Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Synthesis and Characterization of Two Different Azarubrenes

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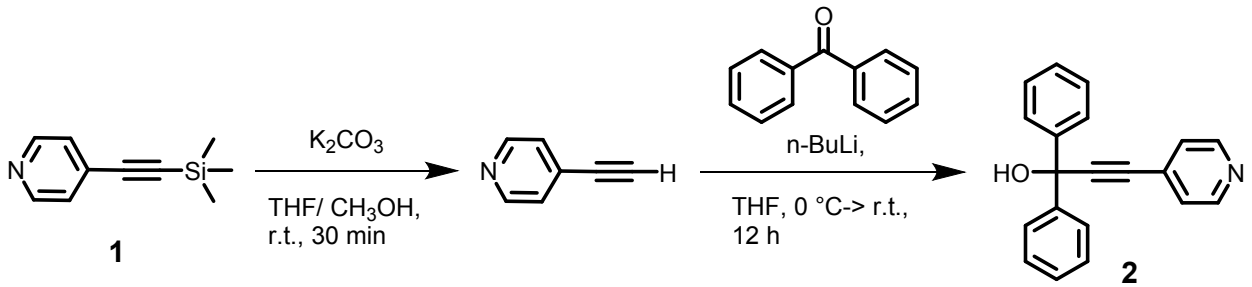
Index:

S1. Experimental Section

Materials and Methods. Thin-layer chromatography (TLC) was carried out on Polygram SILG/UV254 plates from Macherey, Nagel&Co.KG (Düren, Germany) and examined under ultraviolet irradiation (254 and 365 nm). Column chromatography was performed using silica gel from Macherey, Nagel & Co.KG (particle size: 0.032-0.062 mm) or aluminium oxide from Acros Organics (particle size: 0.05-0.20 mm). NMR spectra (^{1}H, ^{13}C) were recorded at Bruker Avance III 300, Bruker Avance III 500 or Bruker Avance III 600. Chemical shifts (δ) are given in parts per million (ppm) relative to internal solvent signals. The following abbreviations describe the signal multiplicities: s = singlet, bs = broad singlet, d = doublet, bd = broad doublet, dd = doublet doublet m = multiplet. IR spectra were recorded on a JASCO FT/IR-4100. High resolution mass spectra (HR-MS) were obtained from electron impact (EI) or electrospray ionization (ESI) on a Bruker ApexQe hybrid 9.4 TFT-ICR-MS. Crystal structure analysis was accomplished on Bruker Smart CCD or Bruker APEX diffractometers. Computational studies were carried out using DFT calculations on Turbomole 6.3.1 and Gaussian09. Geometry optimizations were performed using the BP86 functional and def2-TZVP basis set. At this geometry, the absolute energy and FMO energies were assigned by a single-point approach at the B3LYP/6-311++G** level. Hirshfeld surfaces and fingerprint plots were generated with the program CrystalExplorer 3.1.[1]

Syntheses. All reagents and solvents were obtained from Sigma-Aldrich and ABCR without any further purification. 4-((Trimethylsilyl)ethynyl)pyridine (**1**)[2] and 5,6,11,12-tetrachlorotetracene (**3**)[3] were synthesized according to reported literatures.

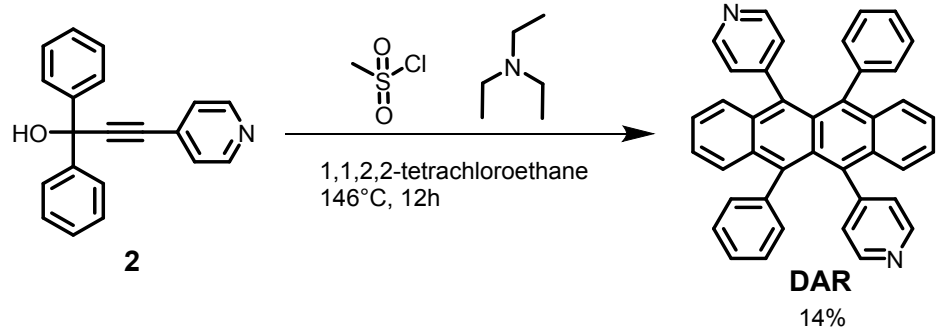
*1,1-Diphenyl-3-pyridyl-2-propyn-1-ol (**2**)*



1 **2** 93%

A solution of **1** (4.92 g, 28.1 mmol, 1.00 eq.) in THF:CH_3OH (28: 28 ml) was treated with K_2CO_3 (8.73 g, 63.2 mmol, 2.25 eq.). After 30 min of stirring at room temperature (r.t.), the mixture was filtered to remove inorganic salts and the solvent was evaporated under reduced pressure. Then the crude product was purified by a flash column chromatography (silica gel, petroleum ether (PE)/ ethyl acetate (EE) = 5:1) to give a colorless solid. The fresh prepared 4-ethynylpridine (2.72 g, 26.3 mmol, 1.20 eq.) was dissolved into dry tetrahydrofuran (THF) (32 mL), followed by adding *n*-butyllithium (*n*-BuLi) (22.0 mmol, 8.78 mL, 2.50 M in hexane, 1.00 eq.) dropwise at -10 °C. The solution was first stirred at -10 °C for 20 min and then at r.t. for 20 min. After that, benzophenone (4.00 g, 22.0 mmol, 1.00 eq.), dissolved in 32 ml THF, was added dropwise at r.t. and the mixture was stirred for 12 h. The mixture was quenched with water (8 mL) and dealt with a short column chromatography using THF as eluent. After evaporation of the solvent, the mixture was separated by a short column chromatography (silica gel, PE/ EE = 5:1) to attain a white powder **2**. Yield: 5.85 g, 20.5 mmol, 93%, Rf = 0.35 (SiO_2, PE/ EE = 1: 1, v/v). Mp: 183 °C. ^{1}H-NMR ($CDCl_3$, 500.13 MHz, 25 °C): δ = 8.55 (bs, 2H), 7.65 (d, *J*= 7.32 Hz, 4H), 7.40-7.34 (m, 6H), 7.33-7.29 (m, 2H), 3.55 (bs, 1H) ppm. ^{13}C-NMR ($CDCl_3$, 125.76 MHz, 25 °C): δ = 149.3, 144.4, 131.1, 128.4, 128.0, 126.0, 125.8, 97.0, 84.2, 74.7 ppm. IR: v = 3068, 2783.5, 1700, 1597,1490, 1445, 1411, 1171, 1046, 996, 829, 753, 692, 643, 605, 552, 418 cm^{-1}. HRMS (ESI^+) m/z: $[M+H]^+$: calcd. for $C_{20}H_{16}NO$: 286.1226; found 286.1229 correct isotope distribution. Elemental analysis calcd. (%) for $C_{20}H_{16}NO$: C 84.19, H 5.30, N 4.91; found: C 84.05, H 5.48, N 4.82.

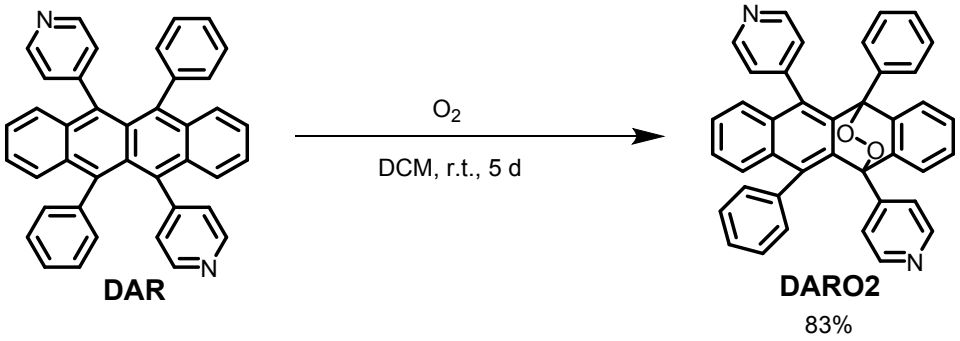
5,11-Di(4-pyridyl)-6,12-diphenyltetraacene (**DAR**)



2 **DAR** 14%

Under nitrogen atmosphere, **1** (0.20 g, 0.70 mmol, 1.00 eq.) was dissolved in 6 ml 1,1,2,2-tetrachloroethane and the solution was cooled to 0 °C. Anhydrous triethylamine (0.20 ml) and methanesulfonyl chloride (0.25 g, 98%, 2.10 mmol, 3.00 eq.) were added to this solution and stirred for 1 h at 0 °C. Then it was heated to 146 °C and stirred for 5 h. After removal of the solvent through reduced pressure distillation, the mixture was first purified using a SiO_2 column chromatography (dichloromethane (DCM)/ EE = 10:1), followed by an alumina column chromatography (DCM/ EE = 3:1). Then the crude product was recrystallized by methanol and hexane to obtain **DAR** as a red powder. Yield: 0.26 g, 0.05 mmol, 14%. Rf = 0.20 (SiO_2, DCM/ EE = 1:1, v/v). Mp: 338 °C (decomposition). ^{1}H-NMR (cyclohexane-d_{12}, 300.51 MHz, 27 °C): δ = 8.28-8.19 (m, 4H), 7.46-7.37 (m, 2H), 7.31-7.25 (m, 2H), 7.16-7.11 (m, 2H), 7.06-6.69 (m, 8H), 6.86-6.76 (m, 4H), 6.67-6.60 (m, 4H) ppm. IR: $\tilde{\nu}$ = 3060, 3027, 1581, 1396, 1068, 1024, 817, 757, 692, 586, 514, 460 cm^{-1}. HRMS (EI$^+$): m/z: [M]$^+$: calcd. for $C_{40}H_{26}N_2^+$: 534.2096; found 534.2081 correct isotope distribution.

5,12-Dihydro-5,11-di(4-pyridyl)-6,12-diphenyl-5,12-epidioxynaphthacene (DARO2)

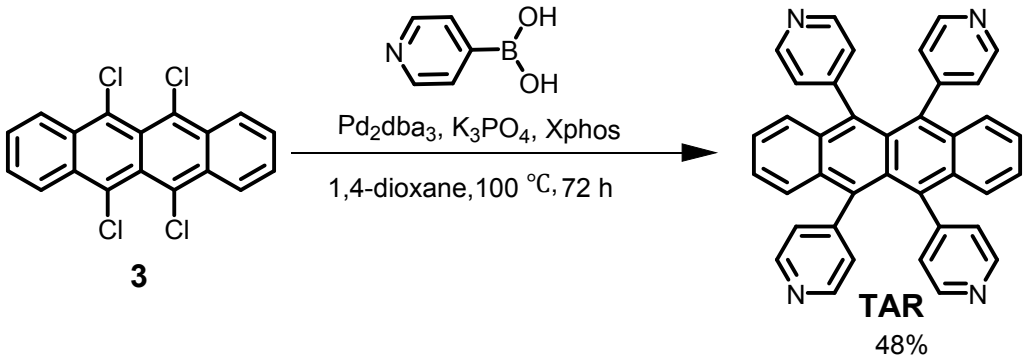


DAR **DARO2** 83%

DAR (0.03 g, 0.06 mmol) was dissolved in 30 mL DCM and stirred at r.t. for 5 d. The solvent was removed under reduced pressure and the crude product was recrystallized by DCM to attain **DARO2** as a colorless powder. Yield: 0.03 g, 0.05 mmol, 83%. Rf = 0.20 (SiO_2, DCM/ EE = 1:1, v/v). Mp: 207 °C (decomposition). ^{1}H-NMR (CD_2Cl_2, 600.24 MHz, 22 °C): δ = 8.45 (bs, 1H), 8.27 (bs, 2H), 8.12 (bs, 1H), 7.54-7.38 (m, 3H), 7.36-7.32 (m, 1H), 7.31-7.13 (m, 12H), 7.12-7.08 (bd,

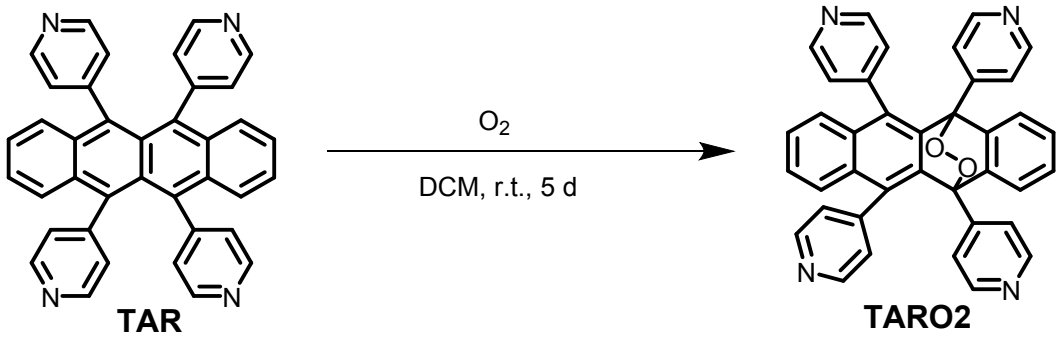
J= 3.85 Hz, 1H), 7.07-6.96 (m, 2H), 6.92-6.87 (m, 1H), 6.74-6.96 (d, *J*= 7.70 Hz, 1H), 6.61-6.53 (bd, *J*= 4.13 Hz, 1H) ppm. ^{13}C-NMR (CD_2Cl_2, 150.93 MHz, 22 °C): δ = 149.8, 148.7, 148.4, 147.1, 142.7, 140.0, 139.3, 138.2, 137.0, 134.9, 133.9, 133.8, 133.6, 133.2, 132.6, 132.2, 131.9, 128.8, 128.8, 128.5, 128.4, 128.0, 127.7, 127.5, 127.2, 127.1, 127.0, 126.9, 125.3, 124.6 ppm. IR: $\tilde{\nu}$ = 3041, 2927, 1589, 1463, 1411, 1270, 1184, 1051, 914, 821, 765, 730, 696, 605, 566 cm^{-1}. HRMS (ESI$^+$) m/z: $[M+H]^+$: calcd. for $C_{40}H_{27}N_2O_2^+$: 567.2067; found 567.2061; m/z: $[M+Na]^+$: calcd. for $C_{40}H_{26}N_2O_2Na^+$: 589.1886; found 589.1880 correct isotope distribution.

5,6,11,12-Tetra(4-pyridyl)tetracene (**TAR**)



Under nitrogen atmosphere, **3** (0.20 g, 0.55 mmol, 1.00 eq.), 4-pyridinylboronic acid (0.48 g, 90%, 3.50 mmol, 6.40 eq.), tris(dibenzylideneacetone)dipalladium(0) (Pd_2dba_3) (0.04 g, 0.04 mmol, 0.07 eq.) and 2-dicyclohexylphosphino-2',4',6'-triisopropylbiphenyl (XPhos) (0.08 g, 0.16 mmol, 0.28 eq.) were added into a 50 mL flask. 16 mL 1,4-dioxane and 4 mL potassium phosphate solution (1.02 g, 4.80 mmol, 8.80 eq., 1.20 M) were degassed for 20 min and added into the flask .The resulting mixture was stirred at 100 ˚C for 72 h. The crude product was extracted with 50 mL DCM and washed three times with 50 mL water. After evaporation of solvent under reduced pressure, the solid was purified by column chromatography (DCM/ CH_3OH = 40: 1 → 10: 1 v/v) to attain **TAR** as a red powder. Yield: 0.14 g, 0.26 mmol, 48%. Rf = 0.30 (SiO_2, DCM/ CH_3OH = 10:1, v/v). Mp: 338 °C. ^{1}H-NMR (tetrahydrofuran-d_8, 500.13 MHz, 25 °C): δ = 8.38-8.25 (m, 8H), 7.43-7.29 (m, 4H), 7.28-7.16 (m, 4H), 6.94-6.80 (m, 8H) ppm. ^{13}C-NMR (THF-d_8, 125.76 MHz, 25 °C): δ = 150.1, 149.5, 135.8, 130.7, 128.4, 127.1, 126.7 ppm. IR: $\tilde{\nu}$ = 3031, 1936, 1589, 1540, 1467, 1403, 1209, 1064, 981, 817, 746, 582, 518, 460 cm^{-1}. HR-MS (EI$^+$): m/z: $[M]^+$: calcd. for $C_{38}H_{24}N_4$: 536.2001; found 536.2002 correct isotope distribution.

5,12-Dihydro-5,6,11,12-tetra(4-pyridyl)-5,12-epidioxynaphthacene (**TARO2**)



TAR (0.03 g, 0.06 mmol) was dissolved in 30 mL DCM and stirred at r.t. for 5 d. The solvent was removed under reduced pressure and the crude product was recrystallized by DCM to attain a **TARO2** as a colorless powder. Yield: 0.02 g, 0.04 mmol, 67%. Rf = 0.30 (SiO_2, DCM/ CH_3OH = 10:1, v/v). Mp: 220 °C. ^{1}H-NMR (CD_2Cl_2, 300.51 MHz, 27 °C): δ = 8.56 (d, J=5.0, 2H), 8.34 (s, 4H), 8.15 (d, J=4.9, 2H), 7.40–7.26 (m, 10H), 7.18 (d, J=3.8, 2H), 7.09 (dd, J=6.6, 3.3, 2H), 6.64 (d, J=3.7, 2H) ppm. ^{13}C-NMR (CD_2Cl_2, 150.93 MHz, 22 °C): δ = 150.1, 149.2, 148.7, 146.3, 141.8, 138.3, 134.2, 133.4, 132.2, 128.8, 127.7, 127.0, 126.9, 124.7, 83.9 ppm. IR: $\tilde{\nu}$ = 3423, 3035, 2911, 1712, 1592, 1407, 1197, 973, 914, 821, 757, 727, 605, 566 cm^{-1}. HRMS (ESI^+) m/z: $[M+H]^+$: calcd. for $C_{38}H_{25}N_4O_2^+$: 569.1972; found 569.1973; m/z: $[M+Na]^+$: calcd. for $C_{38}H_{24}N_4O_2Na^+$: 591.1792; found 591.1793 correct isotope distribution.

S2. Absorption and emission spectra

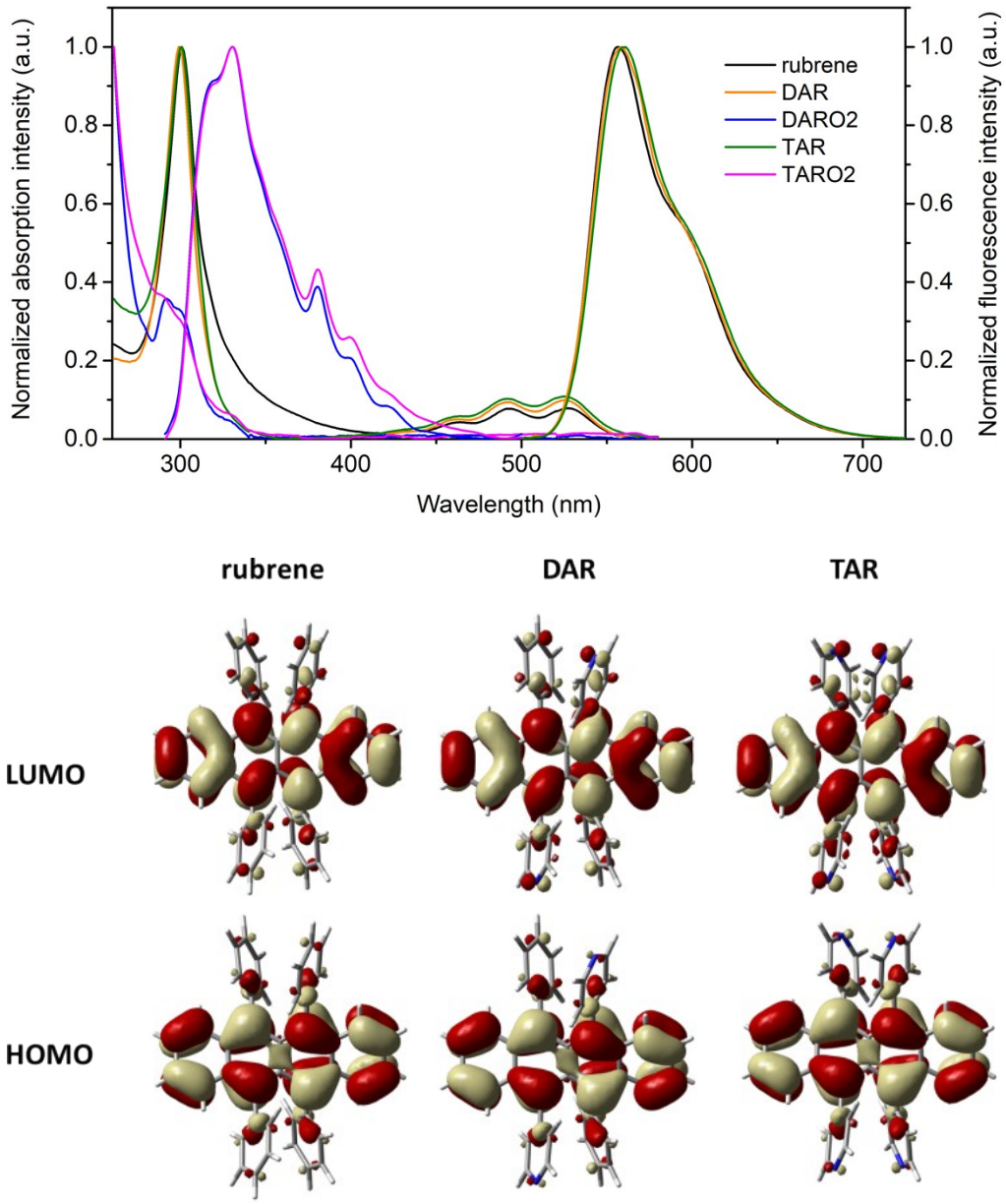


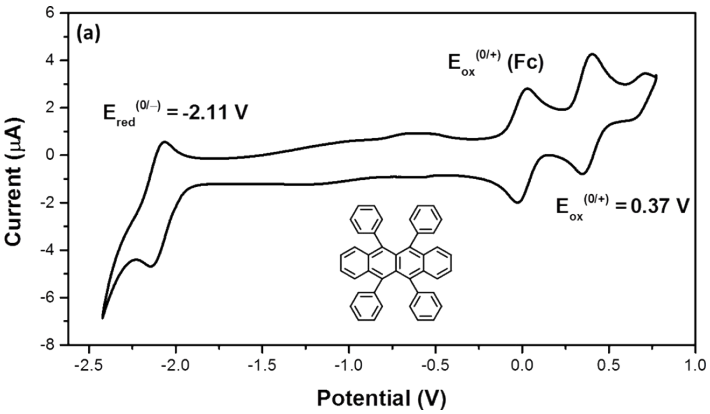
Figure S1. Top: Normalized absorption and emission spectra of **rubrene** and designed compounds measured in dichloromethane. Bottom: Quantum-chemical calculations of the FMOs (LUMOs Top, HOMOs bottom) for rubrene, DAR, and TAR (Gaussian 09 B3LYP/6-311 ++G**//BP86/ def2-TZVP).

S3. Electrochemistry

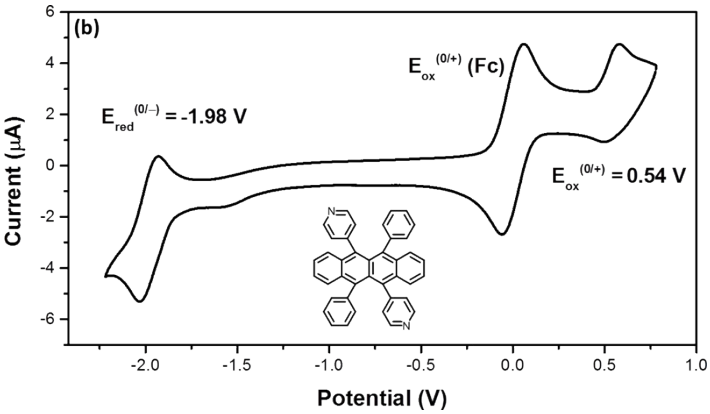
Cyclic Voltammetry (CV). The **CV** experiments were carried out using a platinum working electrode, a platinum/titanium wire auxiliary electrode, a silver wire reference electrode, a 0.1 M NBu_4PF_6 solution in degassed dichloromethane, and ferrocene/ferrocenium as the reference redox system and internal standard (−4.8 eV). To determine the first reduction

potentials ($E_{red}(0/-)$) and oxidation potentials ($E_{ox}(0/+)$) of **rubrene**, **DAR**, **TAR**, the first oxidation potential of ferrocene, the half-wave potentials were used.[4]

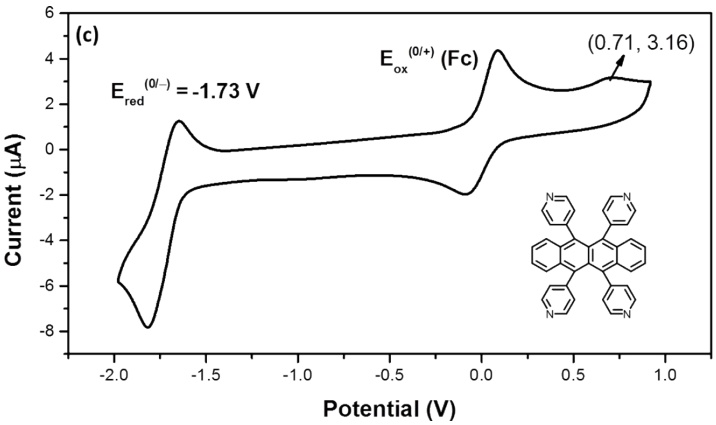
Rubrene with ferrocene **(a)**



DAR with ferrocene **(b)**

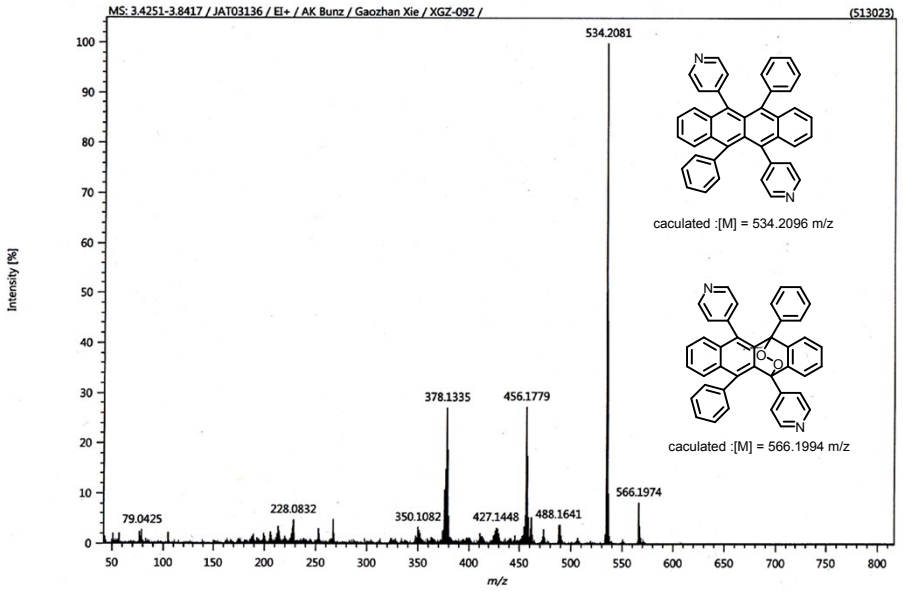


TAR with ferrocene (**c**)

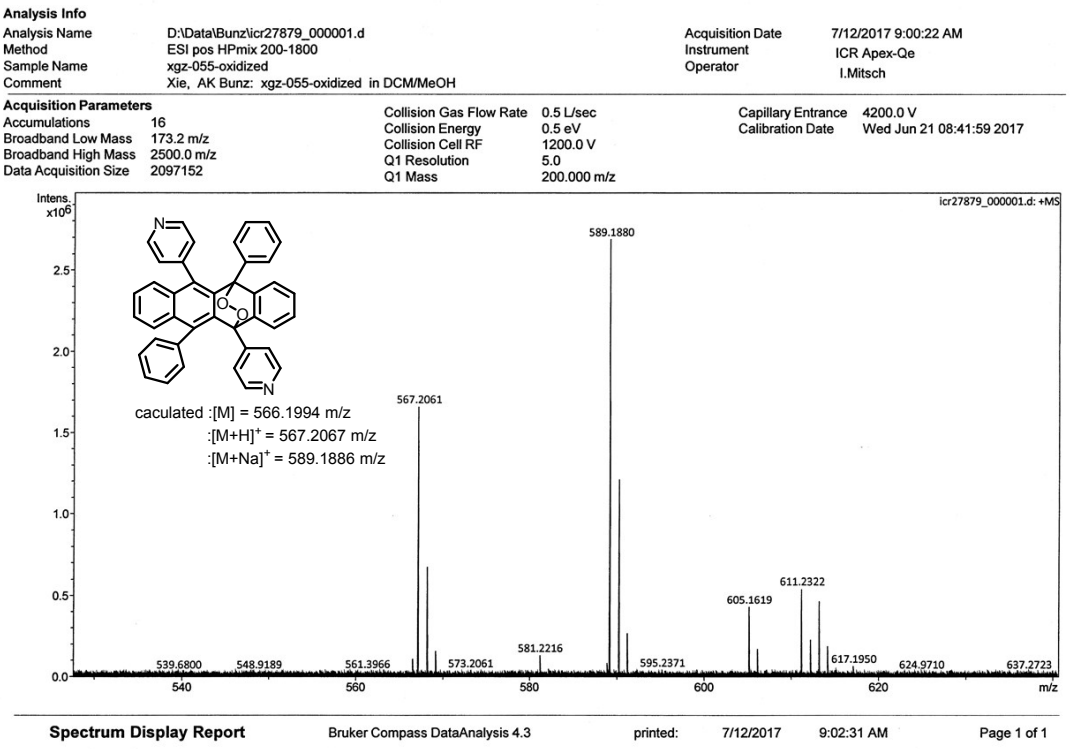


S4. Mass spectrometry

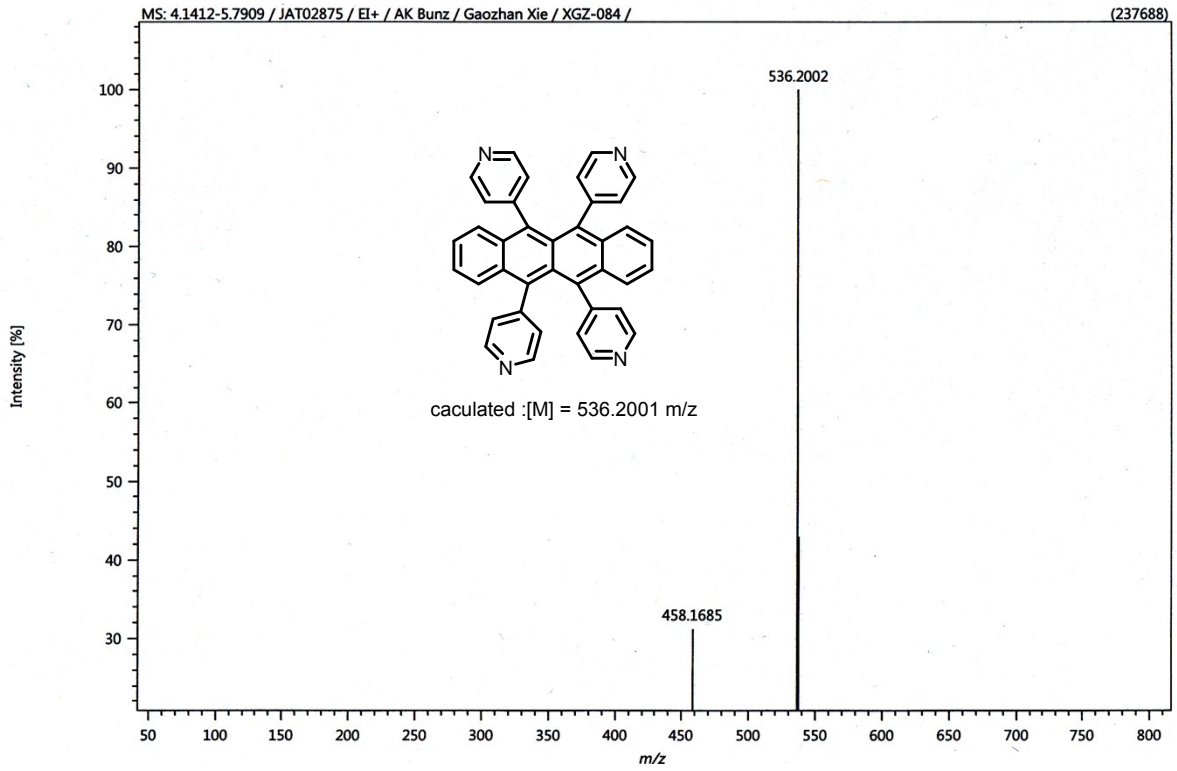
5,11-Di(4-pyridyl)-6,12-diphenyltetracene (**DAR**)



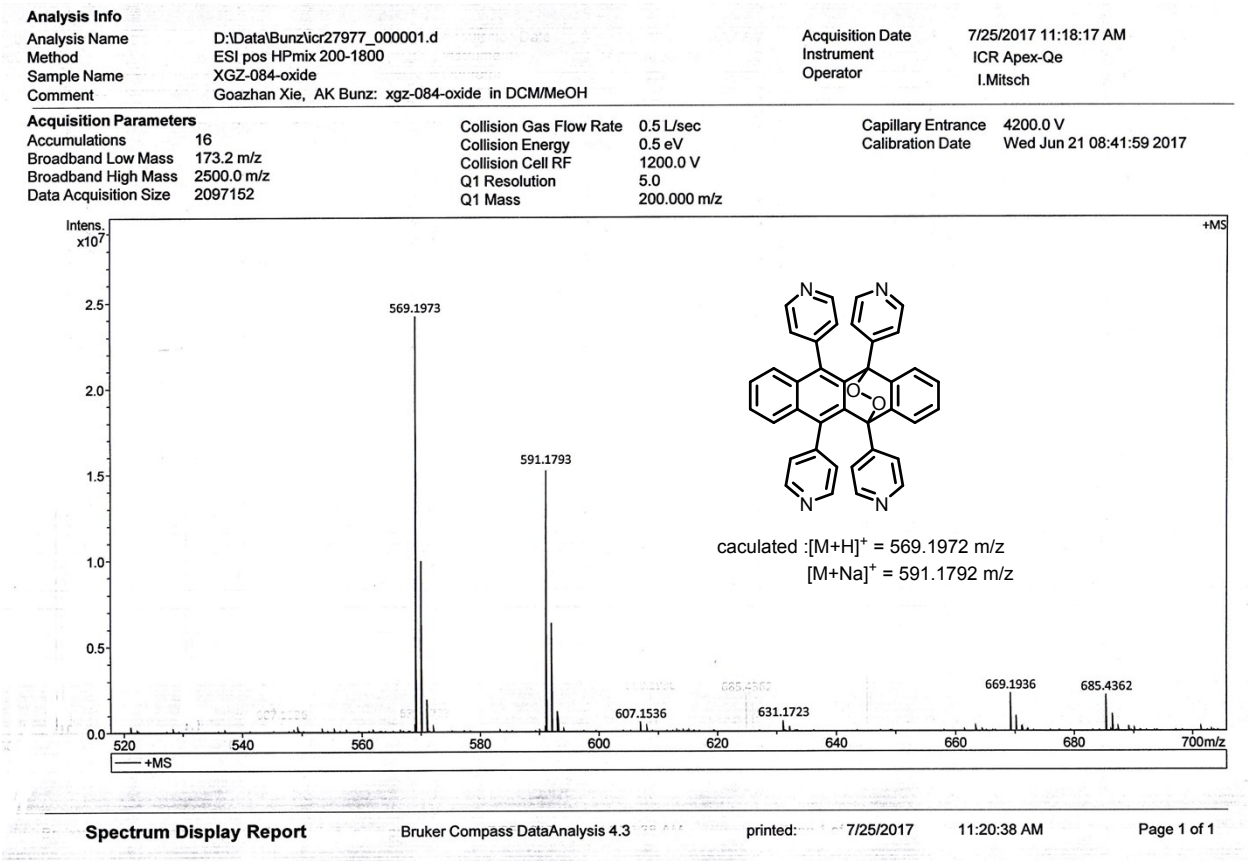
5,12-Dihydro-5,11-di(4-pyridyl)-6,12-diphenyl-5,12-epidioxynaphthacene(**DARO2)**



5,6,11,12-tetra(4-pyridyl)tetracene (**TAR**)

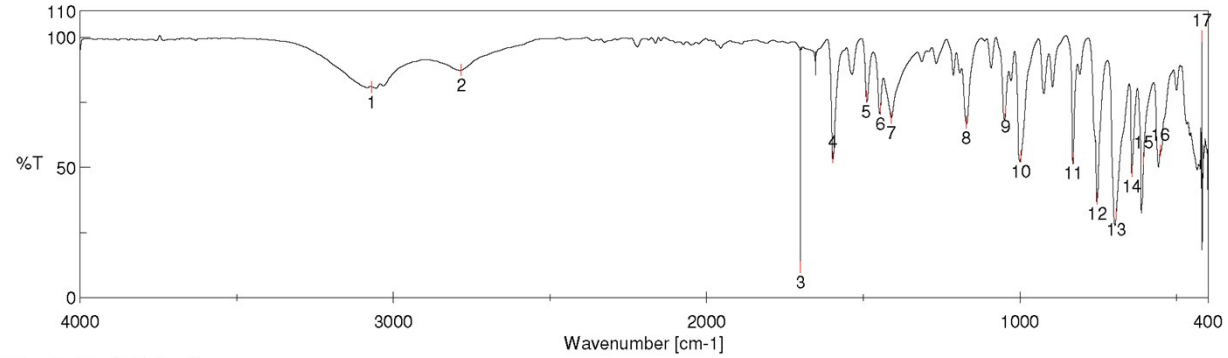


5,12-Dihydro-5,11-di(4-pyridyl)-6,12-diphenyl-5,12-epidioxynaphthacene (**DARO2**)



S5. Infrared spectroscopy

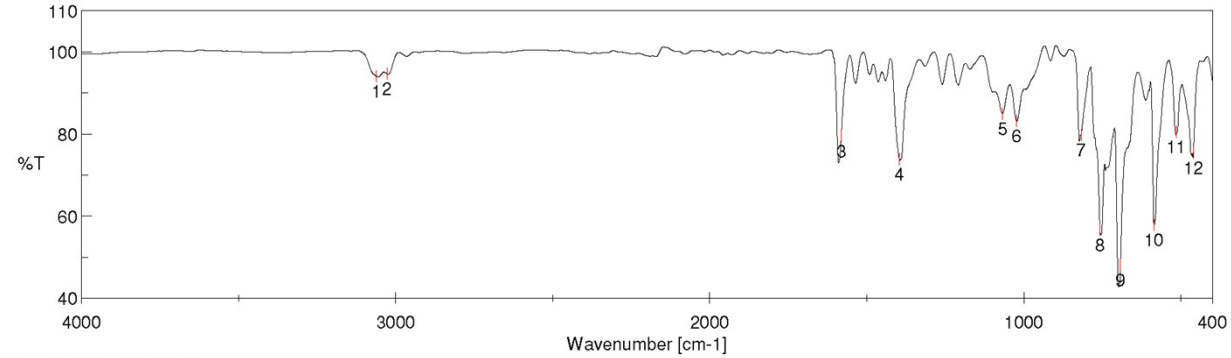
1,1-Diphenyl-3-pyridyl-2- propyn-1-ol **(2)**



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3068.67	80.8558	2	2783.5	87.2559	3	1700.18	11.5568
4	1597.49	53.8423	5	1490.95	77.0292	6	1445.39	72.4798
7	1411.16	69.0682	8	1171.78	66.9949	9	1046.19	71.6092
10	996.776	54.1318	11	829.482	53.6046	12	753.548	38.0443
13	692.802	31.9746	14	643.385	48.5467	15	605.298	53.4384
16	552.024	56.3953	17	418.959	100.34			

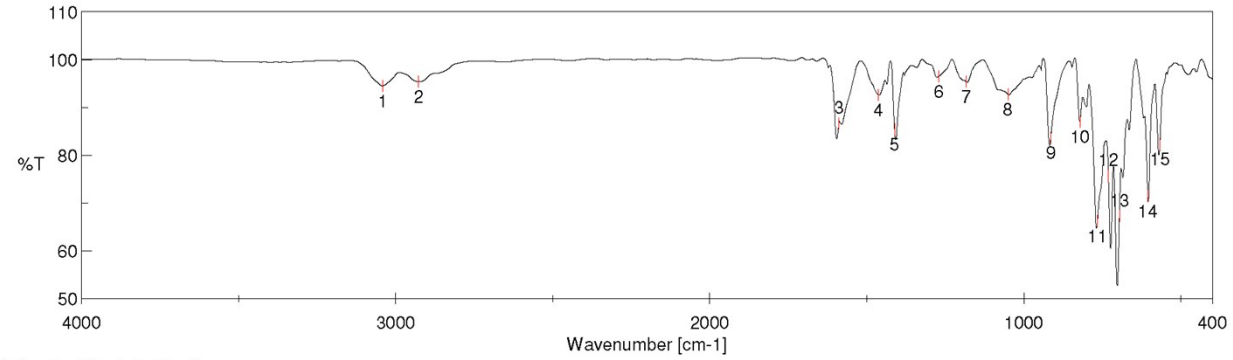
5,11-Di(4-pyridyl)-6,12-diphenyltetracene (**DAR**)



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3060.48	93.9731	2	3027.69	94.6348	3	1581.34	79.387
4	1396.21	73.8393	5	1068.37	84.8804	6	1024.02	83.1783
7	817.67	79.76	8	757.888	56.5568	9	692.32	47.9876
10	586.254	57.8803	11	514.901	80.4411	12	460.904	75.4493

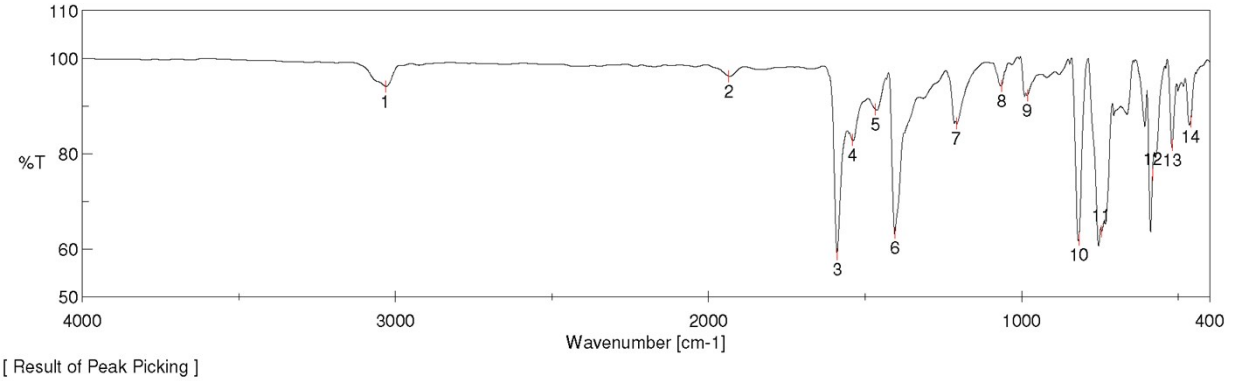
5,12-Dihydro-5,11-di(4-pyridyl)-6,12-diphenyl-5,12-epidioxynaphthacene (**DARO2)**



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3041.19	94.4629	2	2927.41	95.3784	3	1589.06	86.6471
4	1463.71	92.6369	5	1411.64	85.3593	6	1270.86	96.4501
7	1184.08	95.3461	8	1051.01	92.6876	9	914.093	83.709
10	821.527	87.0232	11	765.601	66.1743	12	730.889	75.7114
13	696.177	67.2113	14	605.539	71.3695	15	566.969	82.3527

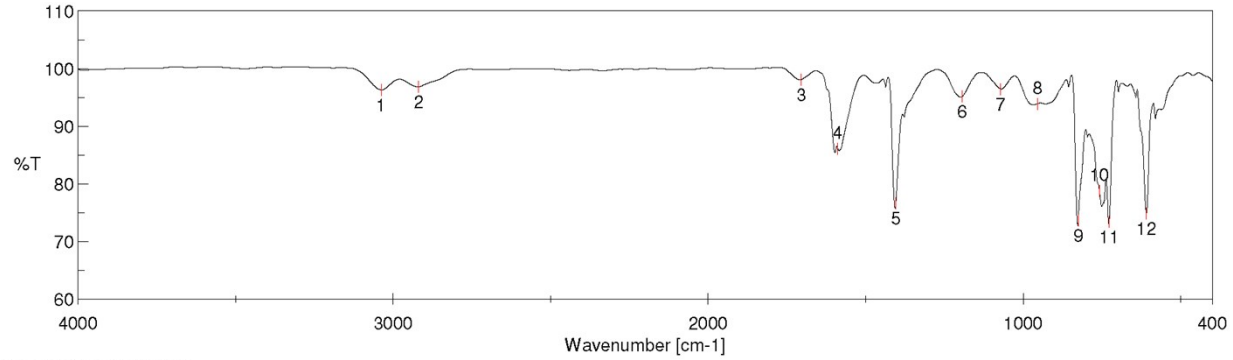
5,6,11,12-tetra(4-pyridyl)tetracene (**TAR**)



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3031.55	94.1191	2	1936.18	96.232	3	1589.06	58.9269
4	1540.85	82.8317	5	1467.56	89.2778	6	1403.92	63.3628
7	1209.15	86.3574	8	1064.51	94.1658	9	981.59	92.1806
10	817.67	61.9788	11	746.317	63.7301	12	582.397	75.566
13	518.758	81.8549	14	460.904	86.7034			

5,12-Dihydro-5,6,11,12-tetra(4-pyridyl)-5,12-epidioxynaphthacene (**TARO2**)



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3037.34	96.2571	2	2919.7	96.8187	3	1704.76	98.0467
4	1589.06	86.1084	5	1403.92	76.5663	6	1193.72	95.119
7	1072.23	96.4348	8	954.591	93.87	9	825.384	73.6656
10	757.888	78.7657	11	727.032	73.403	12	609.396	74.8763

S6. NMR-Spectroscopy

1,1-Diphenyl-3-pyridyl-2- propyn-1-ol ***(2)***

^{1}H-NMR

OriginalDateForRelativeTime	2017-07-20T19:31:06			*Multiplets Integrals Sum*	14.84	*Number of Nuclei*	15 H's		
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DE	6.5	*DS*	2	*Date*	20 Jul 2017 19:31:06			*Date Stamp*	20 Jul 2017 19:31:06
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\d170720ubxgz024\1\1\fid					*Frequency (MHz)*	500.1300	*GB*	0
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Origin	spect	*Original Points Count*	49152	*Owner*	ns	*PC*	1		
PROBHD	<Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)>			*PULPROG*	<zg30>	*Points Count*	65536	*Pulse Sequence*	zg30
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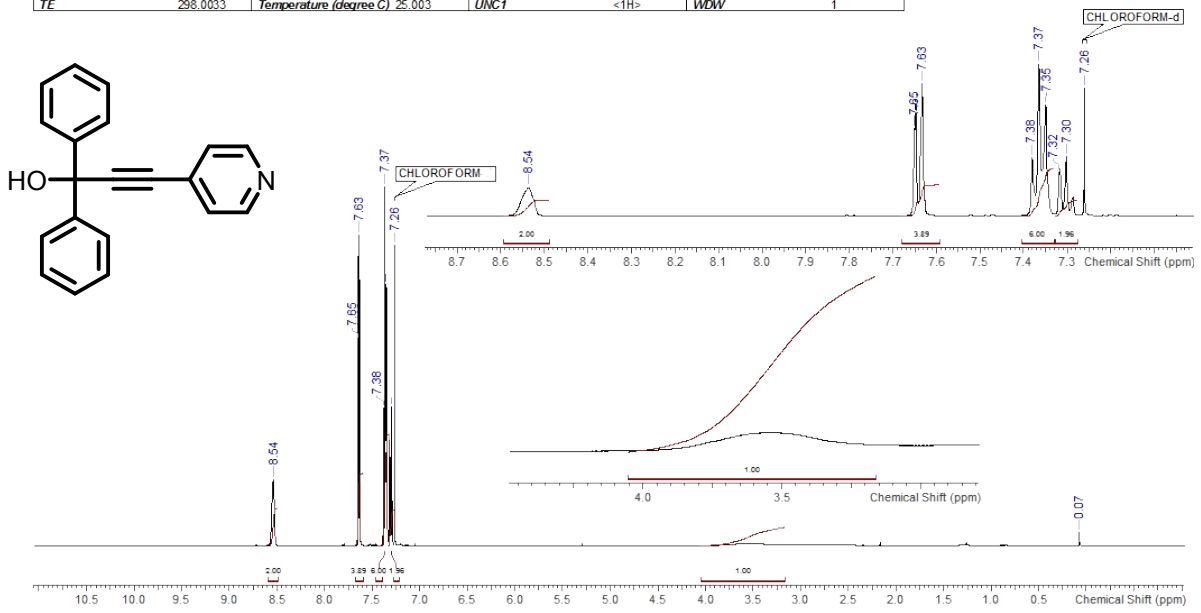
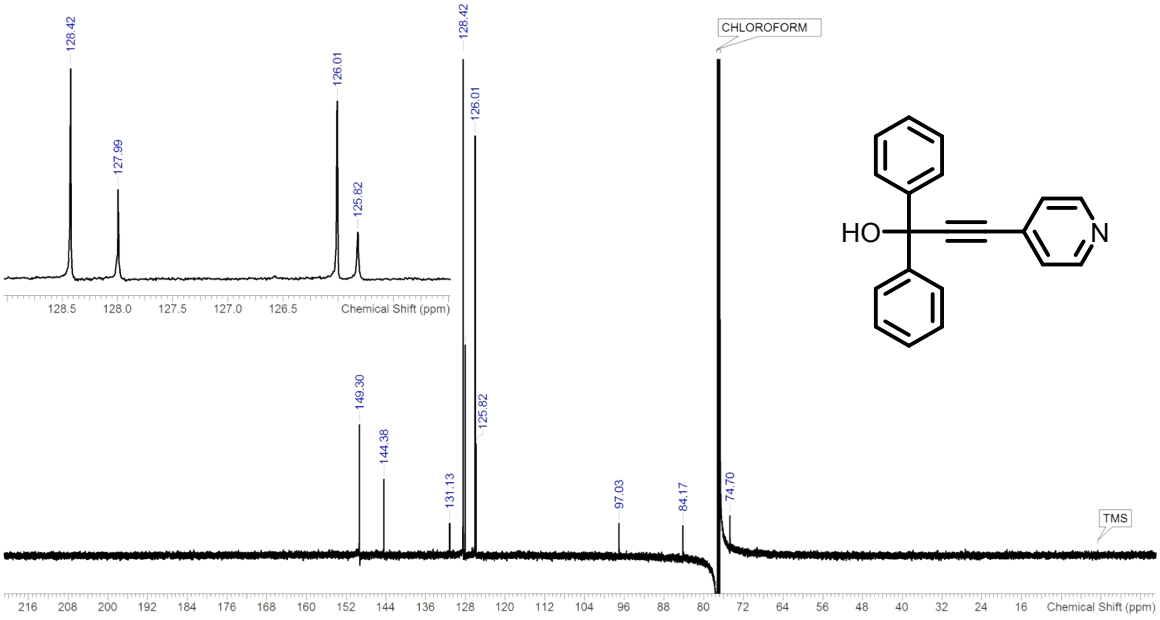
SI	65536	*SSB*	0	*SW(cyclical) (Hz)*	15000.00	*SWH*	15000	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2488.2749	*Spectrum Type*	standard	*Sweep Width (Hz)*	14999.77	*TD*	98304	*TD0*	256
TE	298.0033	*Temperature (degree C)*	25.003	*UNC1*	<1H>	*WDW*	1		



^{13}C-NMR

Acquisition Time (sec)	1.7302	*Comment*	Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)			*D*	1.5	*D1*	1.5
DE	20	*DS*	4	*Date*	20 Jul 2017 23:19:26			*Date Stamp*	20 Jul 2017 23:19:26
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\d170720ubxgz024\2\PDATA\1\1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	0.5	*NS*	4096	*Nucleus*	13C	*Number of Transients*	4096
Origin	spect	*Original Points Count*	65536	*Owner*	ns	*PC*	1.4		
PROBHD	<Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)>			*PULPROG*	<zgpg30>	*Points Count*	65536	*Pulse Sequence*	zgpg30
Receiver Gain	2050.00	*SF*	125.757789	*SFO1*	125.77162235679			*SI*	65536
SSB	0	*SW(cyclical) (Hz)*	37878.79	*SWH*	37878.7878787879			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	13830.6719	*Spectrum Type*	standard	*Sweep Width (Hz)*	37878.21	*TD*	131072	*TD0*	512
TE	298.0268	*Temperature (degree C)*	25.027	*UNC1*	<13C>	*WDW*	1		

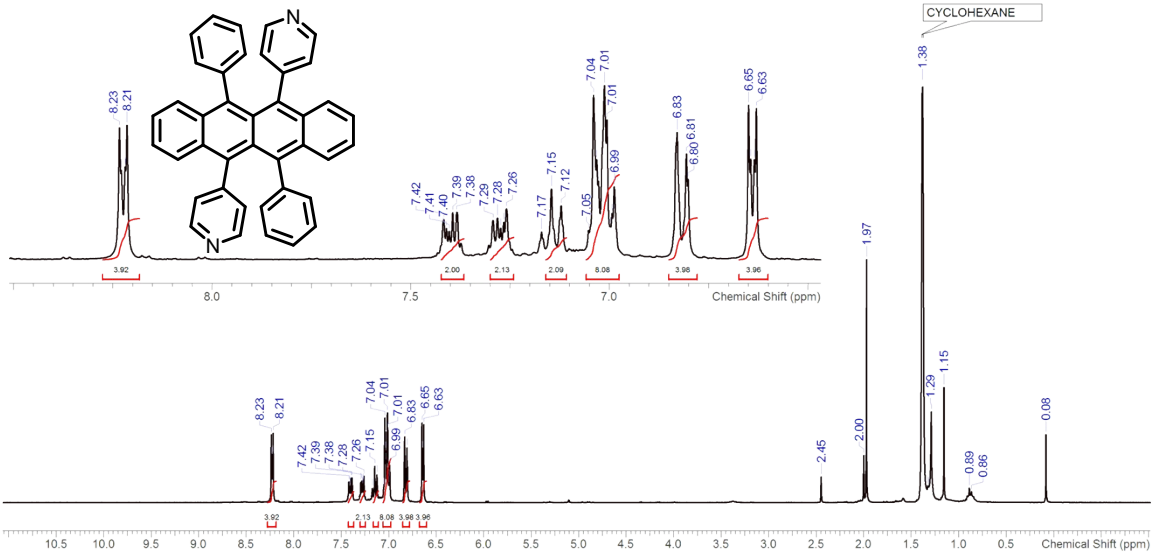


5,11-Di(4-pyridyl)-6,12-diphenyltetracene (**DAR**)

^{1}H-NMR

OriginalDateForRelativeTime	2017-04-24T13:30:54	*Multiplets Integrals Sum*	26.17	*Number of Nuclei*	62 H's / 26 H's (spectrum / structure)		
Formula	$C_{40}H_{26}N_2$	*FW*	534.6478	*[M-H]-*	533.202322	*[M+H]+*	533.201225	*[M+H]-*	535.217972		
[M+H]+	535.216875	*M-*	534.210147	*M+*	534.209050	*Monoisotopic Mass*	534.209599	*Nominal Mass*	534		

Acquisition Time (sec)	3.6351	*Comment*	Z104275_0201 (PA BBO 300S1 BBF-H-D-05 Z)	*D*	0.1	*D1*	0.1
DE	6.5	*DS*	2	*Date*	24 Apr 2017 13:30:54			*Date Stamp*	24 Apr 2017 13:30:54
File Name	G:\a170424ubxgz05507\1\PDATA\1\1r			*Frequency (MHz)*	300.5100	*GB*	0	*INSTRUM*	<spect>
LB	0.3	*NS*	128	*Nucleus*	1H	*Number of Transients*	128	*Origin*	spect
Original Points Count	32768	*Owner*	ns	*PC*	1	*PROBHD*	<Z104275_0201 (PA BBO 300S1 BBF-H-D-05 Z)>		
PULPROG	<zg30>	*Points Count*	65536	*Pulse Sequence*	zg30	*Receiver Gain*	724.00	*SF*	300.51
SFO1	300.51150255			*SI*	65536	*SSB*	0	*SW(cyclical) (Hz)*	9014.42
SWH	9014.42307692308			*Solvent*	C6D12	*Spectrum Offset (Hz)*	1489.0273	*Spectrum Type*	standard
Sweep Width (Hz)	9014.29	*TD*	65536	*TD0*	16	*TE*	300.0014	*Temperature (degree C)*	27.001
UNC1	<1H>	*WDW*	1						

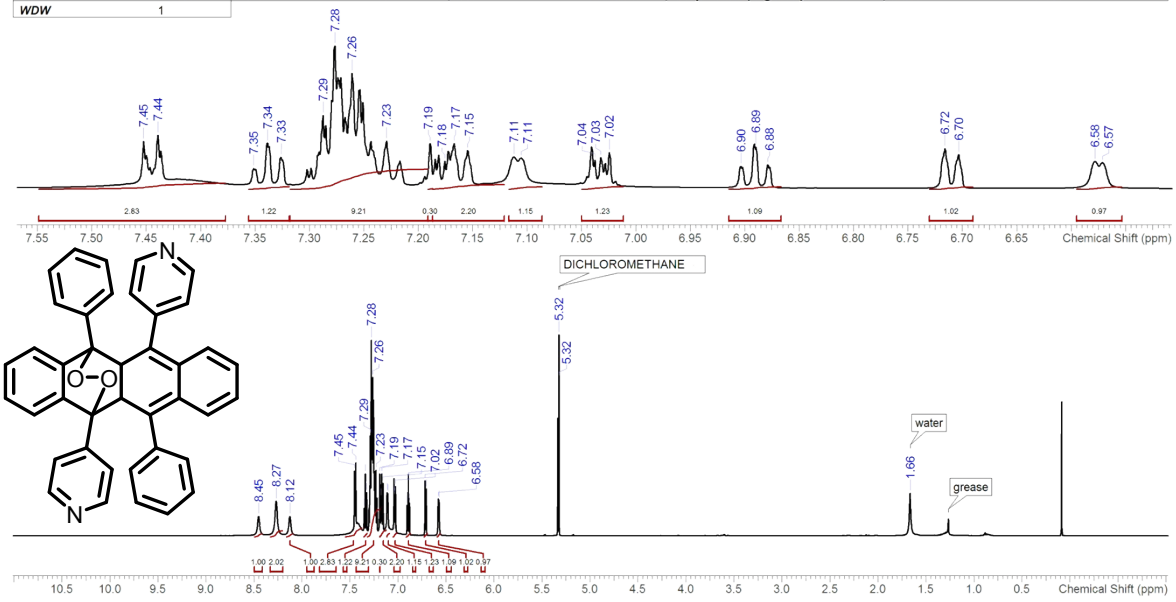


Because **DAR** can be oxidized easily, there is still a little amount of **DARO2** in final product after recrystallization. Fortunately, the solubility of **DAR** is quite better than that of **DARO2** in cyclohexane-d_{12} so that we can get unambiguous ^{1}H-NMR spectrum of **DAR** in this deuterated solvent. However, the dissolved amount of DAR is not sufficient enough to reach the requirement of ^{13}C-NMR measurement.

5,12-Dihydro-5,11-di(4-pyridyl)-6,12-diphenyl-5,12-epidioxynaphthacene (**DARO2)**

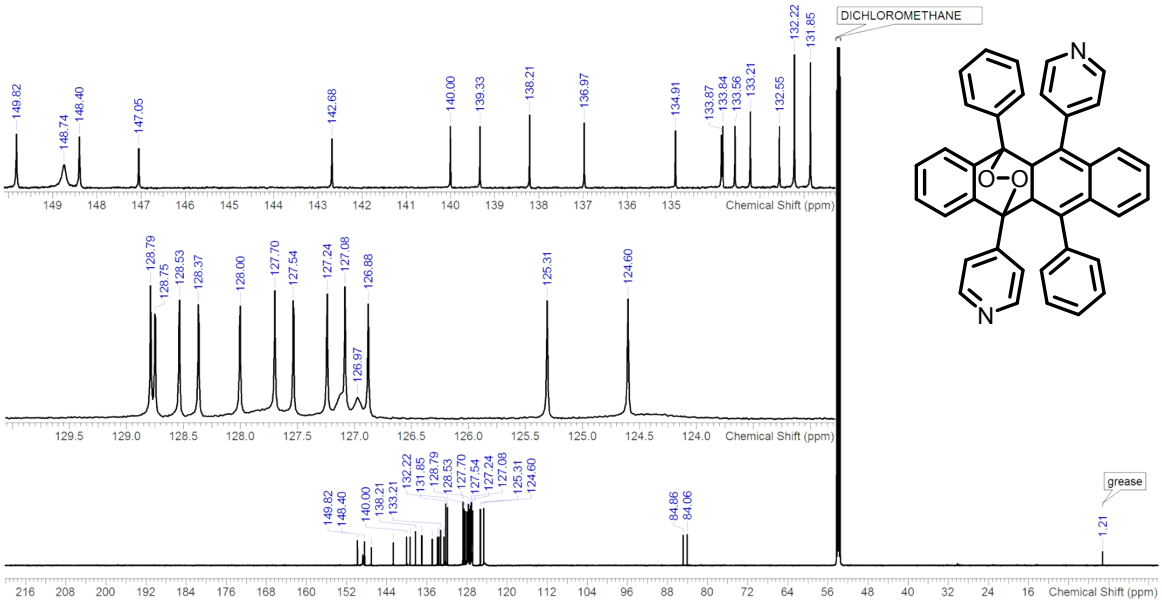
^{1}H-NMR

OriginalDateForRelativeTime	2017-07-07T21:10:32			*Multiplets Integrals Sum*	22.80	*Number of Nuclei*	24 H's		
Acquisition Time (sec)	3.6351	*Comment*	XGZO 055	*D*	0.1	*D1*	0.1	*DE*	12
DS	2	*Date*	07 Jul 2017 21:10:32			*Date Stamp*	07 Jul 2017 21:10:32		
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\e170707ubxgz055-oxidized\2\fid					*Frequency (MHz)*	600.2438	*GB*	0
INSTRUM	<spect>	*LB*	0.3	*NS*	128	*Nucleus*	1H	*Number of Transients*	128
Origin	spect	*Original Points Count*	65536	*Owner*	ns	*PC*	1		
PROBHD	<Z132808_0001 (CP QCI 600S3 H/P/C-N-D-05 Z LT)>					*PULPROG*	<zg30>	*Points Count*	65536
Pulse Sequence	zg30	*Receiver Gain*	15.35	*SF*	600.243829	*SFO1*	600.246830219145		
SI	65536	*SSB*	0	*SW(cyclical) (Hz)*	18028.85	*SWH*	18028.8461538462		
Solvent	DICHLOROMETHANE-d2			*Spectrum Offset (Hz)*	2807.9971	*Spectrum Type*	standard	*Sweep Width (Hz)*	18028.57
TD	131072	*TD0*	16	*TE*	294.9497	*Temperature (degree C)*	21.950	*UNC1*	<1H>
WDW	1								



^{13}C-NMR

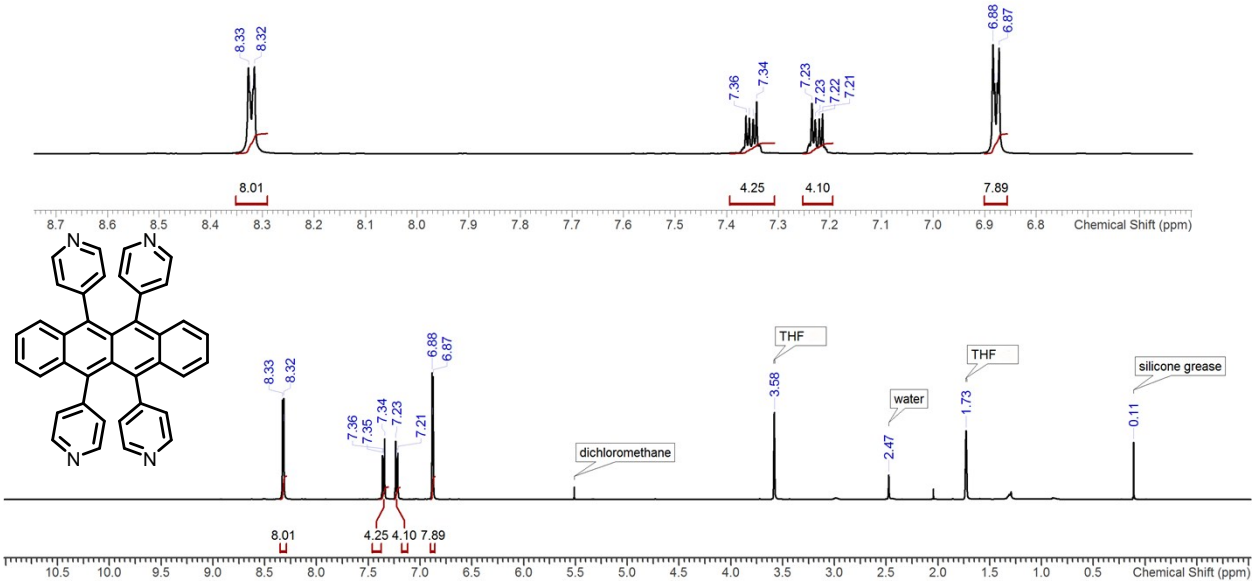
Acquisition Time (sec)	1.0795	*Comment*	XGZO 055	*D*	0.03	*D1*	2	*DE*	18
DS	4	*Date*	07 Jul 2017 21:01:22			*Date Stamp*	07 Jul 2017 21:01:22		
File Name	C:\Users\bunz\Application Data\SSH\temp\1\PDATA\1\1r					*Frequency (MHz)*	150.9314	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	4096	*Nucleus*	13C	*Number of Transients*	4096
Origin	spect	*Original Points Count*	49066	*Owner*	ns	*PC*	1.4		
PROBHD	<Z132808_0001 (CP QCI 600S3 H/P/C-N-D-05 Z LT)>					*PULPROG*	<zgpg30>	*Points Count*	65536
Pulse Sequence	zgpg30	*Receiver Gain*	2050.00	*SF*	150.931431	*SFO1*	150.94803345741		
SI	65536	*SSB*	0	*SW(cyclical) (Hz)*	45454.55	*SWH*	45454.5454545455		
Solvent	DICHLOROMETHANE-d2			*Spectrum Offset (Hz)*	16626.6035	*Spectrum Type*	standard	*Sweep Width (Hz)*	45453.85
TD	98132	*TD0*	512	*TE*	294.9497	*Temperature (degree C)*	21.950	*UNC1*	<13C>
WDW	1								



5,6,11,12-tetra(4-pyridyl)tetracene (**TAR**)

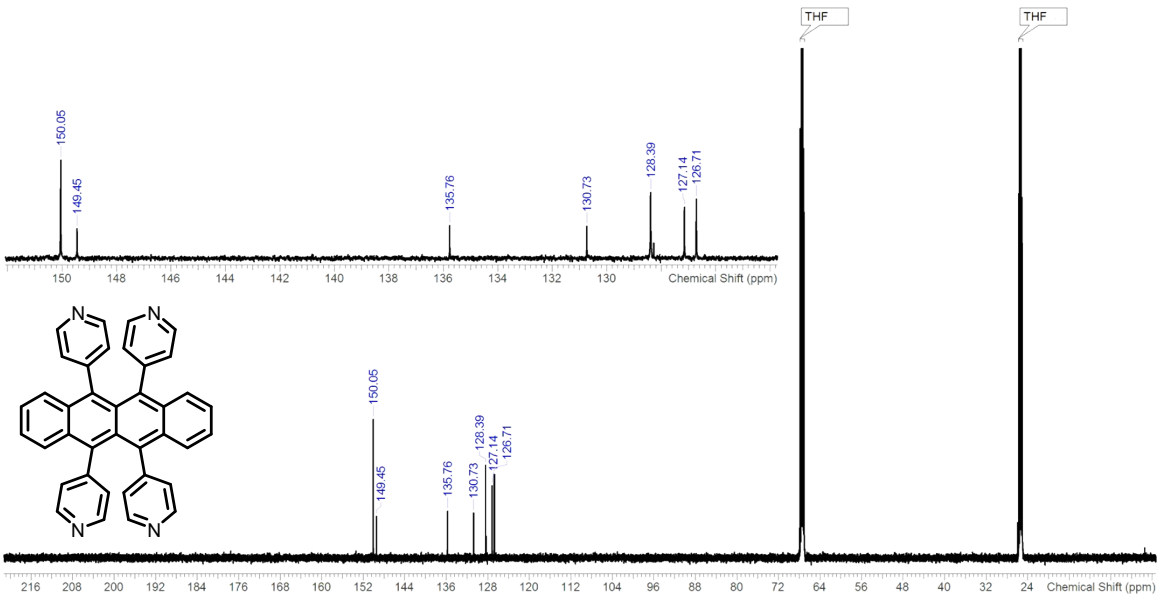
^{1}H-NMR

OriginalDateForRelativeTime 2017-12-06T00:07:28				***Multiplets Integrals Sum***	24.25	***Number of Nuclei***	37 H's
Acquisition Time (sec)	3.2768	***Comment***	Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)		***D*** 0.1	***D1***	0.1
DE	6.5	***DS***	2	***Date***	06 Dec 2017 00:07:28	***Date Stamp***	06 Dec 2017 00:07:28
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\d171205ubxgzTAR\1\PDATA\1\1r				***Frequency (MHz)*** 500.1299	***GB***	0
INSTRUM	<spect>	***LB***	0.3	***NS***	1024	***Nucleus*** 1H	***Number of Transients*** 1024
Origin	spect	***Original Points Count***	49152	***Owner***	ns	***PC*** 1	
PROBHD	<Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)>			***PULPROG***	<zg30>	***Points Count*** 65536	***Pulse Sequence*** zg30
Receiver Gain	256.00	***SF***	500.129953368799			***SFO1*** 500.13250065	
SI	65536	***SSB***	0	***SW(cyclical) (Hz)***	15000.00	***SWH*** 15000	***Solvent*** THF
Spectrum Offset (Hz)	3411.5051	***Spectrum Type***	standard	***Sweep Width (Hz)***	14999.77	***TD*** 98304	***TD0*** 128
TE	298.0014	***Temperature (degree C)***	25.001	***UNC1***	<1H>	***WDW*** 1	



^{13}C-NMR

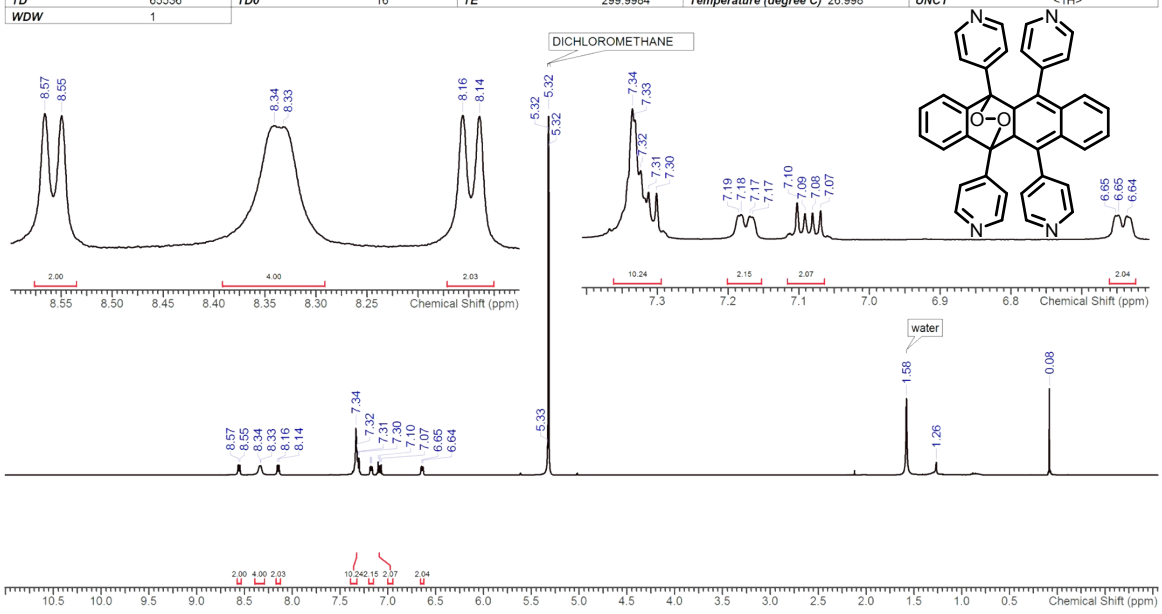
OriginalDateForRelativeTime 2017-12-06T02:01:26				***Multiplets Integrals Sum***	0.00	***Number of Nuclei***	4 C's
Acquisition Time (sec)	1.7302	***Comment***	Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)		***D*** 1.5	***D1***	1.5
DE	20	***DS***	4	***Date***	06 Dec 2017 02:01:26	***Date Stamp***	06 Dec 2017 02:01:26
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\d171205ubxgzTAR\2\PDATA\1\1r				***Frequency (MHz)*** 125.7578	***GB***	0
INSTRUM	<spect>	***LB***	0.5	***NS***	2048	***Nucleus*** 13C	***Number of Transients*** 2048
Origin	spect	***Original Points Count***	65536	***Owner***	ns	***PC*** 1.4	
PROBHD	<Z810701_0032 (PA BBI 500S2 H-BB-D-05 Z)>			***PULPROG***	<zgpg30>	***Points Count*** 65536	***Pulse Sequence*** zgpg30
Receiver Gain	2050.00	***SF***	125.757789	***SFO1***	125.77162235679		***SI*** 65536
SSB	0	***SW(cyclical) (Hz)***	37878.79	***SWH***	37878.7878787879		***Solvent*** THF
Spectrum Offset (Hz)	14197.8975	***Spectrum Type***	standard	***Sweep Width (Hz)***	37878.21	***TD*** 131072	***TD0*** 256
TE	298.0056	***Temperature (degree C)***	25.006	***UNC1***	<13C>	***WDW*** 1	



5,12-Dihydro-5,6,11,12-tetra(4-pyridyl)-5,12-epidioxynaphthacene (**TARO2**)

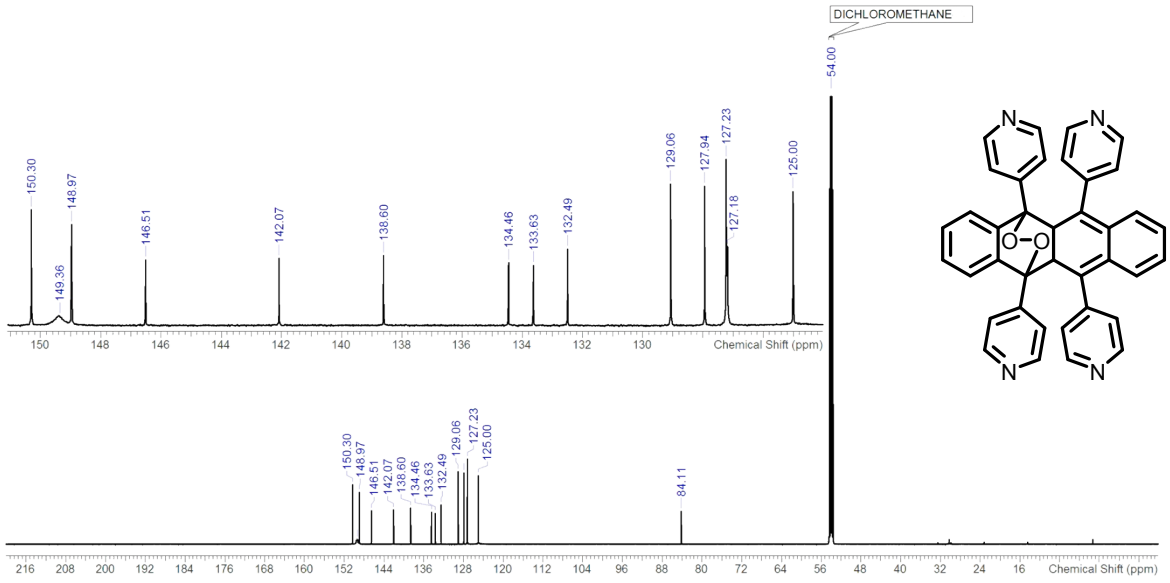
^{1}H-NMR

Acquisition Time (sec)	3.6351	*Comment*	Z104275_0201 (PA BBO 300S1 BBF-H-D-05 Z)			*D*	0.1	*D1*	0.1
DE	6.5	*DS*	2	*Date*	16 Jun 2017 20:08:50				
Date Stamp	16 Jun 2017 20:08:50								
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\Rubren paper\a170616ubxgz084white\1\PDATA\1\1r							*Frequency (MHz)*	300.5100
GB	0	*INSTRUM*	<spect>	*LB*	0.3	*NS*	128	*Nucleus*	1H
Number of Transients	128	*Origin*	spect	*Original Points Count*	32768	*Owner*	ns	*PC*	1
PROBHD	<Z104275_0201 (PA BBO 300S1 BBF-H-D-05 Z)>			*PULPROG*	<zg30>	*Points Count*	65536	*Pulse Sequence*	zg30
Receiver Gain	1030.00	*SF*	300.510036133872			*SFO1*	300.51150255	*SI*	65536
SSB	0	*SW(cyclical) (Hz)*	9014.42	*SWH*	9014.42307692308				
Solvent	DICHLOROMETHANE-d2			*Spectrum Offset (Hz)*	1491.0892	*Spectrum Type*	standard	*Sweep Width (Hz)*	9014.29
TD	65536	*TD0*	16	*TE*	299.9984	*Temperature (degree C)*	26.998	*UNC1*	<1H>
WDW	1								



^{13}C-NMR

OriginalDateForRelativeTime	2017-07-21T21:43:52			*Multiplets Integrals Sum*	0.00	*Number of Nuclei*	0 C's		
Acquisition Time (sec)	1.0795	*Comment*	XG 084	*D*	0.03	*D1*	2	*DE*	18
DS	4	*Date*	21 Jul 2017 21:43:52			*Date Stamp*	21 Jul 2017 21:43:52		
File Name	\\bunz22\Mitarbeiter\Gaozhan XIE\03_analytics\01-NMR\e170721ubxg.084-oxidization\1\PDATA\1\1r							*Frequency (MHz)*	150.9314
GB	0	*INSTRUM*	<spect>	*LB*	1	*NS*	4096	*Nucleus*	13C
Number of Transients	4096	*Origin*	spect	*Original Points Count*	49066	*Owner*	ns	*PC*	1.4
PROBHD	<Z132808_0001 (CP QCI 600S3 H/P/C-N-D-05 Z LT)>			*PULPROG*	<zgpg30>	*Points Count*	65536	*Pulse Sequence*	zgpg30
Receiver Gain	2050.00	*SF*	150.931431	*SFO1*	150.94803345741			*SI*	65536
SSB	0	*SW(cyclical) (Hz)*	45454.55	*SWH*	45454.5454545455				
Solvent	DICHLOROMETHANE-d2			*Spectrum Offset (Hz)*	16642.1660	*Spectrum Type*	standard	*Sweep Width (Hz)*	45453.85
TD	98132	*TD0*	512	*TE*	294.9489	*Temperature (degree C)*	21.949	*UNC1*	<13C>
WDW	1								



S7. Crystal structures

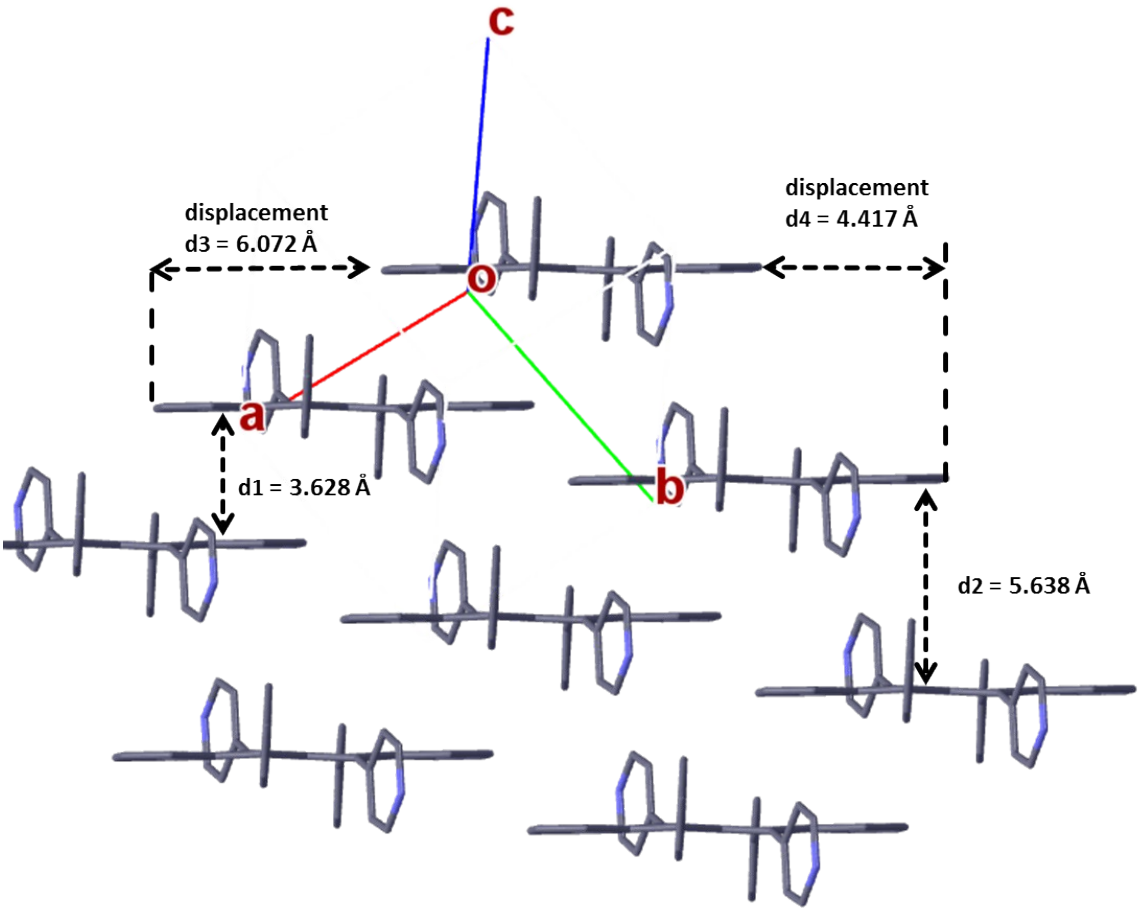


Figure S2. Illustration of the lattice parameters within ab layer of **DAR** crystal. The π - π stacking distances along a and b direction are estimated to be around 3.6 Å and 5.6 Å respectively; The long-axis displacements of adjacent molecules along a and b direction are estimated to be around 6.1 Å and 4.4 Å respectively.

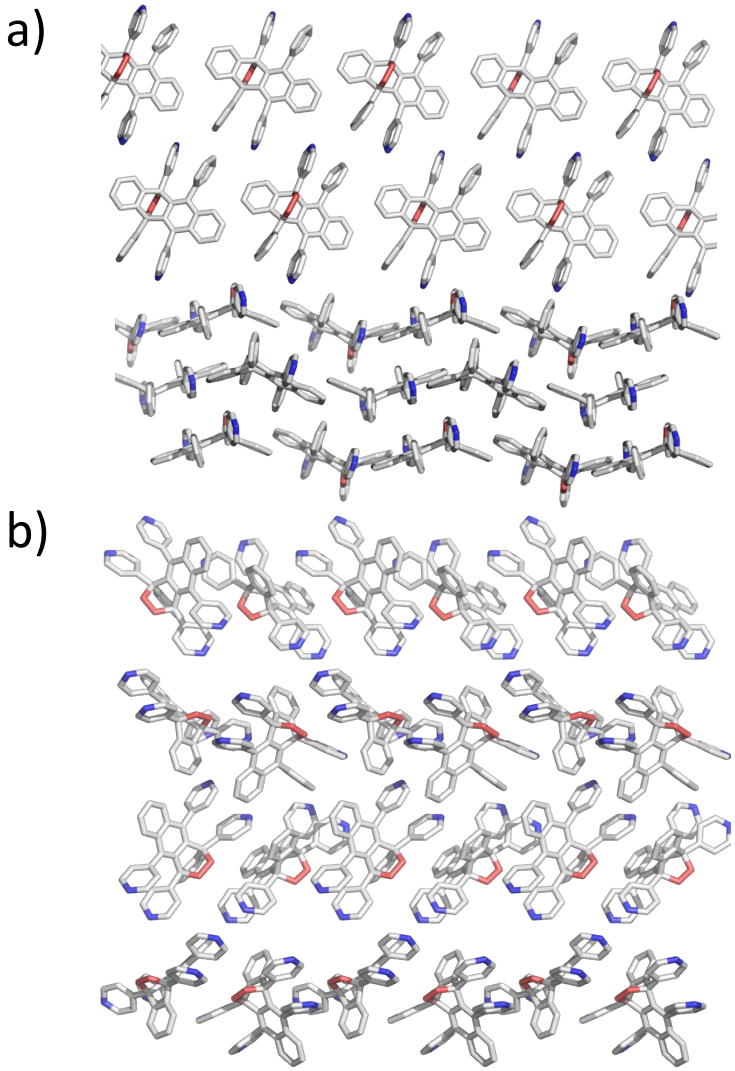
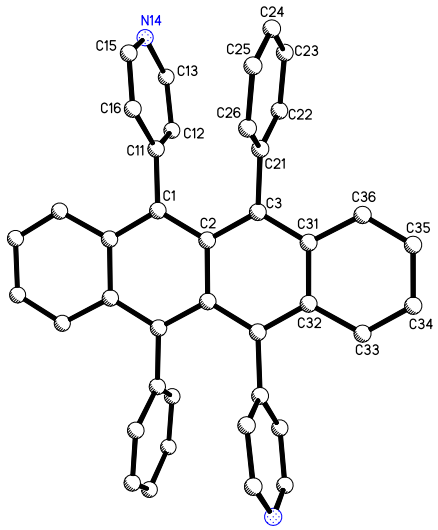


Figure S3. Examples for the visualization of packing of **DARO2** (a) and **TARO2** (b).

5,11-Di(4-pyridyl)-6,12-diphenyltetracene (**DAR**) CCDC 1821077



Identification code	gxi2
Empirical formula	$C_{40}H_{26}N_2$
Formula weight	534.63
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	triclinic
Space group	$P\bar{1}$
Z	1
Unit cell dimensions	a = 7.0727(7) Å α = 90.402(7) deg. b = 8.2696(8) Å β =106.039(7) deg. c = 11.8550(10) Å γ = 97.605(8) deg.
Volume	659.84(11) $Å^3$
Density (calculated)	1.35 g/cm^3
Absorption coefficient	0.60 mm^{-1}
Crystal shape	irregular
Crystal size	0.070 x 0.064 x 0.045 mm^3
Crystal colour	red
Theta range for data collection	3.9 to 61.8 deg.
Index ranges	$-7 \le h \le 7$, $-9 \le k \le 9$, $-13 \le l \le 13$
Reflections collected	7917
Independent reflections	1985 (R(int) = 0.0387)
Observed reflections	998 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.72 and 0.61
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7917 / 0 / 191
Goodness-of-fit on F^2	0.79
Final R indices (I>2sigma(I))	R1 = 0.041, wR2 = 0.086
Largest diff. peak and hole	0.31 and -0.37 $eÅ^{-3}$

Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **DAR**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
C1	0.9026(4)	0.6628(3)	0.5726(2)	0.0180(6)
C2	1.0279(4)	0.5496(3)	0.5550(2)	0.0164(6)
C3	1.2079(4)	0.5277(3)	0.6420(2)	0.0181(6)
C11	0.9641(4)	0.7940(3)	0.6694(2)	0.0187(7)
C12	1.0724(4)	0.9410(3)	0.6549(2)	0.0232(7)
H12	1.1173	0.9552	0.5866	0.028
C13	1.1153(4)	1.0668(3)	0.7392(2)	0.0275(7)
H13	1.1909	1.1657	0.7273	0.033
N14	1.0550(4)	1.0559(3)	0.8378(2)	0.0331(7)
C15	0.9500(4)	0.9121(4)	0.8515(2)	0.0274(7)
H15	0.9080	0.8999	0.9208	0.033
C16	0.9007(4)	0.7825(3)	0.7707(2)	0.0223(7)
H16	0.8235	0.6853	0.7839	0.027
C21	1.2633(4)	0.5997(3)	0.7657(2)	0.0205(7)
C22	1.3972(4)	0.7409(3)	0.8007(2)	0.0236(7)
H22	1.4499	0.7982	0.7445	0.028
C23	1.4552(4)	0.7996(4)	0.9167(2)	0.0291(8)
H23	1.5459	0.8975	0.9391	0.035
C24	1.3821(4)	0.7168(4)	0.9995(2)	0.0264(7)
H24	1.4208	0.7577	1.0788	0.032
C25	1.2535(4)	0.5754(4)	0.9665(2)	0.0283(8)
H25	1.2037	0.5179	1.0237	0.034
C26	1.1938(4)	0.5136(3)	0.8505(2)	0.0237(7)
H26	1.1065	0.4138	0.8292	0.028
C31	1.3360(4)	0.4256(3)	0.6183(2)	0.0177(6)
C32	1.2814(4)	0.3305(3)	0.5092(2)	0.0182(6)
C33	1.4172(4)	0.2243(3)	0.4915(2)	0.0215(7)
H33	1.3841	0.1605	0.4200	0.026
C34	1.5910(4)	0.2125(3)	0.5737(2)	0.0246(7)
H34	1.6792	0.1434	0.5585	0.029
C35	1.6405(4)	0.3025(3)	0.6816(2)	0.0250(7)
H35	1.7604	0.2915	0.7399	0.030
C36	1.5189(4)	0.4042(3)	0.7026(2)	0.0206(7)
H36	1.5558	0.4638	0.7760	0.025

Hydrogen coordinates and isotropic displacement parameters (Å^2) for **DAR**.

Atom	x	y	z	U_{eq}
H12	1.1173	0.9552	0.5866	0.028
H13	1.1909	1.1657	0.7273	0.033
H15	0.9080	0.8999	0.9208	0.033
H16	0.8235	0.6853	0.7839	0.027
H22	1.4499	0.7982	0.7445	0.028
H23	1.5459	0.8975	0.9391	0.035
H24	1.4208	0.7577	1.0788	0.032
H25	1.2037	0.5179	1.0237	0.034
H26	1.1065	0.4138	0.8292	0.028
H33	1.3841	0.1605	0.4200	0.026
H34	1.6792	0.1434	0.5585	0.029
H35	1.7604	0.2915	0.7399	0.030
H36	1.5558	0.4638	0.7760	0.025

Anisotropic displacement parameters ($Å^2$) for **DAR**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0205(17)	0.0195(16)	0.0153(13)	0.0003(11)	0.0061(11)	0.0051(13)
C2	0.0190(16)	0.0162(15)	0.0142(12)	-0.0009(10)	0.0054(11)	0.0013(12)
C3	0.0188(17)	0.0161(15)	0.0192(13)	0.0006(11)	0.0056(11)	0.0012(13)
C11	0.0185(17)	0.0193(16)	0.0176(13)	-0.0010(11)	0.0026(11)	0.0060(13)
C12	0.0264(18)	0.0232(17)	0.0194(13)	0.0021(12)	0.0053(12)	0.0031(14)
C13	0.033(2)	0.0208(17)	0.0268(15)	0.0007(12)	0.0065(13)	-0.0002(14)
N14	0.0358(18)	0.0320(17)	0.0303(13)	-0.0068(11)	0.0080(11)	0.0034(13)
C15	0.0268(19)	0.0288(18)	0.0258(15)	-0.0089(13)	0.0084(12)	-0.0011(14)
C16	0.0211(18)	0.0246(17)	0.0205(14)	-0.0028(12)	0.0054(12)	0.0016(13)
C21	0.0195(17)	0.0232(16)	0.0185(13)	-0.0007(12)	0.0024(12)	0.0085(13)
C22	0.0202(18)	0.0277(18)	0.0241(14)	-0.0033(12)	0.0072(12)	0.0052(14)
C23	0.0240(18)	0.0339(19)	0.0260(15)	-0.0138(13)	0.0015(13)	0.0046(15)
C24	0.0288(19)	0.0355(19)	0.0131(13)	-0.0074(12)	0.0000(12)	0.0108(15)
C25	0.0329(19)	0.038(2)	0.0178(14)	0.0046(13)	0.0083(12)	0.0132(16)
C26	0.0241(18)	0.0237(17)	0.0215(14)	-0.0007(12)	0.0031(12)	0.0042(13)
C31	0.0185(16)	0.0167(15)	0.0166(12)	0.0006(10)	0.0044(11)	-0.0010(13)
C32	0.0225(17)	0.0163(15)	0.0176(13)	0.0016(11)	0.0089(12)	0.0018(13)
C33	0.0265(18)	0.0198(16)	0.0203(13)	-0.0039(11)	0.0094(12)	0.0045(13)
C34	0.0228(18)	0.0222(17)	0.0283(15)	-0.0003(12)	0.0051(13)	0.0063(13)
C35	0.0219(18)	0.0235(17)	0.0266(15)	0.0016(12)	0.0011(12)	0.0053(14)
C36	0.0205(17)	0.0217(17)	0.0181(13)	-0.0008(11)	0.0031(11)	0.0026(13)

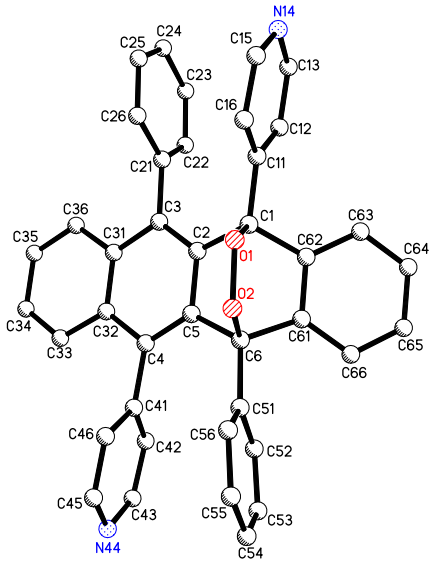
Bond lengths (Å) and angles (deg) for **DAR**.

C1-C32#1	1.400(4)	C31-C32	1.438(3)
C1-C2	1.423(3)	C32-C33	1.439(4)
C1-C11	1.504(3)	C33-C34	1.358(4)
C2-C3	1.433(3)	C33-H33	0.9500
C2-C2#1	1.465(4)	C34-C35	1.408(3)
C3-C31	1.397(3)	C34-H34	0.9500
C3-C21	1.506(3)	C35-C36	1.347(4)
C11-C12	1.387(4)	C35-H35	0.9500
C11-C16	1.393(3)	C36-H36	0.9500
C12-C13	1.382(4)	C32#1-C1-C2	120.6(2)
C12-H12	0.9500	C32#1-C1-C11	115.3(2)
C13-N14	1.351(3)	C2-C1-C11	123.7(2)
C13-H13	0.9500	C1-C2-C3	122.3(2)
N14-C15	1.351(4)	C1-C2-C2#1	119.4(3)
C15-C16	1.375(4)	C3-C2-C2#1	118.3(3)
C15-H15	0.9500	C31-C3-C2	120.8(2)
C16-H16	0.9500	C31-C3-C21	115.7(2)
C21-C22	1.384(4)	C2-C3-C21	123.2(2)
C21-C26	1.395(4)	C12-C11-C16	116.7(2)
C22-C23	1.386(3)	C12-C11-C1	120.0(2)
C22-H22	0.9500	C16-C11-C1	122.9(2)
C23-C24	1.378(4)	C13-C12-C11	120.3(3)
C23-H23	0.9500	C13-C12-H12	119.8
C24-C25	1.365(4)	C11-C12-H12	119.8
C24-H24	0.9500	N14-C13-C12	123.1(3)
C25-C26	1.394(3)	N14-C13-H13	118.4
C25-H25	0.9500	C12-C13-H13	118.4
C26-H26	0.9500	C13-N14-C15	116.2(2)
C31-C36	1.433(4)	N14-C15-C16	123.7(3)

N14-C15-H15	118.2
C16-C15-H15	118.2
C15-C16-C11	119.9(3)
C15-C16-H16	120.0
C11-C16-H16	120.0
C22-C21-C26	118.7(2)
C22-C21-C3	121.8(2)
C26-C21-C3	119.2(2)
C21-C22-C23	120.8(3)
C21-C22-H22	119.6
C23-C22-H22	119.6
C24-C23-C22	120.3(3)
C24-C23-H23	119.8
C22-C23-H23	119.8
C25-C24-C23	119.4(2)
C25-C24-H24	120.3
C23-C24-H24	120.3
C24-C25-C26	121.3(3)
C24-C25-H25	119.3
C26-C25-H25	119.3
C25-C26-C21	119.5(3)
C25-C26-H26	120.3
C21-C26-H26	120.3
C3-C31-C36	122.1(2)
C3-C31-C32	120.3(2)
C36-C31-C32	117.6(2)
C1#1-C32-C31	120.0(2)
C1#1-C32-C33	122.3(2)
C31-C32-C33	117.6(2)
C34-C33-C32	122.0(2)
C34-C33-H33	119.0
C32-C33-H33	119.0
C33-C34-C35	120.0(3)
C33-C34-H34	120.0
C35-C34-H34	120.0
C36-C35-C34	120.4(3)
C36-C35-H35	119.8
C34-C35-H35	119.8
C35-C36-C31	122.4(2)
C35-C36-H36	118.8
C31-C36-H36	118.8

5,12-Dihydro-5,11-di(4-pyridyl)-6,12-diphenyl-5,12-epidioxynaphthacene (**DARO2)**

CCDC 1821078



Identification code	gxi1	
Empirical formula	$C_{40}H_{26}N_2O_2$	
Formula weight	566.63	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	4	
Unit cell dimensions	a = 13.9299(7) Å	α = 90 deg.
	b = 11.2010(5) Å	β = 96.8662(14) deg.
	c = 18.2839(9) Å	γ = 90 deg.
Volume	2832.4(2) Å^3	
Density (calculated)	1.33 g/cm^3	
Absorption coefficient	0.08 mm^{-1}	
Crystal shape	irregular	
Crystal size	0.146 x 0.105 x 0.067 mm^3	
Crystal colour	yellow	
Theta range for data collection	1.7 to 25.1 deg.	
Index ranges	-16≤h≤16, -13≤k≤13, -21≤l≤21	
Reflections collected	26610	
Independent reflections	5024 (R(int) = 0.0392)	
Observed reflections	3757 (I > 2σ(I))	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.92	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5024 / 0 / 397	
Goodness-of-fit on F^2	1.06	
Final R indices (I>2sigma(I))	R1 = 0.042, wR2 = 0.101	
Largest diff. peak and hole	0.17 and -0.21 eÅ^{-3}	

Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **DARO2**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
O1	0.6538(1)	0.5477(1)	0.3150(1)	0.0268(3)
O2	0.5517(1)	0.5334(1)	0.3261(1)	0.0278(3)
C1	0.6793(1)	0.6743(2)	0.3062(1)	0.0211(4)
C2	0.6609(1)	0.7328(2)	0.3796(1)	0.0217(4)
C3	0.7273(1)	0.7885(2)	0.4300(1)	0.0226(4)
C4	0.5335(1)	0.7496(2)	0.4610(1)	0.0242(4)
C5	0.5623(1)	0.7151(2)	0.3944(1)	0.0219(4)
C6	0.5022(1)	0.6488(2)	0.3311(1)	0.0228(4)
C11	0.7818(1)	0.6667(2)	0.2859(1)	0.0216(4)
C12	0.8281(1)	0.7657(2)	0.2606(1)	0.0262(4)
H12	0.7969	0.8414	0.2577	0.031
C13	0.9195(1)	0.7535(2)	0.2396(1)	0.0333(5)
H13	0.9501	0.8228	0.2233	0.040
N14	0.9676(1)	0.6500(2)	0.2410(1)	0.0396(4)
C15	0.9225(1)	0.5560(2)	0.2650(1)	0.0383(5)
H15	0.9547	0.4812	0.2663	0.046
C16	0.8317(1)	0.5598(2)	0.2883(1)	0.0295(4)
H16	0.8038	0.4896	0.3058	0.035
C21	0.8307(1)	0.8144(2)	0.4197(1)	0.0255(4)
C22	0.8568(2)	0.9283(2)	0.3989(1)	0.0353(5)
H22	0.8086	0.9881	0.3890	0.042
C23	0.9522(2)	0.9553(2)	0.3924(1)	0.0458(6)
H23	0.9691	1.0331	0.3778	0.055
C24	1.0228(2)	0.8699(2)	0.4071(1)	0.0460(6)
H24	1.0883	0.8888	0.4027	0.055
C25	0.9984(1)	0.7572(2)	0.4283(1)	0.0400(6)
H25	1.0471	0.6981	0.4380	0.048
C26	0.9026(1)	0.7294(2)	0.4353(1)	0.0309(5)
H26	0.8864	0.6518	0.4509	0.037
C31	0.6981(1)	0.8274(2)	0.4990(1)	0.0256(4)
C32	0.6025(1)	0.8061(2)	0.5149(1)	0.0265(4)
C33	0.5780(1)	0.8396(2)	0.5853(1)	0.0341(5)
H33	0.5145	0.8244	0.5970	0.041
C34	0.6436(2)	0.8932(2)	0.6364(1)	0.0376(5)
H34	0.6256	0.9146	0.6831	0.045
C35	0.7372(2)	0.9165(2)	0.6201(1)	0.0352(5)
H35	0.7823	0.9552	0.6554	0.042
C36	0.7639(1)	0.8837(2)	0.5533(1)	0.0314(5)
H36	0.8281	0.8991	0.5431	0.038
C41	0.4343(1)	0.7342(2)	0.4836(1)	0.0258(4)
C42	0.3727(1)	0.8311(2)	0.4861(1)	0.0337(5)
H42	0.3917	0.9081	0.4716	0.040
C43	0.2836(2)	0.8143(2)	0.5099(1)	0.0428(6)
H43	0.2426	0.8819	0.5108	0.051
N44	0.2509(1)	0.7102(2)	0.5318(1)	0.0468(5)
C45	0.3113(2)	0.6187(2)	0.5311(1)	0.0448(6)
H45	0.2908	0.5433	0.5472	0.054
C46	0.4022(1)	0.6262(2)	0.5085(1)	0.0356(5)
H46	0.4425	0.5576	0.5100	0.043
C51	0.3987(1)	0.6115(2)	0.3380(1)	0.0256(4)
C52	0.3259(1)	0.6978(2)	0.3341(1)	0.0298(5)
H52	0.3420	0.7798	0.3303	0.036
C53	0.2302(1)	0.6645(2)	0.3357(1)	0.0387(5)
H53	0.1810	0.7237	0.3325	0.046
C54	0.2064(2)	0.5461(2)	0.3420(1)	0.0450(6)

H54	0.1409	0.5236	0.3431	0.054
C55	0.2776(2)	0.4604(2)	0.3466(1)	0.0460(6)
H55	0.2611	0.3787	0.3515	0.055
C56	0.3735(1)	0.4924(2)	0.3441(1)	0.0357(5)
H56	0.4221	0.4325	0.3466	0.043
C61	0.5119(1)	0.7110(2)	0.2579(1)	0.0219(4)
C62	0.6079(1)	0.7212(2)	0.2438(1)	0.0214(4)
C63	0.6283(1)	0.7584(2)	0.1750(1)	0.0257(4)
H63	0.6932	0.7604	0.1642	0.031
C64	0.5539(1)	0.7926(2)	0.1222(1)	0.0298(4)
H64	0.5682	0.8210	0.0757	0.036
C65	0.4592(1)	0.7856(2)	0.1367(1)	0.0305(5)
H65	0.4085	0.8104	0.1005	0.037
C66	0.4376(1)	0.7425(2)	0.2042(1)	0.0272(4)
H66	0.3722	0.7348	0.2134	0.033

Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **DARO2**.

Atom	x	y	z	U_{eq}
H12	0.7969	0.8414	0.2577	0.031
H13	0.9501	0.8228	0.2233	0.040
H15	0.9547	0.4812	0.2663	0.046
H16	0.8038	0.4896	0.3058	0.035
H22	0.8086	0.9881	0.3890	0.042
H23	0.9691	1.0331	0.3778	0.055
H24	1.0883	0.8888	0.4027	0.055
H25	1.0471	0.6981	0.4380	0.048
H26	0.8864	0.6518	0.4509	0.037
H33	0.5145	0.8244	0.5970	0.041
H34	0.6256	0.9146	0.6831	0.045
H35	0.7823	0.9552	0.6554	0.042
H36	0.8281	0.8991	0.5431	0.038
H42	0.3917	0.9081	0.4716	0.040
H43	0.2426	0.8819	0.5108	0.051
H45	0.2908	0.5433	0.5472	0.054
H46	0.4425	0.5576	0.5100	0.043
H52	0.3420	0.7798	0.3303	0.036
H53	0.1810	0.7237	0.3325	0.046
H54	0.1409	0.5236	0.3431	0.054
H55	0.2611	0.3787	0.3515	0.055
H56	0.4221	0.4325	0.3466	0.043
H63	0.6932	0.7604	0.1642	0.031
H64	0.5682	0.8210	0.0757	0.036
H65	0.4085	0.8104	0.1005	0.037
H66	0.3722	0.7348	0.2134	0.033

Anisotropic displacement parameters ($Å^2$) for **DARO2**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0192(6)	0.0223(7)	0.0406(8)	0.0032(6)	0.0112(6)	0.0003(5)
O2	0.0194(7)	0.0232(7)	0.0430(8)	0.0020(6)	0.0125(6)	0.0000(5)
C1	0.0213(9)	0.0197(10)	0.0231(9)	0.0012(7)	0.0057(7)	-0.0006(7)
C2	0.0213(9)	0.0227(10)	0.0222(9)	0.0043(7)	0.0067(7)	0.0048(8)

C3	0.0201(9)	0.0265(10)	0.0214(9)	0.0031(8)	0.0035(7)	0.0028(8)
C4	0.0209(9)	0.0287(11)	0.0237(9)	0.0033(8)	0.0050(7)	0.0049(8)
C5	0.0211(9)	0.0239(10)	0.0211(9)	0.0034(8)	0.0046(7)	0.0033(8)
C6	0.0213(9)	0.0233(10)	0.0244(9)	0.0016(8)	0.0058(7)	0.0027(8)
C11	0.0212(9)	0.0267(10)	0.0174(9)	-0.0013(7)	0.0038(7)	-0.0002(8)
C12	0.0249(10)	0.0299(11)	0.0239(9)	0.0032(8)	0.0035(8)	0.0027(8)
C13	0.0290(11)	0.0390(13)	0.0333(11)	0.0075(9)	0.0098(9)	-0.0036(9)
N14	0.0285(9)	0.0457(12)	0.0476(11)	0.0000(9)	0.0168(8)	0.0023(9)
C15	0.0279(11)	0.0343(12)	0.0549(14)	-0.0058(10)	0.0134(10)	0.0054(10)
C16	0.0260(10)	0.0245(11)	0.0393(11)	-0.0012(9)	0.0087(9)	0.0007(8)
C21	0.0217(10)	0.0350(11)	0.0203(9)	-0.0042(8)	0.0039(7)	-0.0005(8)
C22	0.0318(11)	0.0339(12)	0.0419(12)	-0.0076(10)	0.0117(9)	-0.0014(9)
C23	0.0421(13)	0.0413(14)	0.0567(15)	-0.0135(11)	0.0173(11)	-0.0147(11)
C24	0.0234(11)	0.0679(17)	0.0477(14)	-0.0121(12)	0.0081(10)	-0.0114(12)
C25	0.0243(11)	0.0672(17)	0.0281(11)	-0.0009(11)	0.0021(8)	0.0112(11)
C26	0.0265(11)	0.0438(13)	0.0226(10)	0.0024(9)	0.0034(8)	0.0052(9)
C31	0.0232(10)	0.0302(11)	0.0233(9)	0.0007(8)	0.0031(8)	0.0038(8)
C32	0.0252(10)	0.0334(11)	0.0217(9)	0.0015(8)	0.0056(8)	0.0057(8)
C33	0.0283(11)	0.0494(13)	0.0257(10)	0.0005(9)	0.0079(8)	0.0048(10)
C34	0.0371(12)	0.0544(14)	0.0215(10)	-0.0049(10)	0.0050(9)	0.0064(10)
C35	0.0333(11)	0.0454(13)	0.0260(10)	-0.0069(9)	-0.0006(9)	0.0053(10)
C36	0.0258(10)	0.0396(12)	0.0286(10)	-0.0039(9)	0.0026(8)	0.0032(9)
C41	0.0243(10)	0.0347(11)	0.0191(9)	0.0007(8)	0.0057(7)	0.0036(8)
C42	0.0300(11)	0.0368(12)	0.0350(11)	-0.0033(9)	0.0072(9)	0.0042(9)
C43	0.0298(12)	0.0573(16)	0.0428(13)	-0.0132(11)	0.0101(10)	0.0108(11)
N44	0.0318(10)	0.0711(15)	0.0403(11)	0.0020(10)	0.0154(8)	0.0033(10)
C45	0.0378(13)	0.0581(16)	0.0408(13)	0.0182(11)	0.0145(10)	-0.0021(12)
C46	0.0310(11)	0.0417(13)	0.0357(11)	0.0131(10)	0.0108(9)	0.0077(10)
C51	0.0215(10)	0.0336(11)	0.0224(9)	-0.0014(8)	0.0057(8)	-0.0013(8)
C52	0.0250(10)	0.0384(12)	0.0269(10)	-0.0003(9)	0.0060(8)	0.0003(9)
C53	0.0228(11)	0.0602(16)	0.0340(12)	0.0003(10)	0.0064(9)	0.0053(10)
C54	0.0228(11)	0.0615(17)	0.0518(14)	-0.0037(12)	0.0089(10)	-0.0115(11)
C55	0.0359(13)	0.0444(14)	0.0605(15)	-0.0070(11)	0.0173(11)	-0.0139(11)
C56	0.0295(11)	0.0362(12)	0.0431(12)	-0.0026(10)	0.0116(9)	-0.0050(9)
C61	0.0229(9)	0.0218(10)	0.0220(9)	-0.0029(7)	0.0062(7)	0.0002(8)
C62	0.0217(9)	0.0198(10)	0.0232(9)	-0.0019(7)	0.0047(7)	0.0002(7)
C63	0.0240(10)	0.0306(11)	0.0234(9)	-0.0017(8)	0.0065(8)	-0.0031(8)
C64	0.0327(11)	0.0356(12)	0.0212(10)	0.0022(8)	0.0034(8)	-0.0017(9)
C65	0.0289(11)	0.0371(12)	0.0242(10)	0.0011(8)	-0.0019(8)	0.0023(9)
C66	0.0209(10)	0.0328(11)	0.0278(10)	-0.0038(8)	0.0034(8)	0.0002(8)

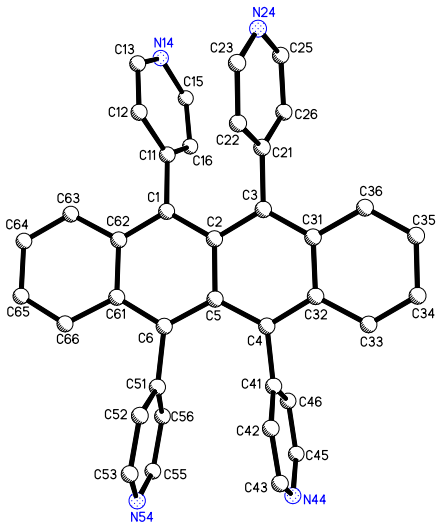
Bond lengths (Å) and angles (deg) for **DARO2**.

O1-O2	1.4694(16)	C11-C12	1.390(3)
O1-C1	1.475(2)	C12-C13	1.380(3)
O2-C6	1.473(2)	C12-H12	0.9500
C1-C62	1.516(2)	C13-N14	1.338(3)
C1-C11	1.521(2)	C13-H13	0.9500
C1-C2	1.541(2)	N14-C15	1.328(3)
C2-C3	1.375(3)	C15-C16	1.383(3)
C2-C5	1.445(2)	C15-H15	0.9500
C3-C31	1.440(2)	C16-H16	0.9500
C3-C21	1.502(2)	C21-C26	1.386(3)
C4-C5	1.381(2)	C21-C22	1.393(3)
C4-C32	1.439(3)	C22-C23	1.381(3)
C4-C41	1.499(2)	C22-H22	0.9500
C5-C6	1.538(2)	C23-C24	1.374(3)
C6-C51	1.521(2)	C23-H23	0.9500
C6-C61	1.529(2)	C24-C25	1.375(3)
C11-C16	1.382(3)	C24-H24	0.9500

C25-C26	1.391(3)	C4-C5-C6	127.54(16)
C25-H25	0.9500	C2-C5-C6	111.65(14)
C26-H26	0.9500	O2-C6-C51	102.71(14)
C31-C32	1.416(3)	O2-C6-C61	104.73(13)
C31-C36	1.416(3)	C51-C6-C61	112.45(14)
C32-C33	1.420(3)	O2-C6-C5	104.67(13)
C33-C34	1.366(3)	C51-C6-C5	120.47(14)
C33-H33	0.9500	C61-C6-C5	109.99(14)
C34-C35	1.395(3)	C16-C11-C12	116.78(16)
C34-H34	0.9500	C16-C11-C1	121.64(16)
C35-C36	1.370(3)	C12-C11-C1	121.51(16)
C35-H35	0.9500	C13-C12-C11	119.56(18)
C36-H36	0.9500	C13-C12-H12	120.2
C41-C46	1.385(3)	C11-C12-H12	120.2
C41-C42	1.388(3)	N14-C13-C12	123.89(19)
C42-C43	1.375(3)	N14-C13-H13	118.1
C42-H42	0.9500	C12-C13-H13	118.1
C43-N44	1.332(3)	C15-N14-C13	115.94(17)
C43-H43	0.9500	N14-C15-C16	124.35(19)
N44-C45	1.327(3)	N14-C15-H15	117.8
C45-C46	1.380(3)	C16-C15-H15	117.8
C45-H45	0.9500	C11-C16-C15	119.46(18)
C46-H46	0.9500	C11-C16-H16	120.3
C51-C56	1.387(3)	C15-C16-H16	120.3
C51-C52	1.396(3)	C26-C21-C22	118.62(18)
C52-C53	1.388(3)	C26-C21-C3	121.45(17)
C52-H52	0.9500	C22-C21-C3	119.78(17)
C53-C54	1.375(3)	C23-C22-C21	120.6(2)
C53-H53	0.9500	C23-C22-H22	119.7
C54-C55	1.376(3)	C21-C22-H22	119.7
C54-H54	0.9500	C24-C23-C22	120.3(2)
C55-C56	1.389(3)	C24-C23-H23	119.9
C55-H55	0.9500	C22-C23-H23	119.9
C56-H56	0.9500	C23-C24-C25	119.9(2)
C61-C66	1.385(2)	C23-C24-H24	120.0
C61-C62	1.396(2)	C25-C24-H24	120.0
C62-C63	1.386(2)	C24-C25-C26	120.3(2)
C63-C64	1.383(3)	C24-C25-H25	119.9
C63-H63	0.9500	C26-C25-H25	119.9
C64-C65	1.380(3)	C21-C26-C25	120.3(2)
C64-H64	0.9500	C21-C26-H26	119.8
C65-C66	1.391(3)	C25-C26-H26	119.8
C65-H65	0.9500	C32-C31-C36	118.54(17)
C66-H66	0.9500	C32-C31-C3	120.01(16)
O2-O1-C1	111.62(11)	C36-C31-C3	121.41(17)
O1-O2-C6	112.43(11)	C31-C32-C33	118.36(17)
O1-C1-C62	105.71(14)	C31-C32-C4	120.08(16)
O1-C1-C11	102.53(13)	C33-C32-C4	121.55(17)
C62-C1-C11	112.74(14)	C34-C33-C32	121.45(19)
O1-C1-C2	104.30(13)	C34-C33-H33	119.3
C62-C1-C2	110.26(14)	C32-C33-H33	119.3
C11-C1-C2	119.64(14)	C33-C34-C35	120.18(18)
C3-C2-C5	120.95(16)	C33-C34-H34	119.9
C3-C2-C1	127.43(15)	C35-C34-H34	119.9
C5-C2-C1	111.46(15)	C36-C35-C34	120.01(19)
C2-C3-C31	119.12(16)	C36-C35-H35	120.0
C2-C3-C21	125.60(16)	C34-C35-H35	120.0
C31-C3-C21	115.29(15)	C35-C36-C31	121.44(18)
C5-C4-C32	119.09(16)	C35-C36-H36	119.3
C5-C4-C41	125.82(17)	C31-C36-H36	119.3
C32-C4-C41	115.10(15)	C46-C41-C42	116.48(17)
C4-C5-C2	120.69(16)	C46-C41-C4	122.40(17)

C42-C41-C4	120.92(17)
C43-C42-C41	119.3(2)
C43-C42-H42	120.4
C41-C42-H42	120.4
N44-C43-C42	124.7(2)
N44-C43-H43	117.7
C42-C43-H43	117.7
C45-N44-C43	115.62(18)
N44-C45-C46	124.2(2)
N44-C45-H45	117.9
C46-C45-H45	117.9
C45-C46-C41	119.7(2)
C45-C46-H46	120.2
C41-C46-H46	120.2
C56-C51-C52	118.76(17)
C56-C51-C6	121.47(17)
C52-C51-C6	119.69(17)
C53-C52-C51	120.4(2)
C53-C52-H52	119.8
C51-C52-H52	119.8
C54-C53-C52	120.2(2)
C54-C53-H53	119.9
C52-C53-H53	119.9
C53-C54-C55	119.96(19)
C53-C54-H54	120.0
C55-C54-H54	120.0
C54-C55-C56	120.4(2)
C54-C55-H55	119.8
C56-C55-H55	119.8
C51-C56-C55	120.3(2)
C51-C56-H56	119.9
C55-C56-H56	119.9
C66-C61-C62	119.91(16)
C66-C61-C6	126.84(16)
C62-C61-C6	112.76(15)
C63-C62-C61	119.85(16)
C63-C62-C1	126.91(16)
C61-C62-C1	112.84(15)
C64-C63-C62	119.96(17)
C64-C63-H63	120.0
C62-C63-H63	120.0
C65-C64-C63	120.22(18)
C65-C64-H64	119.9
C63-C64-H64	119.9
C64-C65-C66	120.28(18)
C64-C65-H65	119.9
C66-C65-H65	119.9
C61-C66-C65	119.65(17)
C61-C66-H66	120.2
C65-C66-H66	120.2

5,6,11,12-tetra(4-pyridyl)tetracene (**TAR**) CCDC 1821075



Identification code	gxi5	
Empirical formula	$C_{42}H_{32}N_4O$	
Formula weight	608.71	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	4	
Unit cell dimensions	a = 7.7635(16) Å	α = 97.536(17) deg.
	b = 18.657(4) Å	β = 90.005(17) deg.
	c = 21.765(5) Å	γ = 100.929(17) deg.
Volume	3067.7(12) Å^3	
Density (calculated)	1.32 g/cm^3	
Absorption coefficient	0.62 mm^{-1}	
Crystal shape	plate	
Crystal size	0.184 x 0.142 x 0.022 mm^3	
Crystal colour	red	
Theta range for data collection	3.4 to 63.2 deg.	
Index ranges	$-8\le h\le 4$, $-20\le k\le 21$, $-24\le l\le 24$	
Reflections collected	31146	
Independent reflections	9492 (R(int) = 0.1020)	
Observed reflections	5709 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.97 and 0.58	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	9492 / 1664 / 892	
Goodness-of-fit on F^2	1.08	
Final R indices (I>2sigma(I))	R1 = 0.111, wR2 = 0.263	
Largest diff. peak and hole	0.44 and -0.37 eÅ^{-3}	

Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **TAR**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
O1	1.1609(7)	0.9677(5)	0.2299(3)	0.113(3)
C2	1.2313(9)	0.9789(5)	0.2898(4)	0.072(2)
H2A	1.2365	0.9311	0.3040	0.087
H2B	1.1573	1.0049	0.3185	0.087
C3	1.4108(10)	1.0241(6)	0.2892(4)	0.075(2)
H3A	1.4971	1.0024	0.3105	0.090
H3B	1.4144	1.0752	0.3090	0.090
C4	1.4453(10)	1.0212(6)	0.2200(4)	0.078(3)
H4A	1.4526	1.0706	0.2070	0.094
H4B	1.5570	1.0045	0.2103	0.094
C5	1.2982(9)	0.9693(5)	0.1881(4)	0.066(2)
H5A	1.2659	0.9861	0.1492	0.079
H5B	1.3279	0.9198	0.1782	0.079
O6	0.0206(14)	0.5012(5)	0.5743(4)	0.064(3)
C7	0.040(3)	0.5656(8)	0.5459(7)	0.053(4)
H7A	0.1419	0.6022	0.5644	0.063
H7B	-0.0666	0.5876	0.5516	0.063
C8	0.066(6)	0.5439(14)	0.4788(8)	0.081(9)
H8A	0.1924	0.5477	0.4696	0.097
H8B	0.0136	0.5741	0.4527	0.097
C9	-0.031(4)	0.4638(11)	0.4696(8)	0.079(7)
H9A	-0.1363	0.4580	0.4426	0.095
H9B	0.0465	0.4311	0.4503	0.095
C10	-0.081(4)	0.4454(11)	0.5326(8)	0.057(5)
H10A	-0.2075	0.4444	0.5388	0.068
H10B	-0.0551	0.3967	0.5383	0.068
O11	0.4717(16)	0.5029(6)	0.0733(4)	0.071(3)
C12	0.532(3)	0.5684(8)	0.0471(6)	0.054(4)
H12A	0.6607	0.5845	0.0539	0.065
H12B	0.4735	0.6083	0.0658	0.065
C13	0.487(7)	0.5497(13)	-0.0207(7)	0.079(9)
H13A	0.5713	0.5800	-0.0457	0.094
H13B	0.3668	0.5560	-0.0300	0.094
C14	0.504(3)	0.4687(10)	-0.0316(7)	0.071(6)
H14A	0.4011	0.4387	-0.0558	0.085
H14B	0.6115	0.4629	-0.0547	0.085
C15	0.513(5)	0.4452(11)	0.0311(8)	0.058(6)
H15A	0.4277	0.3990	0.0335	0.070
H15B	0.6321	0.4370	0.0402	0.070
C11	0.4621(8)	0.6680(3)	0.6185(2)	0.0374(14)
C21	0.3776(8)	0.7240(3)	0.6498(2)	0.0382(14)
C31	0.3826(7)	0.7410(3)	0.7163(2)	0.0374(14)
C41	0.1799(8)	0.8138(3)	0.6459(2)	0.0379(14)
C51	0.2854(8)	0.7666(3)	0.6133(2)	0.0389(14)
C61	0.3087(8)	0.7585(4)	0.5475(2)	0.0406(14)
C111	0.5114(8)	0.6071(3)	0.6499(3)	0.0426(14)
C121	0.6822(8)	0.5994(4)	0.6579(3)	0.0456(15)
H121	0.7763	0.6360	0.6475	0.055
C131	0.7156(9)	0.5374(4)	0.6815(3)	0.0519(17)
H131	0.8344	0.5334	0.6876	0.062
N141	0.5912(8)	0.4837(3)	0.6959(2)	0.0537(14)
C151	0.4262(9)	0.4904(4)	0.6875(3)	0.0533(17)
H151	0.3352	0.4524	0.6977	0.064
C161	0.3797(9)	0.5508(4)	0.6644(3)	0.0475(16)
H161	0.2597	0.5532	0.6586	0.057

C211	0.5046(7)	0.7115(3)	0.7553(2)	0.0389(14)
C221	0.6810(7)	0.7415(4)	0.7580(3)	0.0413(15)
H221	0.7252	0.7804	0.7347	0.050
C231	0.7937(9)	0.7153(4)	0.7944(3)	0.0510(17)
H231	0.9143	0.7379	0.7965	0.061
N241	0.7407(7)	0.6588(3)	0.8274(2)	0.0499(14)
C251	0.5700(8)	0.6312(4)	0.8249(3)	0.0480(16)
H251	0.5292	0.5923	0.8485	0.058
C261	0.4467(8)	0.6548(4)	0.7906(3)	0.0434(15)
H261	0.3259	0.6329	0.7910	0.052
C311	0.2871(8)	0.7908(3)	0.7463(2)	0.0390(14)
C321	0.1800(7)	0.8259(4)	0.7114(2)	0.0388(14)
C331	0.0771(8)	0.8743(4)	0.7437(3)	0.0412(15)
H331	0.0037	0.8970	0.7205	0.049
C341	0.0822(8)	0.8887(4)	0.8067(3)	0.0431(15)
H341	0.0121	0.9208	0.8270	0.052
C351	0.1920(8)	0.8559(4)	0.8423(3)	0.0441(15)
H351	0.1959	0.8663	0.8862	0.053
C361	0.2921(8)	0.8094(4)	0.8131(3)	0.0425(15)
H361	0.3669	0.7887	0.8373	0.051
C411	0.0562(7)	0.8491(3)	0.6127(3)	0.0400(14)
C421	0.1028(8)	0.9200(4)	0.5973(3)	0.0449(15)
H421	0.2182	0.9475	0.6061	0.054
C431	-0.0209(8)	0.9501(4)	0.5689(3)	0.0508(17)
H431	0.0147	0.9979	0.5573	0.061
N441	-0.1877(8)	0.9160(3)	0.5569(3)	0.0552(15)
C451	-0.2322(9)	0.8485(4)	0.5737(3)	0.0590(19)
H451	-0.3495	0.8228	0.5657	0.071
C461	-0.1162(8)	0.8140(4)	0.6021(3)	0.0495(17)
H461	-0.1555	0.7666	0.6142	0.059
C511	0.2389(8)	0.8043(4)	0.5055(3)	0.0457(15)
C521	0.3406(9)	0.8697(4)	0.4915(3)	0.0535(17)
H521	0.4527	0.8882	0.5109	0.064
C531	0.2754(10)	0.9076(4)	0.4486(3)	0.0600(19)
H531	0.3460	0.9519	0.4389	0.072
N541	0.1180(9)	0.8846(4)	0.4204(2)	0.0605(16)
C551	0.0217(11)	0.8214(4)	0.4331(3)	0.0610(19)
H551	-0.0898	0.8043	0.4129	0.073
C561	0.0774(9)	0.7792(4)	0.4747(3)	0.0520(17)
H561	0.0061	0.7340	0.4819	0.062
C611	0.4117(8)	0.7102(4)	0.5188(2)	0.0412(15)
C621	0.4820(8)	0.6620(3)	0.5542(2)	0.0399(14)
C631	0.5725(9)	0.6087(4)	0.5209(3)	0.0489(17)
H631	0.6102	0.5731	0.5425	0.059
C641	0.6054(9)	0.6082(4)	0.4592(3)	0.0519(18)
H641	0.6681	0.5734	0.4386	0.062
C651	0.5462(9)	0.6592(4)	0.4260(3)	0.0511(17)
H651	0.5740	0.6599	0.3835	0.061
C661	0.4508(9)	0.7069(4)	0.4535(3)	0.0491(17)
H661	0.4080	0.7392	0.4296	0.059
C12	0.4264(7)	0.7630(3)	0.0458(2)	0.0379(14)
C22	0.4554(7)	0.7716(3)	0.1120(2)	0.0367(14)
C32	0.6016(7)	0.8196(3)	0.1438(2)	0.0384(14)
C42	0.3325(7)	0.7473(3)	0.2142(2)	0.0372(14)
C52	0.3253(7)	0.7290(3)	0.1481(2)	0.0369(14)
C62	0.1950(7)	0.6708(3)	0.1171(2)	0.0404(14)
C112	0.5320(7)	0.8115(3)	0.0042(2)	0.0382(14)
C122	0.4850(8)	0.8767(4)	-0.0069(3)	0.0424(15)
H122	0.3914	0.8941	0.0146	0.051
C132	0.5776(8)	0.9159(4)	-0.0501(3)	0.0492(17)
H132	0.5431	0.9603	-0.0577	0.059
N142	0.7106(7)	0.8962(3)	-0.0817(3)	0.0548(15)

C152	0.7534(9)	0.8328(4)	-0.0718(3)	0.0530(17)
H152	0.8476	0.8171	-0.0943	0.064
C162	0.6676(8)	0.7882(4)	-0.0303(3)	0.0491(16)
H162	0.7007	0.7427	-0.0256	0.059
C212	0.7585(7)	0.8539(3)	0.1110(3)	0.0405(14)
C222	0.7875(8)	0.9258(3)	0.0975(3)	0.0412(14)
H222	0.7050	0.9564	0.1094	0.049
C232	0.9358(8)	0.9526(4)	0.0671(3)	0.0465(16)
H232	0.9509	1.0018	0.0580	0.056
N242	1.0599(7)	0.9145(3)	0.0494(3)	0.0521(14)
C252	1.0345(9)	0.8464(4)	0.0653(4)	0.0582(19)
H252	1.1222	0.8179	0.0548	0.070
C262	0.8905(8)	0.8149(4)	0.0954(3)	0.0472(16)
H262	0.8814	0.7664	0.1057	0.057
C312	0.6118(7)	0.8327(4)	0.2092(2)	0.0385(14)
C322	0.4706(7)	0.7991(4)	0.2442(2)	0.0398(15)
C332	0.4793(8)	0.8192(4)	0.3110(3)	0.0462(17)
H332	0.3836	0.8001	0.3350	0.055
C342	0.6212(8)	0.8646(4)	0.3395(3)	0.0457(16)
H342	0.6241	0.8763	0.3833	0.055
C352	0.7653(8)	0.8952(4)	0.3053(3)	0.0456(16)
H352	0.8657	0.9257	0.3262	0.055
C362	0.7599(8)	0.8808(4)	0.2422(3)	0.0421(15)
H362	0.8555	0.9029	0.2195	0.051
C412	0.1821(7)	0.7192(4)	0.2532(2)	0.0383(14)
C422	0.0338(7)	0.7492(4)	0.2561(3)	0.0422(15)
H422	0.0263	0.7892	0.2339	0.051
C432	-0.1042(8)	0.7213(4)	0.2910(3)	0.0473(16)
H432	-0.2065	0.7423	0.2914	0.057
N442	-0.1028(7)	0.6657(3)	0.3249(2)	0.0517(14)
C452	0.0435(8)	0.6401(4)	0.3231(3)	0.0468(16)
H452	0.0485	0.6015	0.3471	0.056
C462	0.1906(8)	0.6629(4)	0.2902(3)	0.0428(15)
H462	0.2925	0.6419	0.2923	0.051
C512	0.0897(8)	0.6107(3)	0.1483(2)	0.0395(14)
C522	-0.0880(8)	0.6037(4)	0.1575(3)	0.0432(15)
H522	-0.1487	0.6402	0.1469	0.052
C532	-0.1766(9)	0.5433(4)	0.1822(3)	0.0495(16)
H532	-0.2985	0.5401	0.1891	0.059
N542	-0.1018(8)	0.4889(3)	0.1969(2)	0.0516(14)
C552	0.0696(9)	0.4956(4)	0.1882(3)	0.0482(16)
H552	0.1258	0.4576	0.1985	0.058
C562	0.1716(9)	0.5554(3)	0.1647(3)	0.0460(15)
H562	0.2942	0.5584	0.1600	0.055
C612	0.1732(8)	0.6631(4)	0.0520(2)	0.0406(15)
C622	0.2835(7)	0.7122(3)	0.0172(2)	0.0365(14)
C632	0.2439(8)	0.7071(4)	-0.0483(3)	0.0441(16)
H632	0.3144	0.7398	-0.0723	0.053
C642	0.1093(8)	0.6570(4)	-0.0760(3)	0.0470(17)
H642	0.0833	0.6559	-0.1188	0.056
C652	0.0062(9)	0.6059(4)	-0.0417(3)	0.0511(18)
H652	-0.0869	0.5701	-0.0619	0.061
C662	0.0392(8)	0.6075(4)	0.0195(3)	0.0488(17)
H662	-0.0276	0.5713	0.0413	0.059

Hydrogen coordinates and isotropic displacement parameters (Å^2) for **TAR**.

Atom	x	y	z	U_{eq}
H2A	1.2365	0.9311	0.3040	0.087
H2B	1.1573	1.0049	0.3185	0.087
H3A	1.4971	1.0024	0.3105	0.090
H3B	1.4144	1.0752	0.3090	0.090
H4A	1.4526	1.0706	0.2070	0.094
H4B	1.5570	1.0045	0.2103	0.094
H5A	1.2659	0.9861	0.1492	0.079
H5B	1.3279	0.9198	0.1782	0.079
H7A	0.1419	0.6022	0.5644	0.063
H7B	-0.0666	0.5876	0.5516	0.063
H8A	0.1924	0.5477	0.4696	0.097
H8B	0.0136	0.5741	0.4527	0.097
H9A	-0.1363	0.4580	0.4426	0.095
H9B	0.0465	0.4311	0.4503	0.095
H10A	-0.2075	0.4444	0.5388	0.068
H10B	-0.0551	0.3967	0.5383	0.068
H12A	0.6607	0.5845	0.0539	0.065
H12B	0.4735	0.6083	0.0658	0.065
H13A	0.5713	0.5800	-0.0457	0.094
H13B	0.3668	0.5560	-0.0300	0.094
H14A	0.4011	0.4387	-0.0558	0.085
H14B	0.6115	0.4629	-0.0547	0.085
H15A	0.4277	0.3990	0.0335	0.070
H15B	0.6321	0.4370	0.0402	0.070
H121	0.7763	0.6360	0.6475	0.055
H131	0.8344	0.5334	0.6876	0.062
H151	0.3352	0.4524	0.6977	0.064
H161	0.2597	0.5532	0.6586	0.057
H221	0.7252	0.7804	0.7347	0.050
H231	0.9143	0.7379	0.7965	0.061
H251	0.5292	0.5923	0.8485	0.058
H261	0.3259	0.6329	0.7910	0.052
H331	0.0037	0.8970	0.7205	0.049
H341	0.0121	0.9208	0.8270	0.052
H351	0.1959	0.8663	0.8862	0.053
H361	0.3669	0.7887	0.8373	0.051
H421	0.2182	0.9475	0.6061	0.054
H431	0.0147	0.9979	0.5573	0.061
H451	-0.3495	0.8228	0.5657	0.071
H461	-0.1555	0.7666	0.6142	0.059
H521	0.4527	0.8882	0.5109	0.064
H531	0.3460	0.9519	0.4389	0.072
H551	-0.0898	0.8043	0.4129	0.073
H561	0.0061	0.7340	0.4819	0.062
H631	0.6102	0.5731	0.5425	0.059
H641	0.6681	0.5734	0.4386	0.062
H651	0.5740	0.6599	0.3835	0.061
H661	0.4080	0.7392	0.4296	0.059
H122	0.3914	0.8941	0.0146	0.051
H132	0.5431	0.9603	-0.0577	0.059
H152	0.8476	0.8171	-0.0943	0.064
H162	0.7007	0.7427	-0.0256	0.059
H222	0.7050	0.9564	0.1094	0.049
H232	0.9509	1.0018	0.0580	0.056
H252	1.1222	0.8179	0.0548	0.070
H262	0.8814	0.7664	0.1057	0.057
H332	0.3836	0.8001	0.3350	0.055

H342	0.6241	0.8763	0.3833	0.055
H352	0.8657	0.9257	0.3262	0.055
H362	0.8555	0.9029	0.2195	0.051
H422	0.0263	0.7892	0.2339	0.051
H432	-0.2065	0.7423	0.2914	0.057
H452	0.0485	0.6015	0.3471	0.056
H462	0.2925	0.6419	0.2923	0.051
H522	-0.1487	0.6402	0.1469	0.052
H532	-0.2985	0.5401	0.1891	0.059
H552	0.1258	0.4576	0.1985	0.058
H562	0.2942	0.5584	0.1600	0.055
H632	0.3144	0.7398	-0.0723	0.053
H642	0.0833	0.6559	-0.1188	0.056
H652	-0.0869	0.5701	-0.0619	0.061
H662	-0.0276	0.5713	0.0413	0.059

Anisotropic displacement parameters ($Å^2$) for **TAR**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.057(4)	0.196(8)	0.072(4)	0.036(5)	0.002(3)	-0.023(4)
C2	0.057(5)	0.103(7)	0.059(4)	0.024(5)	0.018(4)	0.010(4)
C3	0.057(5)	0.103(7)	0.060(4)	0.014(5)	0.007(4)	0.006(4)
C4	0.060(5)	0.104(7)	0.062(5)	0.018(5)	0.016(4)	-0.009(4)
C5	0.057(5)	0.078(6)	0.064(5)	0.024(4)	0.008(3)	0.005(4)
O6	0.083(7)	0.065(6)	0.036(5)	0.016(4)	-0.003(5)	-0.008(5)
C7	0.048(10)	0.070(9)	0.038(9)	0.016(7)	-0.002(8)	0.000(8)
C8	0.086(18)	0.111(15)	0.038(9)	0.021(9)	0.015(10)	-0.007(12)
C9	0.078(14)	0.109(15)	0.040(8)	0.001(10)	0.005(9)	-0.001(13)
C10	0.057(13)	0.065(9)	0.047(9)	0.005(7)	0.005(8)	0.010(8)
O11	0.116(9)	0.075(7)	0.034(5)	0.018(5)	0.015(5)	0.037(6)
C12	0.063(10)	0.076(8)	0.026(8)	0.011(7)	0.003(7)	0.020(9)
C13	0.12(3)	0.102(13)	0.026(9)	0.010(8)	0.002(11)	0.050(16)
C14	0.091(15)	0.101(12)	0.025(7)	-0.010(9)	0.000(8)	0.039(13)
C15	0.064(17)	0.076(9)	0.035(8)	0.005(7)	0.005(9)	0.018(10)
C11	0.042(3)	0.047(4)	0.025(3)	0.012(3)	0.005(2)	0.007(3)
C21	0.043(4)	0.050(4)	0.023(3)	0.008(3)	0.000(2)	0.007(3)
C31	0.042(3)	0.050(4)	0.021(3)	0.009(3)	0.005(2)	0.006(3)
C41	0.045(3)	0.044(4)	0.027(3)	0.011(3)	0.003(2)	0.010(3)
C51	0.048(4)	0.045(4)	0.027(3)	0.014(3)	0.005(2)	0.009(3)
C61	0.048(4)	0.055(4)	0.022(3)	0.011(3)	-0.001(2)	0.010(3)
C111	0.056(4)	0.053(4)	0.019(3)	0.000(3)	0.001(3)	0.012(3)
C121	0.059(4)	0.055(4)	0.025(3)	0.008(3)	0.006(3)	0.012(3)
C131	0.069(4)	0.067(5)	0.025(3)	0.012(3)	-0.001(3)	0.019(3)
N141	0.080(4)	0.054(4)	0.026(3)	0.005(3)	-0.003(3)	0.013(3)
C151	0.073(4)	0.057(4)	0.028(3)	0.006(3)	0.000(3)	0.006(3)
C161	0.061(4)	0.054(4)	0.026(3)	0.004(3)	0.000(3)	0.009(3)
C211	0.046(3)	0.053(4)	0.016(3)	0.002(3)	0.000(2)	0.007(3)
C221	0.048(3)	0.049(4)	0.029(3)	0.010(3)	0.003(3)	0.009(3)
C231	0.049(4)	0.057(4)	0.047(4)	0.008(3)	-0.003(3)	0.007(3)
N241	0.063(3)	0.055(4)	0.033(3)	0.008(3)	-0.007(2)	0.012(3)
C251	0.064(4)	0.057(5)	0.024(3)	0.013(3)	-0.002(3)	0.007(3)
C261	0.048(4)	0.056(4)	0.021(3)	0.003(3)	0.003(2)	0.000(3)
C311	0.042(3)	0.051(4)	0.025(3)	0.008(3)	0.003(2)	0.008(3)
C321	0.039(3)	0.054(4)	0.025(3)	0.010(3)	0.005(2)	0.008(3)
C331	0.043(4)	0.052(4)	0.030(3)	0.010(3)	0.002(3)	0.011(3)
C341	0.047(4)	0.052(4)	0.030(3)	0.005(3)	0.008(3)	0.008(3)
C351	0.050(4)	0.057(4)	0.024(3)	0.006(3)	0.003(3)	0.006(3)
C361	0.049(4)	0.052(4)	0.026(3)	0.008(3)	0.000(3)	0.007(3)

C411	0.043(3)	0.055(4)	0.024(3)	0.010(3)	0.005(2)	0.013(3)
C421	0.052(4)	0.054(4)	0.030(3)	0.011(3)	0.003(3)	0.010(3)
C431	0.059(4)	0.062(5)	0.036(4)	0.014(3)	0.006(3)	0.017(3)
N441	0.062(3)	0.065(4)	0.043(3)	0.014(3)	-0.003(3)	0.018(3)
C451	0.051(4)	0.073(5)	0.052(4)	0.012(4)	-0.005(3)	0.007(3)
C461	0.043(3)	0.061(5)	0.046(4)	0.015(3)	0.000(3)	0.006(3)
C511	0.058(4)	0.059(4)	0.022(3)	0.007(3)	0.004(3)	0.018(3)
C521	0.062(4)	0.060(4)	0.043(4)	0.017(3)	0.012(3)	0.014(3)
C531	0.074(5)	0.076(5)	0.039(4)	0.018(4)	0.018(3)	0.029(4)
N541	0.089(4)	0.077(4)	0.023(3)	0.007(3)	0.004(3)	0.036(3)
C551	0.087(5)	0.070(5)	0.032(4)	0.003(3)	-0.009(3)	0.032(4)
C561	0.069(4)	0.058(5)	0.028(3)	0.003(3)	-0.008(3)	0.014(3)
C611	0.047(4)	0.056(4)	0.023(3)	0.010(3)	0.003(2)	0.011(3)
C621	0.048(4)	0.047(4)	0.026(3)	0.009(3)	0.005(2)	0.010(3)
C631	0.065(4)	0.058(5)	0.025(3)	0.000(3)	0.002(3)	0.019(3)
C641	0.069(5)	0.066(5)	0.024(3)	0.003(3)	0.004(3)	0.024(4)
C651	0.063(4)	0.067(5)	0.025(3)	0.009(3)	0.005(3)	0.015(3)
C661	0.062(4)	0.064(5)	0.024(3)	0.011(3)	0.004(3)	0.017(3)
C12	0.042(3)	0.049(4)	0.023(3)	0.009(3)	0.003(2)	0.005(3)
C22	0.036(3)	0.048(4)	0.027(3)	0.009(3)	0.005(2)	0.007(3)
C32	0.039(3)	0.048(4)	0.028(3)	0.007(3)	0.004(2)	0.007(3)
C42	0.036(3)	0.051(4)	0.028(3)	0.012(3)	0.001(2)	0.010(3)
C52	0.039(3)	0.050(4)	0.023(3)	0.011(3)	0.005(2)	0.008(3)
C62	0.041(3)	0.052(4)	0.027(3)	0.008(3)	0.002(2)	0.006(3)
C112	0.042(3)	0.048(4)	0.023(3)	0.008(3)	0.001(2)	0.002(3)
C122	0.040(4)	0.055(4)	0.032(3)	0.011(3)	0.004(3)	0.006(3)
C132	0.052(4)	0.065(5)	0.030(3)	0.019(3)	-0.002(3)	0.003(3)
N142	0.058(4)	0.067(4)	0.036(3)	0.013(3)	0.009(2)	-0.003(3)
C152	0.052(4)	0.066(5)	0.034(4)	0.002(3)	0.014(3)	-0.002(3)
C162	0.051(4)	0.056(4)	0.038(4)	0.009(3)	0.009(3)	0.003(3)
C212	0.044(3)	0.052(4)	0.024(3)	0.008(3)	0.005(2)	0.004(3)
C222	0.048(4)	0.050(4)	0.024(3)	0.004(3)	0.007(2)	0.008(3)
C232	0.045(4)	0.056(4)	0.034(3)	0.003(3)	0.007(3)	0.001(3)
N242	0.048(3)	0.065(4)	0.044(3)	0.016(3)	0.009(2)	0.008(3)
C252	0.046(4)	0.065(5)	0.067(5)	0.015(4)	0.018(3)	0.013(3)
C262	0.042(4)	0.061(4)	0.045(4)	0.025(3)	0.009(3)	0.013(3)
C312	0.040(3)	0.048(4)	0.027(3)	0.007(3)	0.003(2)	0.007(3)
C322	0.039(3)	0.056(4)	0.025(3)	0.006(3)	0.003(2)	0.010(3)
C332	0.049(4)	0.066(5)	0.023(3)	0.006(3)	0.005(2)	0.008(3)
C342	0.049(4)	0.063(5)	0.023(3)	0.004(3)	0.000(2)	0.006(3)
C352	0.045(4)	0.057(4)	0.033(3)	0.005(3)	-0.004(3)	0.006(3)
C362	0.047(4)	0.049(4)	0.028(3)	0.005(3)	0.001(2)	0.004(3)
C412	0.038(3)	0.058(4)	0.018(3)	0.006(3)	0.004(2)	0.005(3)
C422	0.042(3)	0.048(4)	0.034(3)	0.005(3)	0.005(3)	0.003(3)
C432	0.046(4)	0.059(4)	0.035(4)	0.002(3)	0.009(3)	0.009(3)
N442	0.057(3)	0.060(4)	0.038(3)	0.008(3)	0.015(3)	0.009(3)
C452	0.058(4)	0.057(4)	0.025(3)	0.005(3)	0.003(3)	0.009(3)
C462	0.045(4)	0.054(4)	0.030(3)	0.008(3)	0.003(3)	0.009(3)
C512	0.053(3)	0.049(4)	0.015(3)	0.011(3)	0.005(2)	0.001(3)
C522	0.049(3)	0.054(4)	0.023(3)	0.009(3)	-0.001(3)	-0.004(3)
C532	0.058(4)	0.060(4)	0.026(3)	0.010(3)	0.002(3)	-0.002(3)
N542	0.071(4)	0.053(4)	0.028(3)	0.007(3)	0.009(3)	0.002(3)
C552	0.073(4)	0.044(4)	0.026(3)	0.006(3)	0.005(3)	0.006(3)
C562	0.063(4)	0.047(4)	0.026(3)	0.009(3)	0.003(3)	0.004(3)
C612	0.042(3)	0.055(4)	0.024(3)	0.011(3)	0.003(2)	0.002(3)
C622	0.044(3)	0.045(4)	0.021(3)	0.008(3)	0.007(2)	0.007(3)
C632	0.053(4)	0.050(4)	0.028(3)	0.009(3)	0.001(3)	0.005(3)
C642	0.051(4)	0.069(5)	0.020(3)	0.010(3)	0.001(2)	0.007(3)
C652	0.053(4)	0.067(5)	0.026(3)	0.002(3)	0.001(3)	-0.005(3)
C662	0.054(4)	0.061(5)	0.028(3)	0.007(3)	0.003(3)	0.000(3)

Bond lengths (Å) and angles (deg) for **TAR**.

O1-C2	1.389(9)	C151-C161	1.399(8)
O1-C5	1.400(8)	C151-H151	0.9500
C2-C3	1.486(9)	C161-H161	0.9500
C2-H2A	0.9900	C211-C221	1.376(7)
C2-H2B	0.9900	C211-C261	1.394(8)
C3-C4	1.525(10)	C221-C231	1.378(8)
C3-H3A	0.9900	C221-H221	0.9500
C3-H3B	0.9900	C231-N241	1.352(8)
C4-C5	1.459(10)	C231-H231	0.9500
C4-H4A	0.9900	N241-C251	1.326(7)
C4-H4B	0.9900	C251-C261	1.383(8)
C5-H5A	0.9900	C251-H251	0.9500
C5-H5B	0.9900	C261-H261	0.9500
O6-C10	1.403(15)	C311-C321	1.426(7)
O6-C7	1.405(14)	C311-C361	1.449(7)
C7-C8	1.489(15)	C321-C331	1.434(7)
C7-H7A	0.9900	C331-C341	1.363(7)
C7-H7B	0.9900	C331-H331	0.9500
C8-C9	1.528(19)	C341-C351	1.422(8)
C8-H8A	0.9900	C341-H341	0.9500
C8-H8B	0.9900	C351-C361	1.368(8)
C9-C10	1.490(14)	C351-H351	0.9500
C9-H9A	0.9900	C361-H361	0.9500
C9-H9B	0.9900	C411-C461	1.379(8)
C10-H10A	0.9900	C411-C421	1.389(8)
C10-H10B	0.9900	C421-C431	1.383(8)
O11-C15	1.405(15)	C421-H421	0.9500
O11-C12	1.417(13)	C431-N441	1.339(8)
C12-C13	1.495(15)	C431-H431	0.9500
C12-H12A	0.9900	N441-C451	1.340(8)
C12-H12B	0.9900	C451-C461	1.390(8)
C13-C14	1.529(19)	C451-H451	0.9500
C13-H13A	0.9900	C461-H461	0.9500
C13-H13B	0.9900	C511-C561	1.391(8)
C14-C15	1.493(14)	C511-C521	1.392(8)
C14-H14A	0.9900	C521-C531	1.391(8)
C14-H14B	0.9900	C521-H521	0.9500
C15-H15A	0.9900	C531-N541	1.337(8)
C15-H15B	0.9900	C531-H531	0.9500
C11-C621	1.400(7)	N541-C551	1.333(9)
C11-C21	1.434(7)	C551-C561	1.393(8)
C11-C111	1.508(7)	C551-H551	0.9500
C21-C31	1.440(7)	C561-H561	0.9500
C21-C51	1.470(8)	C611-C621	1.438(8)
C31-C311	1.393(7)	C611-C661	1.449(7)
C31-C211	1.496(7)	C621-C631	1.444(8)
C41-C321	1.415(7)	C631-C641	1.367(8)
C41-C51	1.435(7)	C631-H631	0.9500
C41-C411	1.497(7)	C641-C651	1.409(8)
C51-C61	1.435(7)	C641-H641	0.9500
C61-C611	1.402(7)	C651-C661	1.345(8)
C61-C511	1.498(7)	C651-H651	0.9500
C111-C121	1.374(8)	C661-H661	0.9500
C111-C161	1.389(8)	C12-C622	1.401(7)
C121-C131	1.393(8)	C12-C22	1.440(7)
C121-H121	0.9500	C12-C112	1.498(7)
C131-N141	1.323(8)	C22-C32	1.421(7)
C131-H131	0.9500	C22-C52	1.460(7)
N141-C151	1.325(8)	C32-C312	1.413(7)

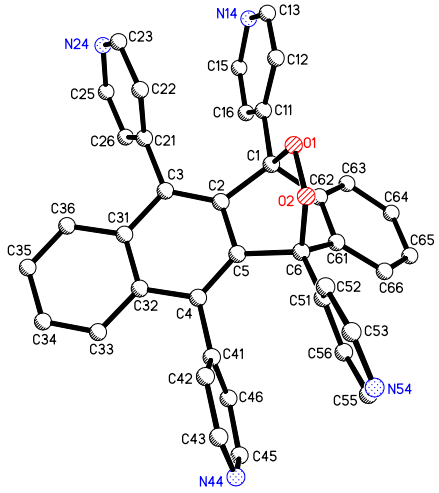
C32-C212	1.493(7)	C642-C652	1.416(8)
C42-C322	1.397(7)	C642-H642	0.9500
C42-C52	1.433(7)	C652-C662	1.351(8)
C42-C412	1.498(7)	C652-H652	0.9500
C52-C62	1.431(7)	C662-H662	0.9500
C62-C612	1.414(7)	C2-O1-C5	108.7(6)
C62-C512	1.497(7)	O1-C2-C3	107.9(6)
C112-C122	1.385(8)	O1-C2-H2A	110.1
C112-C162	1.397(8)	C3-C2-H2A	110.1
C122-C132	1.386(8)	O1-C2-H2B	110.1
C122-H122	0.9500	C3-C2-H2B	110.1
C132-N142	1.324(8)	H2A-C2-H2B	108.4
C132-H132	0.9500	C2-C3-C4	102.4(6)
N142-C152	1.332(8)	C2-C3-H3A	111.3
C152-C162	1.392(8)	C4-C3-H3A	111.3
C152-H152	0.9500	C2-C3-H3B	111.3
C162-H162	0.9500	C4-C3-H3B	111.3
C212-C262	1.383(8)	H3A-C3-H3B	109.2
C212-C222	1.388(8)	C5-C4-C3	106.5(6)
C222-C232	1.372(7)	C5-C4-H4A	110.4
C222-H222	0.9500	C3-C4-H4A	110.4
C232-N242	1.331(8)	C5-C4-H4B	110.4
C232-H232	0.9500	C3-C4-H4B	110.4
N242-C252	1.339(8)	H4A-C4-H4B	108.6
C252-C262	1.371(8)	O1-C5-C4	104.9(7)
C252-H252	0.9500	O1-C5-H5A	110.8
C262-H262	0.9500	C4-C5-H5A	110.8
C312-C322	1.428(7)	O1-C5-H5B	110.8
C312-C362	1.443(7)	C4-C5-H5B	110.8
C322-C332	1.450(7)	H5A-C5-H5B	108.9
C332-C342	1.351(8)	C10-O6-C7	105.9(13)
C332-H332	0.9500	O6-C7-C8	106.9(15)
C342-C352	1.415(8)	O6-C7-H7A	110.3
C342-H342	0.9500	C8-C7-H7A	110.3
C352-C362	1.363(7)	O6-C7-H7B	110.3
C352-H352	0.9500	C8-C7-H7B	110.3
C362-H362	0.9500	H7A-C7-H7B	108.6
C412-C422	1.371(8)	C7-C8-C9	101.3(13)
C412-C462	1.416(8)	C7-C8-H8A	111.5
C422-C432	1.375(7)	C9-C8-H8A	111.5
C422-H422	0.9500	C7-C8-H8B	111.5
C432-N442	1.351(8)	C9-C8-H8B	111.5
C432-H432	0.9500	H8A-C8-H8B	109.3
N442-C452	1.311(7)	C10-C9-C8	106.1(12)
C452-C462	1.375(8)	C10-C9-H9A	110.5
C452-H452	0.9500	C8-C9-H9A	110.5
C462-H462	0.9500	C10-C9-H9B	110.5
C512-C522	1.377(7)	C8-C9-H9B	110.5
C512-C562	1.393(8)	H9A-C9-H9B	108.7
C522-C532	1.379(8)	O6-C10-C9	105.6(13)
C522-H522	0.9500	O6-C10-H10A	110.6
C532-N542	1.334(8)	C9-C10-H10A	110.6
C532-H532	0.9500	O6-C10-H10B	110.6
N542-C552	1.328(8)	C9-C10-H10B	110.6
C552-C562	1.396(8)	H10A-C10-H10B	108.8
C552-H552	0.9500	C15-O11-C12	106.0(13)
C562-H562	0.9500	O11-C12-C13	105.8(15)
C612-C622	1.425(7)	O11-C12-H12A	110.6
C612-C662	1.434(8)	C13-C12-H12A	110.6
C622-C632	1.446(7)	O11-C12-H12B	110.6
C632-C642	1.345(8)	C13-C12-H12B	110.6
C632-H632	0.9500	H12A-C12-H12B	108.7

C12-C13-C14	101.1(13)	N241-C251-C261	125.0(6)
C12-C13-H13A	111.6	N241-C251-H251	117.5
C14-C13-H13A	111.6	C261-C251-H251	117.5
C12-C13-H13B	111.6	C251-C261-C211	118.2(6)
C14-C13-H13B	111.6	C251-C261-H261	120.9
H13A-C13-H13B	109.4	C211-C261-H261	120.9
C15-C14-C13	106.1(11)	C31-C311-C321	120.4(5)
C15-C14-H14A	110.5	C31-C311-C361	122.3(5)
C13-C14-H14A	110.5	C321-C311-C361	117.4(5)
C15-C14-H14B	110.5	C41-C321-C311	119.8(5)
C13-C14-H14B	110.5	C41-C321-C331	121.1(5)
H14A-C14-H14B	108.7	C311-C321-C331	119.1(5)
O11-C15-C14	106.1(12)	C341-C331-C321	121.5(6)
O11-C15-H15A	110.5	C341-C331-H331	119.3
C14-C15-H15A	110.5	C321-C331-H331	119.3
O11-C15-H15B	110.5	C331-C341-C351	120.2(6)
C14-C15-H15B	110.5	C331-C341-H341	119.9
H15A-C15-H15B	108.7	C351-C341-H341	119.9
C621-C11-C21	120.3(5)	C361-C351-C341	119.9(5)
C621-C11-C111	116.1(5)	C361-C351-H351	120.0
C21-C11-C111	123.1(5)	C341-C351-H351	120.0
C11-C21-C31	122.1(5)	C351-C361-C311	121.8(6)
C11-C21-C51	119.5(5)	C351-C361-H361	119.1
C31-C21-C51	118.4(5)	C311-C361-H361	119.1
C311-C31-C21	121.4(5)	C461-C411-C421	117.4(5)
C311-C31-C211	117.4(5)	C461-C411-C41	119.8(6)
C21-C31-C211	120.9(5)	C421-C411-C41	122.4(5)
C321-C41-C51	121.4(5)	C431-C421-C411	119.1(6)
C321-C41-C411	116.5(5)	C431-C421-H421	120.4
C51-C41-C411	122.0(5)	C411-C421-H421	120.4
C61-C51-C41	124.7(5)	N441-C431-C421	124.1(7)
C61-C51-C21	117.4(5)	N441-C431-H431	117.9
C41-C51-C21	117.8(5)	C421-C431-H431	117.9
C611-C61-C51	121.4(5)	C431-N441-C451	116.1(6)
C611-C61-C511	115.1(5)	N441-C451-C461	123.6(6)
C51-C61-C511	123.3(5)	N441-C451-H451	118.2
C121-C111-C161	117.6(6)	C461-C451-H451	118.2
C121-C111-C11	122.8(6)	C411-C461-C451	119.5(6)
C161-C111-C11	119.0(5)	C411-C461-H461	120.3
C111-C121-C131	119.2(6)	C451-C461-H461	120.3
C111-C121-H121	120.4	C561-C511-C521	118.0(6)
C131-C121-H121	120.4	C561-C511-C61	120.8(6)
N141-C131-C121	123.7(6)	C521-C511-C61	121.0(6)
N141-C131-H131	118.1	C531-C521-C511	118.9(7)
C121-C131-H131	118.1	C531-C521-H521	120.6
C131-N141-C151	117.3(6)	C511-C521-H521	120.6
N141-C151-C161	123.1(7)	N541-C531-C521	123.1(7)
N141-C151-H151	118.4	N541-C531-H531	118.4
C161-C151-H151	118.4	C521-C531-H531	118.4
C111-C161-C151	119.0(6)	C551-N541-C531	118.0(6)
C111-C161-H161	120.5	N541-C551-C561	122.9(7)
C151-C161-H161	120.5	N541-C551-H551	118.6
C221-C211-C261	117.6(5)	C561-C551-H551	118.6
C221-C211-C31	119.8(5)	C511-C561-C551	119.1(7)
C261-C211-C31	122.6(5)	C511-C561-H561	120.4
C211-C221-C231	120.1(6)	C551-C561-H561	120.4
C211-C221-H221	120.0	C61-C611-C621	120.1(5)
C231-C221-H221	120.0	C61-C611-C661	121.9(5)
N241-C231-C221	123.1(6)	C621-C611-C661	117.9(5)
N241-C231-H231	118.5	C11-C621-C611	120.1(5)
C221-C231-H231	118.5	C11-C621-C631	122.5(5)
C251-N241-C231	116.0(5)	C611-C621-C631	117.5(5)

C641-C631-C621	121.7(6)
C641-C631-H631	119.2
C621-C631-H631	119.2
C631-C641-C651	120.0(6)
C631-C641-H641	120.0
C651-C641-H641	120.0
C661-C651-C641	121.0(6)
C661-C651-H651	119.5
C641-C651-H651	119.5
C651-C661-C611	121.6(6)
C651-C661-H661	119.2
C611-C661-H661	119.2
C622-C12-C22	120.8(5)
C622-C12-C112	115.5(5)
C22-C12-C112	123.4(5)
C32-C22-C12	123.8(5)
C32-C22-C52	118.5(5)
C12-C22-C52	117.6(5)
C312-C32-C22	121.2(5)
C312-C32-C212	116.0(5)
C22-C32-C212	122.6(5)
C322-C42-C52	121.3(5)
C322-C42-C412	116.8(5)
C52-C42-C412	121.5(5)
C62-C52-C42	121.9(5)
C62-C52-C22	119.8(5)
C42-C52-C22	118.3(5)
C612-C62-C52	119.8(5)
C612-C62-C512	115.7(5)
C52-C62-C512	124.1(5)
C122-C112-C162	117.6(5)
C122-C112-C12	120.9(5)
C162-C112-C12	121.0(6)
C112-C122-C132	118.5(6)
C112-C122-H122	120.8
C132-C122-H122	120.8
N142-C132-C122	124.9(7)
N142-C132-H132	117.6
C122-C132-H132	117.6
C132-N142-C152	116.5(6)
N142-C152-C162	123.6(6)
N142-C152-H152	118.2
C162-C152-H152	118.2
C152-C162-C112	118.9(6)
C152-C162-H162	120.6
C112-C162-H162	120.6
C262-C212-C222	116.1(5)
C262-C212-C32	119.9(6)
C222-C212-C32	123.9(5)
C232-C222-C212	119.8(6)
C232-C222-H222	120.1
C212-C222-H222	120.1
N242-C232-C222	124.6(7)
N242-C232-H232	117.7
C222-C232-H232	117.7
C232-N242-C252	115.1(6)
N242-C252-C262	124.4(6)
N242-C252-H252	117.8
C262-C252-H252	117.8
C252-C262-C212	119.9(6)
C252-C262-H262	120.1
C212-C262-H262	120.1
C32-C312-C322	119.6(5)
C32-C312-C362	121.8(5)
C322-C312-C362	118.5(5)
C42-C322-C312	120.0(5)
C42-C322-C332	122.2(5)
C312-C322-C332	117.8(5)
C342-C332-C322	121.1(5)
C342-C332-H332	119.4
C322-C332-H332	119.4
C332-C342-C352	121.2(5)
C332-C342-H342	119.4
C352-C342-H342	119.4
C362-C352-C342	119.9(6)
C362-C352-H352	120.1
C342-C352-H352	120.1
C352-C362-C312	121.3(5)
C352-C362-H362	119.4
C312-C362-H362	119.4
C422-C412-C462	117.7(5)
C422-C412-C42	120.9(5)
C462-C412-C42	121.4(5)
C412-C422-C432	119.8(6)
C412-C422-H422	120.1
C432-C422-H422	120.1
N442-C432-C422	123.9(6)
N442-C432-H432	118.1
C422-C432-H432	118.1
C452-N442-C432	114.7(5)
N442-C452-C462	127.4(6)
N442-C452-H452	116.3
C462-C452-H452	116.3
C452-C462-C412	116.5(6)
C452-C462-H462	121.8
C412-C462-H462	121.8
C522-C512-C562	117.7(5)
C522-C512-C62	123.5(5)
C562-C512-C62	118.6(5)
C512-C522-C532	119.3(6)
C512-C522-H522	120.3
C532-C522-H522	120.3
N542-C532-C522	124.0(6)
N542-C532-H532	118.0
C522-C532-H532	118.0
C552-N542-C532	116.7(6)
N542-C552-C562	123.5(6)
N542-C552-H552	118.2
C562-C552-H552	118.2
C512-C562-C552	118.6(6)
C512-C562-H562	120.7
C552-C562-H562	120.7
C62-C612-C622	119.9(5)
C62-C612-C662	121.6(5)
C622-C612-C662	118.5(5)
C12-C622-C612	120.7(5)
C12-C622-C632	121.6(5)
C612-C622-C632	117.7(5)
C642-C632-C622	121.4(6)
C642-C632-H632	119.3
C622-C632-H632	119.3
C632-C642-C652	120.4(5)
C632-C642-H642	119.8
C652-C642-H642	119.8

C662-C652-C642	120.6(6)
C662-C652-H652	119.7
C642-C652-H652	119.7
C652-C662-C612	121.1(6)
C652-C662-H662	119.5
C612-C662-H662	119.5

5,12-Dihydro-5,6,11,12-tetra(4-pyridyl)-5,12-epidioxynaphthacene (**TARO2**) CCDC 1821076



Identification code	gxi3sq
Empirical formula	$C_{38}H_{24}N_4O_2$
Formula weight	568.61
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	tetragonal
Space group	P4/n
Z	16
Unit cell dimensions	a = 29.9853(18) Å α = 90 deg. b = 29.9853(18) Å β = 90 deg. c = 14.2542(9) Å γ = 90 deg.
Volume	12816.2(17) Å^3
Density (calculated)	1.18 g/cm^3
Absorption coefficient	0.07 mm^{-1}
Crystal shape	plate
Crystal size	0.15 x 0.10 x 0.03 mm^3
Crystal colour	colourless
Theta range for data collection	1.0 to 20.4 deg.
Index ranges	-29≤h≤29, -29≤k≤29, -13≤l≤13
Reflections collected	52616
Independent reflections	6330 (R(int) = 0.1772)
Observed reflections	3410 (I > 2σ(I))
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.91
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6330 / 780 / 793
Goodness-of-fit on F^2	1.04
Final R indices (I>2sigma(I))	R1 = 0.070, wR2 = 0.177
Largest diff. peak and hole	0.30 and -0.33 eÅ^{-3}

Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **TARO2**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
O11	0.6350(2)	0.4533(2)	0.6176(3)	0.0386(13)
O21	0.6577(2)	0.4850(2)	0.6796(3)	0.0363(12)
C11	0.6320(2)	0.4712(2)	0.5210(5)	0.0329(16)
C21	0.6795(2)	0.4833(2)	0.4928(5)	0.0331(17)
C31	0.7062(2)	0.4628(2)	0.4265(5)	0.0342(17)
C41	0.7375(2)	0.5378(2)	0.5322(5)	0.0335(17)
C51	0.6965(2)	0.5190(2)	0.5506(5)	0.0309(17)
C61	0.6650(2)	0.5292(2)	0.6343(5)	0.0319(16)
C121	0.5921(2)	0.3963(2)	0.5104(5)	0.041(2)
H121	0.5970	0.3913	0.5755	0.049
C111	0.6073(2)	0.4349(2)	0.4681(5)	0.0336(17)
C131	0.5697(2)	0.3650(3)	0.4569(6)	0.047(2)
H131	0.5597	0.3385	0.4869	0.056
N141	0.5614(2)	0.3699(2)	0.3659(5)	0.0478(18)
C151	0.5749(2)	0.4080(3)	0.3259(6)	0.047(2)
H151	0.5689	0.4126	0.2612	0.057
C161	0.5970(2)	0.4406(2)	0.3741(5)	0.0369(18)
H161	0.6053	0.4674	0.3430	0.044
C211	0.6941(2)	0.4224(2)	0.3716(6)	0.0395(19)
C221	0.6924(3)	0.3816(3)	0.4125(7)	0.061(2)
H221	0.6981	0.3784	0.4777	0.073
C231	0.6820(3)	0.3437(3)	0.3567(7)	0.072(3)
H231	0.6803	0.3152	0.3855	0.086
N241	0.6745(3)	0.3474(3)	0.2647(7)	0.084(3)
C251	0.6777(3)	0.3870(3)	0.2253(7)	0.066(3)
H251	0.6731	0.3895	0.1595	0.079
C261	0.6872(3)	0.4244(3)	0.2752(6)	0.052(2)
H261	0.6892	0.4523	0.2438	0.063
C311	0.7497(2)	0.4816(2)	0.4094(5)	0.0343(18)
C321	0.7647(2)	0.5200(2)	0.4576(5)	0.0328(17)
C331	0.8066(2)	0.5384(3)	0.4357(5)	0.0405(19)
H331	0.8161	0.5647	0.4669	0.049
C341	0.8337(2)	0.5191(3)	0.3703(5)	0.044(2)
H341	0.8619	0.5321	0.3565	0.053
C351	0.8201(2)	0.4804(3)	0.3237(5)	0.045(2)
H351	0.8392	0.4669	0.2787	0.053
C361	0.7795(2)	0.4621(2)	0.3430(5)	0.040(2)
H361	0.7708	0.4356	0.3114	0.049
C411	0.7560(2)	0.5771(2)	0.5813(5)	0.0334(18)
C421	0.7846(2)	0.5733(3)	0.6591(5)	0.0408(19)
H421	0.7922	0.5447	0.6830	0.049
C431	0.8013(2)	0.6112(3)	0.7005(6)	0.047(2)
H431	0.8200	0.6078	0.7538	0.056
N441	0.7931(2)	0.6522(2)	0.6707(5)	0.0574(19)
C451	0.7668(3)	0.6558(3)	0.5957(6)	0.058(2)
H451	0.7608	0.6848	0.5719	0.070
C461	0.7478(3)	0.6196(3)	0.5503(5)	0.048(2)
H461	0.7290	0.6243	0.4975	0.057
C511	0.6839(2)	0.5554(2)	0.7167(5)	0.0335(17)
C521	0.7014(2)	0.5345(3)	0.7952(5)	0.0421(19)
H521	0.7036	0.5029	0.7968	0.051
C531	0.7154(2)	0.5593(3)	0.8707(5)	0.046(2)
H531	0.7272	0.5440	0.9236	0.055
N541	0.7134(2)	0.6040(2)	0.8737(5)	0.0508(18)
C551	0.6974(2)	0.6240(3)	0.7957(6)	0.048(2)

H551	0.6962	0.6557	0.7950	0.057
C561	0.6827(2)	0.6016(3)	0.7175(6)	0.044(2)
H561	0.6719	0.6176	0.6646	0.052
C611	0.6203(2)	0.5433(2)	0.5950(5)	0.0313(16)
C621	0.6026(2)	0.5127(2)	0.5318(5)	0.0346(17)
C631	0.5612(2)	0.5198(2)	0.4932(5)	0.0374(19)
H631	0.5493	0.4992	0.4493	0.045
C641	0.5366(2)	0.5574(3)	0.5185(6)	0.044(2)
H641	0.5081	0.5625	0.4914	0.053
C651	0.5535(2)	0.5870(2)	0.5824(5)	0.0381(19)
H651	0.5368	0.6127	0.5989	0.046
C661	0.5950(2)	0.5798(2)	0.6234(5)	0.0358(19)
H661	0.6059	0.5995	0.6702	0.043
O12	0.9677(2)	0.3967(2)	-0.1152(3)	0.0454(13)
O22	1.0051(2)	0.3868(2)	-0.1789(3)	0.0407(13)
C12	0.9768(2)	0.3792(2)	-0.0209(5)	0.0360(17)
C22	1.0211(2)	0.3984(2)	0.0074(5)	0.0335(17)
C32	1.0300(2)	0.4299(2)	0.0760(5)	0.0295(16)
C42	1.1005(2)	0.3940(2)	-0.0341(5)	0.0313(17)
C52	1.0570(2)	0.3829(2)	-0.0523(5)	0.0302(16)
C62	1.0387(2)	0.3568(2)	-0.1360(5)	0.0338(16)
C112	0.9350(2)	0.3895(3)	0.0337(6)	0.046(2)
C122	0.8974(3)	0.4066(3)	-0.0080(7)	0.077(3)
H122	0.8975	0.4149	-0.0723	0.092
C132	0.8602(3)	0.4115(5)	0.0449(8)	0.129(5)
H132	0.8345	0.4233	0.0148	0.154
N142	0.8565(3)	0.4011(4)	0.1352(7)	0.116(4)
C152	0.8925(3)	0.3840(3)	0.1754(7)	0.071(3)
H152	0.8911	0.3757	0.2397	0.086
C162	0.9319(3)	0.3780(2)	0.1278(6)	0.047(2)
H162	0.9570	0.3659	0.1594	0.056
C212	0.9949(2)	0.4533(2)	0.1315(5)	0.0312(17)
C222	0.9645(2)	0.4805(2)	0.0892(6)	0.046(2)
H222	0.9650	0.4844	0.0230	0.055
C232	0.9328(3)	0.5024(3)	0.1436(7)	0.065(3)
H232	0.9116	0.5206	0.1123	0.078
N242	0.9302(2)	0.4996(2)	0.2369(6)	0.062(2)
C252	0.9596(3)	0.4730(3)	0.2759(6)	0.055(2)
H252	0.9585	0.4695	0.3421	0.066
C262	0.9919(2)	0.4500(2)	0.2282(5)	0.0410(19)
H262	1.0123	0.4317	0.2617	0.049
C312	1.0757(2)	0.4433(2)	0.0929(5)	0.0319(17)
C322	1.1107(2)	0.4243(2)	0.0410(5)	0.0321(17)
C332	1.1547(2)	0.4374(2)	0.0603(5)	0.042(2)
H332	1.1784	0.4235	0.0272	0.050
C342	1.1645(2)	0.4691(2)	0.1243(5)	0.041(2)
H342	1.1946	0.4776	0.1350	0.049
C352	1.1300(2)	0.4895(2)	0.1747(5)	0.042(2)
H352	1.1365	0.5120	0.2195	0.050
C362	1.0869(2)	0.4768(2)	0.1591(5)	0.042(2)
H362	1.0638	0.4909	0.1936	0.050
C412	1.1404(2)	0.3771(2)	-0.0878(5)	0.0325(17)
C422	1.1578(2)	0.4001(2)	-0.1639(5)	0.0356(18)
H422	1.1441	0.4267	-0.1859	0.043
C432	1.1950(2)	0.3835(3)	-0.2062(6)	0.048(2)
H432	1.2060	0.3992	-0.2592	0.058
N442	1.2173(2)	0.3471(2)	-0.1798(5)	0.0499(18)
C452	1.2010(3)	0.3261(3)	-0.1056(6)	0.054(2)
H452	1.2166	0.3006	-0.0837	0.065
C462	1.1627(2)	0.3389(2)	-0.0572(5)	0.043(2)
H462	1.1521	0.3221	-0.0052	0.052
C512	1.0692(2)	0.3491(2)	-0.2185(5)	0.0344(17)

C522	1.0702(2)	0.3777(2)	-0.2957(5)	0.0386(19)
H522	1.0514	0.4033	-0.2966	0.046
C532	1.0980(2)	0.3692(3)	-0.3706(5)	0.043(2)
H532	1.0977	0.3895	-0.4219	0.052
N542	1.1252(2)	0.3342(2)	-0.3750(5)	0.0492(17)
C552	1.1251(3)	0.3074(3)	-0.3009(6)	0.046(2)
H552	1.1447	0.2826	-0.3017	0.056
C562	1.0988(2)	0.3131(2)	-0.2238(5)	0.0348(18)
H562	1.1006	0.2924	-0.1734	0.042
C612	1.0130(2)	0.3164(2)	-0.1008(5)	0.0366(18)
C622	0.9811(2)	0.3283(2)	-0.0339(5)	0.0394(18)
C632	0.9532(3)	0.2967(3)	0.0024(6)	0.056(2)
H632	0.9303	0.3051	0.0449	0.067
C642	0.9582(3)	0.2525(3)	-0.0225(7)	0.070(3)
H642	0.9401	0.2303	0.0060	0.084
C652	0.9896(3)	0.2405(3)	-0.0890(6)	0.060(2)
H652	0.9926	0.2102	-0.1069	0.072
C662	1.0164(2)	0.2723(2)	-0.1291(5)	0.045(2)
H662	1.0373	0.2641	-0.1763	0.053

Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **TARO2**.

Atom	x	y	z	U_{eq}
H121	0.5970	0.3913	0.5755	0.049
H131	0.5597	0.3385	0.4869	0.056
H151	0.5689	0.4126	0.2612	0.057
H161	0.6053	0.4674	0.3430	0.044
H221	0.6981	0.3784	0.4777	0.073
H231	0.6803	0.3152	0.3855	0.086
H251	0.6731	0.3895	0.1595	0.079
H261	0.6892	0.4523	0.2438	0.063
H331	0.8161	0.5647	0.4669	0.049
H341	0.8619	0.5321	0.3565	0.053
H351	0.8392	0.4669	0.2787	0.053
H361	0.7708	0.4356	0.3114	0.049
H421	0.7922	0.5447	0.6830	0.049
H431	0.8200	0.6078	0.7538	0.056
H451	0.7608	0.6848	0.5719	0.070
H461	0.7290	0.6243	0.4975	0.057
H521	0.7036	0.5029	0.7968	0.051
H531	0.7272	0.5440	0.9236	0.055
H551	0.6962	0.6557	0.7950	0.057
H561	0.6719	0.6176	0.6646	0.052
H631	0.5493	0.4992	0.4493	0.045
H641	0.5081	0.5625	0.4914	0.053
H651	0.5368	0.6127	0.5989	0.046
H661	0.6059	0.5995	0.6702	0.043
H122	0.8975	0.4149	-0.0723	0.092
H132	0.8345	0.4233	0.0148	0.154
H152	0.8911	0.3757	0.2397	0.086
H162	0.9570	0.3659	0.1594	0.056
H222	0.9650	0.4844	0.0230	0.055
H232	0.9116	0.5206	0.1123	0.078
H252	0.9585	0.4695	0.3421	0.066
H262	1.0123	0.4317	0.2617	0.049
H332	1.1784	0.4235	0.0272	0.050
H342	1.1946	0.4776	0.1350	0.049
H352	1.1365	0.5120	0.2195	0.050

H362	1.0638	0.4909	0.1936	0.050
H422	1.1441	0.4267	-0.1859	0.043
H432	1.2060	0.3992	-0.2592	0.058
H452	1.2166	0.3006	-0.0837	0.065
H462	1.1521	0.3221	-0.0052	0.052
H522	1.0514	0.4033	-0.2966	0.046
H532	1.0977	0.3895	-0.4219	0.052
H552	1.1447	0.2826	-0.3017	0.056
H562	1.1006	0.2924	-0.1734	0.042
H632	0.9303	0.3051	0.0449	0.067
H642	0.9401	0.2303	0.0060	0.084
H652	0.9926	0.2102	-0.1069	0.072
H662	1.0373	0.2641	-0.1763	0.053

Anisotropic displacement parameters ($Å^2$) for **TARO2**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O11	0.045(3)	0.034(3)	0.037(3)	0.003(2)	-0.002(2)	-0.013(2)
O21	0.045(3)	0.030(3)	0.035(3)	-0.001(2)	0.002(2)	-0.005(2)
C11	0.033(4)	0.039(4)	0.027(4)	0.001(3)	0.003(3)	-0.003(3)
C21	0.033(4)	0.036(4)	0.030(4)	0.005(3)	-0.003(3)	0.002(3)
C31	0.037(4)	0.038(4)	0.028(4)	0.003(3)	-0.002(3)	0.003(3)
C41	0.028(4)	0.041(4)	0.031(4)	-0.003(3)	-0.003(3)	-0.004(3)
C51	0.032(4)	0.028(4)	0.033(4)	0.004(3)	0.002(3)	0.004(3)
C61	0.031(4)	0.029(4)	0.035(4)	0.000(3)	0.005(3)	0.001(3)
C121	0.047(5)	0.041(4)	0.035(5)	0.007(3)	-0.001(4)	-0.011(4)
C111	0.024(4)	0.038(4)	0.040(4)	0.006(3)	0.000(3)	-0.005(3)
C131	0.048(5)	0.037(5)	0.055(5)	0.006(4)	-0.005(4)	-0.011(4)
N141	0.046(4)	0.047(4)	0.051(4)	0.004(3)	-0.013(4)	-0.011(3)
C151	0.039(5)	0.049(5)	0.054(5)	0.000(4)	-0.005(4)	-0.005(4)
C161	0.033(5)	0.042(5)	0.036(4)	0.005(4)	0.004(4)	0.000(4)
C211	0.033(5)	0.036(4)	0.049(5)	-0.002(3)	0.008(4)	0.003(4)
C221	0.074(6)	0.035(4)	0.073(6)	0.004(4)	0.011(5)	0.005(4)
C231	0.084(7)	0.040(5)	0.092(6)	0.000(5)	0.024(6)	-0.004(5)
N241	0.087(6)	0.073(5)	0.092(6)	-0.024(5)	0.007(5)	-0.010(5)
C251	0.056(6)	0.078(6)	0.063(6)	-0.031(5)	0.009(5)	-0.004(5)
C261	0.055(6)	0.055(5)	0.048(5)	-0.014(4)	0.005(4)	0.002(4)
C311	0.032(4)	0.039(4)	0.032(5)	0.008(3)	-0.001(3)	0.007(3)
C321	0.028(4)	0.038(4)	0.032(4)	0.011(3)	0.001(3)	0.009(3)
C331	0.033(4)	0.052(5)	0.036(5)	0.005(4)	0.001(3)	-0.005(4)
C341	0.031(5)	0.064(5)	0.037(5)	0.013(4)	0.005(4)	-0.005(4)
C351	0.031(4)	0.060(5)	0.043(5)	0.005(4)	0.005(4)	0.010(4)
C361	0.041(4)	0.044(5)	0.037(5)	0.000(4)	0.003(4)	-0.004(4)
C411	0.025(4)	0.038(4)	0.037(5)	0.005(3)	-0.002(3)	-0.006(3)
C421	0.036(5)	0.043(4)	0.044(5)	0.010(4)	-0.004(4)	-0.008(4)
C431	0.034(5)	0.049(5)	0.058(6)	-0.001(4)	-0.005(4)	-0.006(4)
N441	0.056(5)	0.051(4)	0.066(5)	-0.006(4)	-0.012(4)	-0.007(4)
C451	0.066(6)	0.035(5)	0.073(6)	0.010(4)	-0.020(5)	-0.004(4)
C461	0.053(5)	0.044(4)	0.046(5)	0.008(4)	-0.011(4)	-0.004(4)
C511	0.022(4)	0.043(4)	0.035(4)	-0.007(3)	0.003(3)	0.002(3)
C521	0.031(5)	0.054(5)	0.041(5)	-0.002(4)	0.003(4)	-0.002(4)
C531	0.047(5)	0.056(5)	0.034(5)	0.006(4)	0.007(4)	-0.009(4)
N541	0.046(4)	0.062(4)	0.045(4)	-0.009(4)	-0.003(3)	0.005(4)
C551	0.040(5)	0.045(5)	0.058(5)	-0.010(4)	-0.008(4)	0.009(4)
C561	0.037(5)	0.046(4)	0.049(5)	-0.010(4)	-0.003(4)	0.003(4)
C611	0.027(4)	0.039(4)	0.028(4)	0.011(3)	0.010(3)	-0.004(3)
C621	0.032(4)	0.041(4)	0.031(5)	0.006(3)	0.008(3)	-0.005(3)

C631	0.037(4)	0.044(5)	0.031(5)	0.003(4)	0.004(3)	-0.004(4)
C641	0.027(5)	0.053(5)	0.054(6)	0.000(4)	-0.003(4)	0.002(4)
C651	0.029(4)	0.044(5)	0.041(5)	0.004(4)	0.007(4)	-0.001(4)
C661	0.027(4)	0.049(5)	0.031(5)	-0.002(4)	0.006(3)	-0.003(3)
O12	0.032(3)	0.062(4)	0.042(3)	-0.002(3)	-0.003(2)	0.018(3)
O22	0.038(3)	0.049(3)	0.035(3)	0.001(2)	0.002(2)	0.017(3)
C12	0.028(4)	0.044(4)	0.036(4)	-0.001(4)	-0.003(3)	0.007(3)
C22	0.031(4)	0.035(4)	0.034(4)	0.007(3)	0.002(3)	0.009(3)
C32	0.031(4)	0.028(4)	0.030(4)	0.008(3)	0.003(3)	0.008(3)
C42	0.034(4)	0.029(4)	0.032(4)	0.002(3)	0.005(3)	0.005(3)
C52	0.031(4)	0.027(4)	0.033(4)	0.006(3)	0.006(3)	0.000(3)
C62	0.034(4)	0.034(4)	0.034(4)	0.003(3)	-0.003(3)	0.011(3)
C112	0.031(4)	0.051(5)	0.056(5)	-0.003(4)	0.007(4)	0.011(4)
C122	0.034(5)	0.130(9)	0.068(6)	-0.019(6)	-0.009(4)	0.038(5)
C132	0.045(6)	0.264(16)	0.077(7)	-0.050(9)	-0.006(5)	0.062(8)
N142	0.038(5)	0.228(12)	0.083(6)	-0.044(7)	0.009(5)	0.021(6)
C152	0.046(5)	0.099(8)	0.069(7)	-0.034(5)	0.018(4)	-0.015(5)
C162	0.036(4)	0.050(5)	0.054(5)	-0.006(4)	0.005(4)	-0.001(4)
C212	0.027(4)	0.030(4)	0.036(4)	0.005(3)	0.007(3)	0.003(3)
C222	0.042(5)	0.047(5)	0.048(5)	0.020(4)	0.017(4)	0.011(4)
C232	0.057(6)	0.055(6)	0.082(6)	0.028(5)	0.035(5)	0.022(4)
N242	0.069(5)	0.042(5)	0.074(5)	0.004(4)	0.036(4)	0.012(4)
C252	0.067(6)	0.057(6)	0.042(5)	-0.008(4)	0.018(4)	-0.003(4)
C262	0.045(5)	0.045(5)	0.033(4)	-0.002(4)	0.001(4)	-0.001(4)
C312	0.030(4)	0.035(4)	0.031(4)	0.004(3)	0.001(3)	0.005(3)
C322	0.030(4)	0.033(4)	0.033(4)	0.002(3)	-0.003(3)	0.007(3)
C332	0.033(4)	0.051(5)	0.040(5)	-0.005(4)	0.003(4)	0.000(4)
C342	0.033(4)	0.055(5)	0.036(5)	-0.003(4)	-0.006(4)	0.003(4)
C352	0.038(4)	0.044(5)	0.042(5)	-0.011(4)	-0.003(4)	0.001(4)
C362	0.035(4)	0.046(5)	0.043(5)	-0.004(4)	-0.001(4)	0.005(4)
C412	0.035(4)	0.029(4)	0.033(4)	-0.007(3)	-0.002(3)	0.001(3)
C422	0.032(4)	0.032(4)	0.042(5)	0.000(3)	0.000(3)	0.000(3)
C432	0.041(5)	0.050(5)	0.053(6)	0.005(4)	0.010(4)	0.002(4)
N442	0.038(4)	0.050(4)	0.062(5)	-0.002(4)	0.014(3)	0.009(3)
C452	0.048(5)	0.047(5)	0.068(6)	0.009(4)	0.009(4)	0.014(4)
C462	0.042(5)	0.040(5)	0.048(5)	0.006(4)	0.001(4)	0.005(4)
C512	0.029(4)	0.034(4)	0.041(4)	-0.002(3)	-0.001(3)	-0.001(3)
C522	0.039(5)	0.038(5)	0.039(5)	0.002(4)	-0.005(4)	0.002(4)
C532	0.051(5)	0.043(5)	0.037(5)	0.002(4)	-0.007(4)	0.001(4)
N542	0.060(5)	0.044(4)	0.043(4)	-0.003(3)	0.005(4)	0.009(3)
C552	0.055(5)	0.037(5)	0.047(5)	-0.004(4)	0.007(4)	0.016(4)
C562	0.034(4)	0.036(4)	0.035(4)	-0.005(4)	-0.001(3)	-0.004(3)
C612	0.038(5)	0.036(4)	0.036(5)	-0.004(3)	0.000(3)	0.002(3)
C622	0.034(5)	0.042(4)	0.042(5)	-0.006(4)	0.000(3)	-0.001(3)
C632	0.051(6)	0.051(5)	0.066(6)	-0.010(4)	0.012(4)	-0.010(4)
C642	0.070(7)	0.047(5)	0.093(8)	-0.016(5)	0.030(5)	-0.029(5)
C652	0.067(6)	0.037(5)	0.074(7)	-0.015(4)	0.014(5)	-0.011(4)
C662	0.044(5)	0.041(4)	0.048(5)	-0.009(4)	-0.002(4)	-0.006(4)

Bond lengths (Å) and angles (deg) for **TARO2**.

O11-O21	1.465(6)	C31-C211	1.488(10)
O11-C11	1.481(8)	C41-C51	1.376(9)
O21-C61	1.491(8)	C41-C321	1.442(9)
C11-C111	1.517(10)	C41-C411	1.479(9)
C11-C21	1.524(9)	C51-C61	1.553(9)
C11-C621	1.533(9)	C61-C611	1.513(9)
C21-C31	1.383(9)	C61-C511	1.522(9)
C21-C51	1.444(9)	C121-C111	1.382(9)
C31-C311	1.442(9)	C121-C131	1.383(10)

C121-H121	0.9500	C12-C112	1.507(10)
C111-C161	1.386(9)	C12-C622	1.541(10)
C131-N141	1.330(9)	C22-C32	1.386(9)
C131-H131	0.9500	C22-C52	1.448(9)
N141-C151	1.341(9)	C32-C312	1.449(9)
C151-C161	1.365(10)	C32-C212	1.491(9)
C151-H151	0.9500	C42-C52	1.371(9)
C161-H161	0.9500	C42-C322	1.437(9)
C211-C221	1.354(10)	C42-C412	1.509(9)
C211-C261	1.391(10)	C52-C62	1.528(9)
C221-C231	1.422(11)	C62-C512	1.507(9)
C221-H221	0.9500	C62-C612	1.520(10)
C231-N241	1.335(11)	C112-C122	1.376(10)
C231-H231	0.9500	C112-C162	1.389(10)
N241-C251	1.317(11)	C122-C132	1.354(12)
C251-C261	1.359(10)	C122-H122	0.9500
C251-H251	0.9500	C132-N142	1.329(13)
C261-H261	0.9500	C132-H132	0.9500
C311-C321	1.414(10)	N142-C152	1.326(12)
C311-C361	1.427(9)	C152-C162	1.374(10)
C321-C331	1.407(9)	C152-H152	0.9500
C331-C341	1.366(10)	C162-H162	0.9500
C331-H331	0.9500	C212-C222	1.364(9)
C341-C351	1.399(10)	C212-C262	1.385(9)
C341-H341	0.9500	C222-C232	1.393(10)
C351-C361	1.364(9)	C222-H222	0.9500
C351-H351	0.9500	C232-N242	1.334(10)
C361-H361	0.9500	C232-H232	0.9500
C411-C461	1.372(9)	N242-C252	1.312(10)
C411-C421	1.406(9)	C252-C262	1.369(10)
C421-C431	1.377(10)	C252-H252	0.9500
C421-H421	0.9500	C262-H262	0.9500
C431-N441	1.324(9)	C312-C322	1.405(9)
C431-H431	0.9500	C312-C362	1.418(9)
N441-C451	1.332(10)	C322-C332	1.402(9)
C451-C461	1.386(10)	C332-C342	1.350(9)
C451-H451	0.9500	C332-H332	0.9500
C461-H461	0.9500	C342-C352	1.398(9)
C511-C521	1.385(10)	C342-H342	0.9500
C511-C561	1.387(9)	C352-C362	1.364(9)
C521-C531	1.375(10)	C352-H352	0.9500
C521-H521	0.9500	C362-H362	0.9500
C531-N541	1.341(9)	C412-C422	1.387(9)
C531-H531	0.9500	C412-C462	1.396(9)
N541-C551	1.352(9)	C422-C432	1.362(9)
C551-C561	1.374(10)	C422-H422	0.9500
C551-H551	0.9500	C432-N442	1.333(9)
C561-H561	0.9500	C432-H432	0.9500
C611-C621	1.390(9)	N442-C452	1.325(9)
C611-C661	1.393(9)	C452-C462	1.393(10)
C621-C631	1.375(9)	C452-H452	0.9500
C631-C641	1.395(9)	C462-H462	0.9500
C631-H631	0.9500	C512-C522	1.394(9)
C641-C651	1.368(10)	C512-C562	1.401(9)
C641-H641	0.9500	C522-C532	1.379(10)
C651-C661	1.390(9)	C522-H522	0.9500
C651-H651	0.9500	C532-N542	1.332(9)
C661-H661	0.9500	C532-H532	0.9500
O12-C12	1.469(8)	N542-C552	1.325(9)
O12-O22	1.473(6)	C552-C562	1.363(9)
O22-C62	1.483(8)	C552-H552	0.9500
C12-C22	1.503(9)	C562-H562	0.9500

C612-C662	1.386(9)
C612-C622	1.399(9)
C622-C632	1.366(10)
C632-C642	1.378(10)
C632-H632	0.9500
C642-C652	1.383(11)
C642-H642	0.9500
C652-C662	1.372(10)
C652-H652	0.9500
C662-H662	0.9500
O21-O11-C11	110.7(4)
O11-O21-C61	112.6(4)
O11-C11-C111	103.4(5)
O11-C11-C21	106.0(5)
C111-C11-C21	119.8(6)
O11-C11-C621	103.6(5)
C111-C11-C621	110.5(6)
C21-C11-C621	111.8(6)
C31-C21-C51	121.0(7)
C31-C21-C11	127.9(7)
C51-C21-C11	110.9(6)
C21-C31-C311	117.7(7)
C21-C31-C211	125.5(7)
C311-C31-C211	116.7(6)
C51-C41-C321	119.6(6)
C51-C41-C411	124.8(6)
C321-C41-C411	115.6(6)
C41-C51-C21	120.7(6)
C41-C51-C61	127.6(6)
C21-C51-C61	111.6(6)
O21-C61-C611	106.2(5)
O21-C61-C511	100.4(5)
C611-C61-C511	118.1(6)
O21-C61-C51	104.4(5)
C611-C61-C51	108.0(6)
C511-C61-C51	117.9(6)
C111-C121-C131	119.2(7)
C111-C121-H121	120.4
C131-C121-H121	120.4
C121-C111-C161	116.9(7)
C121-C111-C11	123.0(7)
C161-C111-C11	120.1(7)
N141-C131-C121	123.7(7)
N141-C131-H131	118.2
C121-C131-H131	118.2
C131-N141-C151	116.9(7)
N141-C151-C161	122.9(8)
N141-C151-H151	118.6
C161-C151-H151	118.6
C151-C161-C111	120.5(7)
C151-C161-H161	119.8
C111-C161-H161	119.8
C221-C211-C261	117.4(8)
C221-C211-C31	121.2(8)
C261-C211-C31	121.3(7)
C211-C221-C231	119.3(9)
C211-C221-H221	120.4
C231-C221-H221	120.4
N241-C231-C221	121.3(9)
N241-C231-H231	119.3
C221-C231-H231	119.3
C251-N241-C231	118.7(9)
N241-C251-C261	122.5(9)
N241-C251-H251	118.8
C261-C251-H251	118.8
C251-C261-C211	120.7(9)
C251-C261-H261	119.6
C211-C261-H261	119.6
C321-C311-C361	117.1(7)
C321-C311-C31	121.6(7)
C361-C311-C31	121.3(7)
C331-C321-C311	119.7(7)
C331-C321-C41	121.5(7)
C311-C321-C41	118.7(6)
C341-C331-C321	121.1(7)
C341-C331-H331	119.4
C321-C331-H331	119.4
C331-C341-C351	120.1(7)
C331-C341-H341	119.9
C351-C341-H341	119.9
C361-C351-C341	119.9(7)
C361-C351-H351	120.1
C341-C351-H351	120.1
C351-C361-C311	121.9(7)
C351-C361-H361	119.1
C311-C361-H361	119.1
C461-C411-C421	116.1(7)
C461-C411-C41	121.3(7)
C421-C411-C41	122.5(7)
C431-C421-C411	119.5(7)
C431-C421-H421	120.3
C411-C421-H421	120.3
N441-C431-C421	124.3(8)
N441-C431-H431	117.9
C421-C431-H431	117.9
C431-N441-C451	116.2(7)
N441-C451-C461	123.8(8)
N441-C451-H451	118.1
C461-C451-H451	118.1
C411-C461-C451	120.1(7)
C411-C461-H461	119.9
C451-C461-H461	119.9
C521-C511-C561	117.0(7)
C521-C511-C61	122.0(7)
C561-C511-C61	120.9(7)
C531-C521-C511	120.3(8)
C531-C521-H521	119.9
C511-C521-H521	119.9
N541-C531-C521	123.5(8)
N541-C531-H531	118.3
C521-C531-H531	118.3
C531-N541-C551	115.7(7)
N541-C551-C561	124.4(8)
N541-C551-H551	117.8
C561-C551-H551	117.8
C551-C561-C511	119.1(8)
C551-C561-H561	120.4
C511-C561-H561	120.4
C621-C611-C661	119.8(7)
C621-C611-C61	113.2(6)
C661-C611-C61	126.5(7)
C631-C621-C611	120.1(7)
C631-C621-C11	127.3(7)
C611-C621-C11	112.3(6)

C621-C631-C641	120.0(7)	C222-C232-H232	117.8
C621-C631-H631	120.0	C252-N242-C232	115.0(7)
C641-C631-H631	120.0	N242-C252-C262	124.8(8)
C651-C641-C631	120.0(7)	N242-C252-H252	117.6
C651-C641-H641	120.0	C262-C252-H252	117.6
C631-C641-H641	120.0	C252-C262-C212	120.3(8)
C641-C651-C661	120.7(7)	C252-C262-H262	119.9
C641-C651-H651	119.6	C212-C262-H262	119.9
C661-C651-H651	119.6	C322-C312-C362	117.5(7)
C651-C661-C611	119.2(7)	C322-C312-C32	120.4(7)
C651-C661-H661	120.4	C362-C312-C32	122.1(6)
C611-C661-H661	120.4	C332-C322-C312	118.9(7)
C12-O12-O22	110.6(4)	C332-C322-C42	121.7(7)
O12-O22-C62	112.6(5)	C312-C322-C42	119.3(6)
O12-C12-C22	105.8(6)	C342-C332-C322	122.4(7)
O12-C12-C112	104.1(6)	C342-C332-H332	118.8
C22-C12-C112	121.2(6)	C322-C332-H332	118.8
O12-C12-C622	105.0(5)	C332-C342-C352	119.6(7)
C22-C12-C622	109.8(6)	C332-C342-H342	120.2
C112-C12-C622	109.5(6)	C352-C342-H342	120.2
C32-C22-C52	119.4(6)	C362-C352-C342	119.6(7)
C32-C22-C12	128.4(6)	C362-C352-H352	120.2
C52-C22-C12	112.0(6)	C342-C352-H352	120.2
C22-C32-C312	119.3(6)	C352-C362-C312	122.0(7)
C22-C32-C212	124.0(6)	C352-C362-H362	119.0
C312-C32-C212	116.7(6)	C312-C362-H362	119.0
C52-C42-C322	119.9(6)	C422-C412-C462	118.2(7)
C52-C42-C412	125.2(6)	C422-C412-C42	121.9(6)
C322-C42-C412	114.9(6)	C462-C412-C42	119.8(7)
C42-C52-C22	121.1(7)	C432-C422-C412	118.2(7)
C42-C52-C62	127.8(6)	C432-C422-H422	120.9
C22-C52-C62	110.9(6)	C412-C422-H422	120.9
O22-C62-C512	100.5(5)	N442-C432-C422	125.8(8)
O22-C62-C612	106.0(5)	N442-C432-H432	117.1
C512-C62-C612	116.3(6)	C422-C432-H432	117.1
O22-C62-C52	104.8(5)	C452-N442-C432	115.4(7)
C512-C62-C52	118.0(6)	N442-C452-C462	124.6(7)
C612-C62-C52	109.4(6)	N442-C452-H452	117.7
C122-C112-C162	117.0(8)	C462-C452-H452	117.7
C122-C112-C12	122.5(8)	C452-C462-C412	117.7(7)
C162-C112-C12	120.3(7)	C452-C462-H462	121.1
C132-C122-C112	118.4(10)	C412-C462-H462	121.1
C132-C122-H122	120.8	C522-C512-C562	114.8(7)
C112-C122-H122	120.8	C522-C512-C62	122.3(6)
N142-C132-C122	125.6(10)	C562-C512-C62	122.9(6)
N142-C132-H132	117.2	C532-C522-C512	120.6(7)
C122-C132-H132	117.2	C532-C522-H522	119.7
C152-N142-C132	116.2(9)	C512-C522-H522	119.7
N142-C152-C162	122.5(10)	N542-C532-C522	123.5(7)
N142-C152-H152	118.7	N542-C532-H532	118.2
C162-C152-H152	118.7	C522-C532-H532	118.2
C152-C162-C112	120.2(8)	C552-N542-C532	116.0(7)
C152-C162-H162	119.9	N542-C552-C562	124.7(7)
C112-C162-H162	119.9	N542-C552-H552	117.7
C222-C212-C262	116.1(7)	C562-C552-H552	117.7
C222-C212-C32	121.2(7)	C552-C562-C512	120.3(7)
C262-C212-C32	122.7(7)	C552-C562-H562	119.8
C212-C222-C232	119.5(8)	C512-C562-H562	119.8
C212-C222-H222	120.3	C662-C612-C622	119.5(7)
C232-C222-H222	120.3	C662-C612-C62	128.8(7)
N242-C232-C222	124.4(8)	C622-C612-C62	111.6(6)
N242-C232-H232	117.8	C632-C622-C612	120.0(7)

C632-C622-C12	126.3(7)
C612-C622-C12	113.0(6)
C622-C632-C642	120.2(8)
C622-C632-H632	119.9
C642-C632-H632	119.9
C632-C642-C652	120.0(8)
C632-C642-H642	120.0
C652-C642-H642	120.0
C662-C652-C642	120.3(8)
C662-C652-H652	119.9
C642-C652-H652	119.9
C652-C662-C612	119.8(8)
C652-C662-H662	120.1
C612-C662-H662	120.1

S8. Cartesian Coordinates of computational studied molecules

Coordinates of rubrene:

C	-0.03043	1.84339	-4.59077
C	0.50666	2.97722	-3.91902
C	0.67419	2.95796	-2.5579
C	0.32328	1.80782	-1.77581
C	-0.08119	0.60341	-2.48009
C	-0.31131	0.6966	-3.89297
C	0.32442	1.82604	-0.36527
C	0.00829	0.63451	0.36038
C	0.00049	-0.63476	-0.35874
C	-0.19974	-0.61272	-1.77524
C	-0.30061	0.6271	1.75724
C	-0.30253	-0.59178	2.46728
C	0.08657	-1.81852	1.79337
C	0.19332	-1.84048	0.38678
C	-0.64225	-0.66787	3.8588
C	-0.47756	-1.82636	4.57423
C	0.04436	-2.9901	3.94292
C	0.31366	-2.98417	2.59805
C	-0.70008	-1.81431	-2.50804
C	-0.79087	1.85645	2.44995
C	0.82213	3.05057	0.33054
C	0.67122	-3.09377	-0.27086
C	-2.0049	-2.26737	-2.24617
C	-2.55672	-3.3252	-2.97094
C	-1.81044	-3.95576	-3.96945
C	-0.51117	-3.51683	-4.23891
C	0.03541	-2.45182	-3.52078
C	0.13786	4.27682	0.29857
C	0.68529	5.41678	0.8895
C	1.93577	5.35713	1.51101
C	2.63206	4.14636	1.54197
C	2.0786	3.00455	0.95997
C	-2.04598	2.37635	2.08762
C	-2.59489	3.4663	2.76565
C	-1.89508	4.06234	3.81766
C	-0.64591	3.55628	4.18785
C	-0.10302	2.4596	3.51597
C	-0.08403	-4.27785	-0.29277
C	0.43897	-5.44951	-0.84228
C	1.73451	-5.46495	-1.36665
C	2.50087	-4.29715	-1.34254
C	1.97247	-3.12313	-0.80259
H	-0.20514	1.88259	-5.66706
H	0.77143	3.86993	-4.48778
H	1.06407	3.83736	-2.04799
H	-0.7005	-0.17443	-4.41758
H	-1.02085	0.22502	4.35358
H	-0.73335	-1.85258	5.63457
H	0.21644	-3.89434	4.52881
H	0.69079	-3.88539	2.1176
H	-2.59226	-1.77175	-1.47143
H	-3.57491	-3.65438	-2.75679
H	-2.23889	-4.78398	-4.53576
H	0.08147	-4.0065	-5.01322
H	1.05013	-2.1148	-3.73594
H	-0.83869	4.32958	-0.18411
H	0.13171	6.3567	0.8642
H	2.36528	6.25033	1.9672
H	3.61268	4.09015	2.01757
H	2.62811	2.06185	0.9786
H	-2.59775	1.90735	1.27133
H	-3.57463	3.8475	2.47287
H	-2.32095	4.91566	4.34745
H	-0.0896	4.01819	5.00498
H	0.87273	2.07075	3.80954
H	-1.09582	-4.27211	0.1142
H	-0.16922	-6.35519	-0.86135
H	2.14431	-6.38302	-1.79044
H	3.51636	-4.29965	-1.74211
H	2.57538	-2.214	-0.77844

Coordinates of DAR:

C	0.15423	1.89312	-4.56675
C	0.65919	3.02396	-3.86601
C	0.78494	2.99152	-2.5008
C	0.42066	1.82949	-1.74257
C	0.04555	0.63077	-2.47203
C	-0.13919	0.73688	-3.89043
C	0.38057	1.82768	-0.33264
C	0.04945	0.62794	0.37188
C	0.06123	-0.63182	-0.36294
C	-0.09193	-0.59337	-1.78493
C	-0.2959	0.60513	1.7599
C	-0.32425	-0.62165	2.45531
C	0.0727	-1.84393	1.77828
C	0.22181	-1.84637	0.37543
C	-0.70182	-0.70924	3.83605
C	-0.56964	-1.87742	4.54201
C	-0.04427	-3.03966	3.91125
C	0.26347	-3.02166	2.57491
C	-0.55557	-1.79118	-2.54619
C	-0.78897	1.83208	2.45367
C	0.86074	3.04476	0.38662
C	0.71802	-3.09462	-0.27663
C	-1.862	-2.26351	-2.33113
C	-2.37114	-3.3283	-3.07649
C	-1.5789	-3.94715	-4.04643
C	-0.27837	-3.48681	-4.27121
C	0.22461	-2.41319	-3.53488
C	0.19135	4.27672	0.36669
C	0.76914	5.38003	0.99682
N	1.9579	5.35232	1.6206
C	2.60115	4.17442	1.62839
C	2.10274	3.01128	1.04013
C	-2.02626	2.37433	2.06398
C	-2.5705	3.47251	2.73248
C	-1.88205	4.05536	3.7993
C	-0.65159	3.52529	4.19822
C	-0.11534	2.41838	3.53822
C	-0.02267	-4.28316	-0.34746
C	0.56446	-5.42421	-0.89646

N	1.82487	-5.47348	-1.35698
C	2.53447	-4.33707	-1.27841
C	2.03521	-3.14159	-0.75962
H	0.01367	1.94293	-5.64744
H	0.93287	3.92544	-4.41616
H	1.15104	3.8703	-1.97267
H	-0.50398	-0.13176	-4.43597
H	-1.08346	0.18251	4.33037
H	-0.85463	-1.9132	5.59443
H	0.1	-3.95294	4.49032
H	0.64394	-3.92319	2.09782
H	-2.48424	-1.77866	-1.57688
H	-3.39098	-3.67375	-2.89943
H	-1.97221	-4.78366	-4.62568
H	0.34943	-3.96839	-5.02223
H	1.2406	-2.0593	-3.71482
H	-0.77765	4.37113	-0.12395
H	0.24919	6.34261	0.99776
H	3.573	4.1606	2.13117
H	2.68008	2.08623	1.07595
H	-2.56763	1.91756	1.23386
H	-3.53647	3.87195	2.41925
H	-2.30188	4.91779	4.31875
H	-0.10419	3.97823	5.02596
H	0.84581	2.01062	3.85393
H	-1.05223	-4.31466	0.00982
H	-0.00889	-6.35327	-0.96721
H	3.56308	-4.38593	-1.64848
H	2.66761	-2.25374	-0.71758

Coordinates of TAR:

C	0.04725	1.80382	-4.61019
C	0.54849	2.95216	-3.93597
C	0.68531	2.94743	-2.57163
C	0.33625	1.79768	-1.7884
C	-0.03807	0.58264	-2.49074
C	-0.23364	0.6591	-3.90962
C	0.31257	1.82339	-0.37845
C	-0.00335	0.63663	0.35434
C	0.00229	-0.6375	-0.35412
C	-0.16349	-0.62613	-1.77483
C	-0.32379	0.63809	1.74814
C	-0.34062	-0.5732	2.47046
C	0.04391	-1.80846	1.81004
C	0.17385	-1.83722	0.40574
C	-0.69216	-0.63376	3.85963
C	-0.54888	-1.78904	4.58419
C	-0.03845	-2.96443	3.96584
C	0.24562	-2.9719	2.62433
C	0.66186	-3.09542	-0.23234
C	-0.81509	1.87281	2.42851
C	0.79179	3.0566	0.31292
C	-0.63979	-1.8353	-2.50896
C	0.11116	4.28214	0.28099
C	0.68224	5.39786	0.89583
N	1.87522	5.38633	1.51221
C	2.53044	4.21554	1.5286
C	2.03816	3.04056	0.9584
C	-2.06359	2.40301	2.06745
C	-2.5677	3.50468	2.76054
N	-1.92223	4.11449	3.76636
C	-0.72731	3.606	4.10836
C	-0.14454	2.49851	3.48931
C	-0.07789	-4.28598	-0.27281
C	0.49924	-5.43156	-0.82372
N	1.7498	-5.48168	-1.31044
C	2.4596	-4.34425	-1.25821
C	1.96843	-3.14367	-0.743
C	-1.94238	-2.30657	-2.28287
C	-2.42337	-3.38096	-3.03263
N	-1.7071	-4.01803	-3.97129
C	-0.46038	-3.56687	-4.18339
C	0.10687	-2.49045	-3.49876
H	-0.1005	1.83066	-5.69059
H	0.81051	3.84448	-4.50608
H	1.04886	3.83874	-2.06332
H	-0.59618	-0.22073	-4.43824
H	-1.0629	0.2661	4.34729
H	-0.81332	-1.80397	5.64233
H	0.11371	-3.86696	4.55927
H	0.61515	-3.88283	2.15686
H	-0.86153	4.36249	-0.20513
H	0.15312	6.35505	0.89227
H	3.50602	4.21715	2.02416
H	2.62374	2.12098	1.00165
H	-2.64145	1.94911	1.26095
H	-3.54506	3.91865	2.4947
H	-0.20627	4.11278	4.9255
H	0.82927	2.13603	3.81969
H	-1.09943	-4.31614	0.10725
H	-0.07391	-6.36158	-0.87632
H	3.48045	-4.3959	-1.64862
H	2.59924	-2.25385	-0.72482
H	-2.57868	-1.82833	-1.53659
H	-3.4414	-3.74859	-2.87212
H	0.11808	-4.09584	-4.94608
H	1.12597	-2.1746	-3.72381

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