622** |
| Formula | C$_{48}$H$_{62}$N$_4$O$_{6.5}$ |
| $D_{calc.}$/ g cm$^{-3}$ | 1.370 |
| $\mu$/ mm$^{-1}$ | 3.278 |
| Formula Weight | 1037.06 |
| Colour | Red |
| Shape | Prism |
| Size/$mm^3$ | 0.69 × 0.19 × 0.07 |
| T/K | 180(2) |
| Crystal System | monoclinic |
| Space Group | $P 2_1/n$ |
| a/A | 18.0525(18) |
| b/A | 13.4858(13) |
| c/A | 20.817(2) |
| $\alpha$/° | 90 |
| $\beta$/° | 97.379(3) |
| $\gamma$/° | 90 |
| $V$ / A$^3$ | 5026.1(9) |
| Z | 4 |
| $\Theta_{min}$/° | 1.60 |
| $\Theta_{max}$/° | 24.55 |
| Measured Refl. | 26745 |
| Independent Refl. | 8268 |
| Reflections Used | 6341 |
| R$_{int}$ | 0.0669 |
| Parameters | 481 |
| Restraints | 7 |
| Largest Peak Largest Peak | 2.544 |
| Deepest Hole | -2.230 |
| GooF | 1.055 |
| wR$_2$(all data) | 0.1427 |
| wR$_2$ | 0.1371 |
| R$_1$(all data) | 0.0717 |
| R$_1$ | 0.0550 |

**Crystal Data**. C$_{48}$H$_{62}$N$_4$O$_{6.5}$U, M = 1037.06, monoclinic, $P2_1/n$ (No. 14, $a$ = 18.0525(18) A, $b$ = 13.4858(13) A, $c$ = 20.817(2) A, $\beta$ = 97.379°, $\alpha$ = $\gamma$ = 90°, $V$ = 5026.1(9)$A^3$, $T$ = 180(2) K, $Z$ = 4, $\mu$(Mo K$\alpha$) = 3.278, 26745 reflections measured, 8268 unique ($R_{int}$ = 0.0669) which were used in all calculations. The final $wR2$ was 0.1427 (all data) and $R1$ was 0.0550 ($> 2\sigma(I)$). C$_{48}$H$_{62}$N$_4$O$_{6.5}$U

**Experimental**. Single crystals of (**UO$_2$[di-tert-butylsal-phenazine]**) were obtained by recrystallization using slow evaporation from a concentrated solution. A suitable crystal (0.69 × 0.19 × 0.07$mm^3$) was selected and mounted on a borosilicate fiber using paratone N as the cryoprotectant on a Bruker Apex diffractometer. The crystal was kept at 180(2) K during data collection. Using Bruker Apex2, the structure was solved with the ShelXP structure solution program, using direct methods. The model was refined with the ShelXL refinement package using least squares minimization. SQUEEZE was performed with a total potential solvent area volume found to be 1,731.1 Å$^3$.

Table 5: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($A^2 \times 10^3$) for **UO$_2$[L]**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| U1 | 1461.70(17) | 1587.0(2) | 1713.00(16) | 30.07(12) |
| O1 | 2707(3) | 1708(4) | 1701(3) | 41.8(15) |
| O2 | 387(3) | 960(4) | 1960(3) | 39.0(15) |
| N3 | 1129(4) | 6500(5) | 765(3) | 36.0(17) |
| N4 | −398(4) | 5990(5) | 717(3) | 33.0(17) |
| N1 | 1779(4) | 3051(5) | 1029(3) | 31.2(16) |
| C24 | −182(5) | 6936(6) | 654(4) | 33(2) |
| C7 | 4393(5) | 1677(7) | 950(5) | 44(2) |
| C20 | 773(6) | 8215(6) | 667(4) | 41(2) |
| C17 | 1449(5) | 4778(6) | 871(4) | 33(2) |
| C26 | −46(4) | 4295(6) | 914(4) | 32(2) |
| C19 | 586(5) | 7192(6) | 702(4) | 32(2) |
| C14 | 3039(5) | 2604(6) | 814(4) | 34(2) |
| C30 | −638(5) | 1330(6) | 1171(4) | 30.5(19) |
| C18 | 910(5) | 5551(6) | 800(4) | 30.7(19) |
| C27 | 491(4) | 3581(6) | 991(4) | 31(2) |
| C31 | −1375(5) | 1137(6) | 887(4) | 35(2) |
| C16 | 1258(5) | 3832(6) | 947(4) | 30.4(19) |
| C38 | −721(5) | −21(6) | 1940(4) | 33(2) |
| C25 | 154(4) | 5298(6) | 799(4) | 30.6(19) |
| C1 | 3200(5) | 1888(6) | 1301(4) | 32(2) |
| C8 | 4254(5) | 2393(7) | 457(5) | 41(2) |
| C15 | 2360(5) | 3152(6) | 738(4) | 36(2) |
| C37 | −1445(5) | −162(7) | 1633(4) | 39(2) |
| C23 | −731(5) | 7688(7) | 546(5) | 44(2) |
| C2 | 3919(5) | 1412(6) | 1377(4) | 37(2) |
| C32 | −1786(5) | 382(7) | 1094(4) | 38(2) |
| C39 | −402(6) | −647(8) | 2513(5) | 48(3) |
| C28 | −319(5) | 2231(6) | 968(4) | 31.1(19) |
| C21 | 244(6) | 8902(7) | 562(5) | 43(2) |
| C3 | 4117(5) | 593(7) | 1880(5) | 43(2) |
| C9 | 4833(6) | 2613(8) | 0(5) | 57(3) |
| C22 | −517(6) | 8644(6) | 497(5) | 48(3) |
| C13 | 3572(5) | 2841(7) | 407(5) | 41(2) |
| C33 | −2580(5) | 137(8) | 788(5) | 54(3) |
| C35 | −3123(7) | 407(14) | 1248(7) | 110(6) |
| C41 | 301(7) | −1194(9) | 2361(6) | 69(3) |
| C42 | −946(8) | −1429(10) | 2694(7) | 86(4) |
| C11 | 5007(9) | 1664(11) | −342(8) | 107(6) |
| C40 | −184(8) | 8(10) | 3108(6) | 83(4) |
| C10 | 5560(8) | 2948(13) | 407(7) | 102(5) |
| C34 | −2791(8) | 687(14) | 160(7) | 117(6) |
| C12 | 4583(10) | 3374(15) | −487(10) | 167(11) |
| C5 | 3599(7) | −308(8) | 1699(5) | 67(3) |
| C4 | 4018(7) | 938(9) | 2567(5) | 64(3) |
| C6 | 4916(6) | 226(10) | 1897(6) | 78(4) |
| O8 | 1413(4) | 779(4) | 1045(3) | 41.9(15) |
| O3 | 1501(4) | 2444(4) | 2370(3) | 44.1(16) |
| C36 | −2637(7) | −951(11) | 626(10) | 134(8) |
| N2 | 352(4) | 2573(5) | 1153(3) | 28.1(15) |
| C43 | −305(5) | 764(6) | 1692(4) | 33(2) |
| O5 | | 368(6) | 2543(4) | 63(2) |

Table 6: Anisotropic Displacement Parameters ($\times 10^4$) $\mathbf{UO_2[L]}$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*\times b\times U_{12}]$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|------|---------|---------|---------|---------|---------|---------|
| U1 | 28.85(19) | 28.19(18) | 32.17(19) | 3.41(15) | 0.03(13) | 0.44( |
| O1 | 42(4) | 39(4) | 45(4) | 12(3) | 11(3) | 13(3) |
| O2 | 37(4) | 40(4) | 39(4) | 14(3) | 0(3) | −2(3) |
| N3 | 47(5) | 26(4) | 36(4) | 5(3) | 6(3) | 0(3) |
| N4 | 27(4) | 29(4) | 42(4) | −1(3) | −1(3) | 4(3) |
| N1 | 26(4) | 28(4) | 39(4) | 2(3) | 2(3) | 6(3) |
| C24 | 42(5) | 27(4) | 28(5) | −5(3) | −1(4) | 13(4) |
| C7 | 38(5) | 45(6) | 49(6) | 3(5) | 8(5) | 12(4) |
| C20 | 58(6) | 26(5) | 39(6) | 2(4) | 9(5) | −1(4) |
| C17 | 35(5) | 25(4) | 39(5) | −6(4) | 2(4) | 3(4) |
| C26 | 16(4) | 33(5) | 48(6) | 1(4) | 3(4) | −1(4) |
| C19 | 40(5) | 29(5) | 25(5) | −3(4) | 1(4) | 4(4) |
| C14 | 29(5) | 34(5) | 39(5) | 7(4) | 8(4) | 2(4) |
| C30 | 25(4) | 31(5) | 36(5) | 3(4) | 3(4) | 4(3) |
| C18 | 41(5) | 32(5) | 18(4) | 7(3) | 1(4) | −1(4) |
| C27 | 26(4) | 20(4) | 46(5) | 4(4) | 0(4) | 7(3) |
| C31 | 37(5) | 32(5) | 37(5) | −6(4) | 6(4) | −1(4) |
| C16 | 30(5) | 23(4) | 36(5) | 2(4) | −2(4) | 8(4) |
| C38 | 35(5) | 35(5) | 31(5) | 3(4) | 6(4) | −2(4) |
| C25 | 27(5) | 32(5) | 32(5) | 4(4) | −1(4) | 2(4) |
| C1 | 34(5) | 34(5) | 30(5) | 0(4) | 12(4) | 2(4) |
| C8 | 37(5) | 44(5) | 43(6) | 2(4) | 16(4) | 5(4) |
| C15 | 42(5) | 28(5) | 39(5) | 1(4) | 5(4) | 5(4) |
| C37 | 33(5) | 40(5) | 47(6) | 0(4) | 14(4) | −11(4) |
| C23 | 37(5) | 39(5) | 54(6) | 5(4) | 0(5) | 7(4) |
| C2 | 34(5) | 35(5) | 40(5) | 4(4) | 7(4) | 1(4) |
| C32 | 29(5) | 39(5) | 44(6) | −10(4) | 3(4) | −1(4) |
| C39 | 50(6) | 53(6) | 42(6) | 12(5) | 6(5) | −12(5) |
| C28 | 32(5) | 34(5) | 28(5) | 0(4) | 4(4) | −1(4) |
| C21 | 58(7) | 24(5) | 49(6) | −1(4) | 15(5) | 6(5) |
| C3 | 34(5) | 47(6) | 50(6) | 14(5) | 7(4) | 10(4) |
| C9 | 51(7) | 66(7) | 57(7) | 10(6) | 20(5) | 5(6) |
| C22 | 63(7) | 22(5) | 59(7) | 1(4) | 5(5) | 17(4) |
| C13 | 43(6) | 35(5) | 45(6) | 7(4) | 11(5) | 0(4) |
| C33 | 35(6) | 62(6) | 64(7) | 1(5) | 3(5) | −6(5) |
| C35 | 44(8) | 183(17) | 106(12) | −4(12) | 16(8) | −13(9) |
| C41 | 85(9) | 61(7) | 60(8) | 26(6) | 6(7) | 15(7) |
| C42 | 86(10) | 90(10) | 79(9) | 37(8) | 0(8) | −34(8) |
| C11 | 119(13) | 119(13) | 95(12) | −30(10) | 64(10) | −10(10) |
| C40 | 102(11) | 99(10) | 44(7) | 4(7) | −2(7) | −17(8) |
| C10 | 76(10) | 158(15) | 80(10) | −8(10) | 43(8) | −45(10) |
| C34 | 65(9) | 188(18) | 86(11) | 35(11) | −31(8) | −33(10) |
| C12 | 113(14) | 230(20) | 190(20) | 157(18) | 109(14) | 91(14) |
| C5 | 103(10) | 40(6) | 57(7) | 9(5) | 7(7) | 8(6) |
| C4 | 86(9) | 77(8) | 27(6) | 13(5) | 1(6) | 22(7) |
| C6 | 57(7) | 92(9) | 87(9) | 39(8) | 18(7) | 45(7) |
| O8 | 55(4) | 40(4) | 32(3) | 0(3) | 6(3) | 7(3) |
| O3 | 47(4) | 40(4) | 47(4) | −10(3) | 8(3) | 0(3) |
| C36 | 49(8) | 76(9) | 260(20) | −57(13) | −33(11) | −9(7) |
| N2 | 24(4) | 24(4) | 36(4) | 6(3) | 3(3) | 1(3) |
| C43 | 30(5) | 32(5) | 35(5) | −1(4) | 0(4) | −5(4) |
| O5 | 54(5) | 67(5) | 66(5) | 26(4) | −2(4) | |

Table 7: Bond Lengths in A for **UO₂[L]**.

| Atom | Atom | Length/A | Atom | Atom | Length/A |
|------|------|----------|------|------|----------|
| U1 | O8 | 1.760(6) | C30 | C28 | 1.432(11) |
| U1 | O3 | 1.786(6) | C18 | C25 | 1.406(11) |
| U1 | O2 | 2.237(6) | C27 | N2 | 1.431(10) |
| U1 | O1 | 2.258(6) | C27 | C16 | 1.438(11) |
| U1 | O5 | 2.454(6) | C31 | C32 | 1.362(12) |
| U1 | N1 | 2.542(7) | C38 | C37 | 1.392(12) |
| U1 | N2 | 2.558(6) | C38 | C43 | 1.433(11) |
| O1 | C1 | 1.317(10) | C38 | C39 | 1.514(12) |
| O2 | C43 | 1.327(10) | C1 | C2 | 1.438(12) |
| N3 | C18 | 1.344(10) | C8 | C13 | 1.364(12) |
| N3 | C19 | 1.348(11) | C8 | C9 | 1.532(13) |
| N4 | C24 | 1.345(11) | C37 | C32 | 1.415(13) |
| N4 | C25 | 1.360(10) | C23 | C22 | 1.354(13) |
| N1 | C15 | 1.284(11) | C2 | C3 | 1.532(12) |
| N1 | C16 | 1.408(10) | C32 | C33 | 1.528(13) |
| C24 | C23 | 1.417(12) | C39 | C42 | 1.520(14) |
| C24 | C19 | 1.420(12) | C39 | C40 | 1.530(15) |
| C7 | C2 | 1.359(13) | C39 | C41 | 1.535(15) |
| C7 | C8 | 1.407(13) | C28 | N2 | 1.308(10) |
| C20 | C21 | 1.327(13) | C21 | C22 | 1.407(14) |
| C20 | C19 | 1.424(11) | C3 | C6 | 1.521(13) |
| C17 | C16 | 1.336(11) | C3 | C4 | 1.538(14) |
| C17 | C18 | 1.422(11) | C3 | C5 | 1.550(14) |
| C26 | C27 | 1.361(11) | C9 | C12 | 1.471(17) |
| C26 | C25 | 1.429(11) | C9 | C11 | 1.517(17) |
| C14 | C13 | 1.399(12) | C9 | C10 | 1.535(17) |
| C14 | C1 | 1.403(12) | C33 | C35 | 1.501(16) |
| C14 | C15 | 1.423(12) | C33 | C36 | 1.506(16) |
| C30 | C43 | 1.396(11) | C33 | C34 | 1.508(17) |
| C30 | C31 | 1.410(12) | | | |

Table 8: Bond Angles in ° for **bam149_0m_sq**.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|------|------|------|---------|------|------|------|---------|
| O8 | U1 | O3 | 177.9(3) | C37 | C38 | C39 | 121.7(8) |
| O8 | U1 | O2 | 89.4(3) | C43 | C38 | C39 | 122.1(8) |
| O3 | U1 | O2 | 91.1(3) | N4 | C25 | C18 | 122.0(7) |
| O8 | U1 | O1 | 89.2(3) | N4 | C25 | C26 | 118.3(7) |
| O3 | U1 | O1 | 91.1(3) | C18 | C25 | C26 | 119.7(7) |
| O2 | U1 | O1 | 157.6(2) | O1 | C1 | C14 | 119.3(7) |
| O8 | U1 | O5 | 96.8(3) | O1 | C1 | C2 | 121.4(7) |
| O3 | U1 | O5 | 85.3(3) | C14 | C1 | C2 | 119.2(7) |
| O2 | U1 | O5 | 79.2(2) | C13 | C8 | C7 | 115.8(8) |
| O1 | U1 | O5 | 78.8(2) | C13 | C8 | C9 | 123.2(9) |
| O8 | U1 | N1 | 91.8(3) | C7 | C8 | C9 | 121.0(8) |
| O3 | U1 | N1 | 86.4(3) | N1 | C15 | C14 | 129.4(8) |
| O2 | U1 | N1 | 133.4(2) | C38 | C37 | C32 | 125.5(8) |
| O1 | U1 | N1 | 69.0(2) | C22 | C23 | C24 | 119.5(9) |
| O5 | U1 | N1 | 146.4(2) | C7 | C2 | C1 | 116.5(8) |
| O8 | U1 | N2 | 90.3(3) | C7 | C2 | C3 | 121.7(8) |
| O3 | U1 | N2 | 88.0(3) | C1 | C2 | C3 | 121.7(8) |
| O2 | U1 | N2 | 69.5(2) | C31 | C32 | C37 | 116.1(8) |
| O1 | U1 | N2 | 132.8(2) | C31 | C32 | C33 | 123.4(9) |
| O5 | U1 | N2 | 147.8(2) | C37 | C32 | C33 | 120.5(8) |
| N1 | U1 | N2 | 63.9(2) | C38 | C39 | C42 | 112.9(9) |
| C1 | O1 | U1 | 140.8(6) | C38 | C39 | C40 | 110.3(9) |
| C43 | O2 | U1 | 140.8(5) | C42 | C39 | C40 | 107.9(9) |
| C18 | N3 | C19 | 116.7(8) | C38 | C39 | C41 | 110.3(8) |
| C24 | N4 | C25 | 116.5(7) | C42 | C39 | C41 | 107.2(10) |
| C15 | N1 | C16 | 115.9(7) | C40 | C39 | C41 | 108.1(10) |
| C15 | N1 | U1 | 127.1(5) | N2 | C28 | C30 | 127.2(8) |
| C16 | N1 | U1 | 117.0(5) | C20 | C21 | C22 | 121.1(9) |
| N4 | C24 | C23 | 119.3(8) | C6 | C3 | C2 | 112.9(8) |
| N4 | C24 | C19 | 121.1(7) | C6 | C3 | C4 | 107.4(9) |
| C23 | C24 | C19 | 119.6(8) | C2 | C3 | C4 | 111.9(8) |
| C2 | C7 | C8 | 126.1(9) | C6 | C3 | C5 | 107.0(9) |
| C21 | C20 | C19 | 120.9(9) | C2 | C3 | C5 | 108.6(8) |
| C16 | C17 | C18 | 121.9(8) | C4 | C3 | C5 | 108.9(9) |
| C27 | C26 | C25 | 119.9(7) | C12 | C9 | C11 | 109.3(14) |
| N3 | C19 | C24 | 122.0(7) | C12 | C9 | C8 | 112.9(9) |
| N3 | C19 | C20 | 120.1(8) | C11 | C9 | C8 | 109.0(9) |
| C24 | C19 | C20 | 117.9(8) | C12 | C9 | C10 | 109.9(13) |
| C13 | C14 | C1 | 120.1(8) | C11 | C9 | C10 | 107.0(11) |
| C13 | C14 | C15 | 117.5(8) | C8 | C9 | C10 | 108.4(9) |
| C1 | C14 | C15 | 122.3(8) | C23 | C22 | C21 | 120.9(9) |
| C43 | C30 | C31 | 120.9(8) | C8 | C13 | C14 | 122.4(9) |
| C43 | C30 | C28 | 123.0(8) | C35 | C33 | C36 | 110.4(12) |
| C31 | C30 | C28 | 115.2(8) | C35 | C33 | C34 | 108.7(12) |
| N3 | C18 | C25 | 121.5(8) | C36 | C33 | C34 | 106.5(13) |
| N3 | C18 | C17 | 120.1(8) | C35 | C33 | C32 | 109.6(10) |
| C25 | C18 | C17 | 118.3(7) | C36 | C33 | C32 | 109.8(9) |
| C26 | C27 | N2 | 123.7(7) | C34 | C33 | C32 | 111.9(9) |
| C26 | C27 | C16 | 120.2(7) | C28 | N2 | C27 | 116.8(7) |
| N2 | C27 | C16 | 116.0(6) | C28 | N2 | U1 | 126.3(5) |
| C32 | C31 | C30 | 121.9(9) | C27 | N2 | U1 | 116.8(5) |
| C17 | C16 | N1 | 123.3(8) | O2 | C43 | C30 | 120.4(7) |
| C17 | C16 | C27 | 119.8(7) | O2 | C43 | C38 | 120.3(8) |
| N1 | C16 | C27 | 116.7(7) | C30 | C43 | C38 | 119.3(8) |
| C37 | C38 | C43 | 116.2(8) | | | | |

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