Electronic Supplementary Information (ESI) for:

Synthesis and Spectroscopic Properties of Propeller Typed 2,4,6-Tri(anthracen-9-yl)-1,3,5-triazine

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1. Materials and methods

Ether and tetrahydrofuran (THF) for use on vacuum line were freshly distilled from sodium/benzophenone prior to use. *t*-BuLi (pentane) were obtained from Energy Chemical; prior to use, its concentration was determined by titration with *N*-pivaloyl-*o*-toluidine[s1]. Column chromatography was carried out on silica gel (300-400 mesh). Analytical thin-layer chromatography was performed on glass plates of Silica Gel GF-254 with detection by UV. Standard techniques for synthesis under inert atmosphere, using gasbag and Schlenk glassware equipped with an 8-mm PTFE vacuum stop-cock (Synthware) were employed. All starting materials and reagents were commercially available. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker AVANCE 400M spectrometer. The chemical shift references were as following: (^{1}H) $CDCl_3$, 7.26 ppm ($CHCl_3$); (^{13}C) $CDCl_3$, 77.00 ppm ($CDCl_3$). IR spectra were obtained using an FT-IR instrument (Nicolet, AVATAR360). HRMS analysis was carried out at

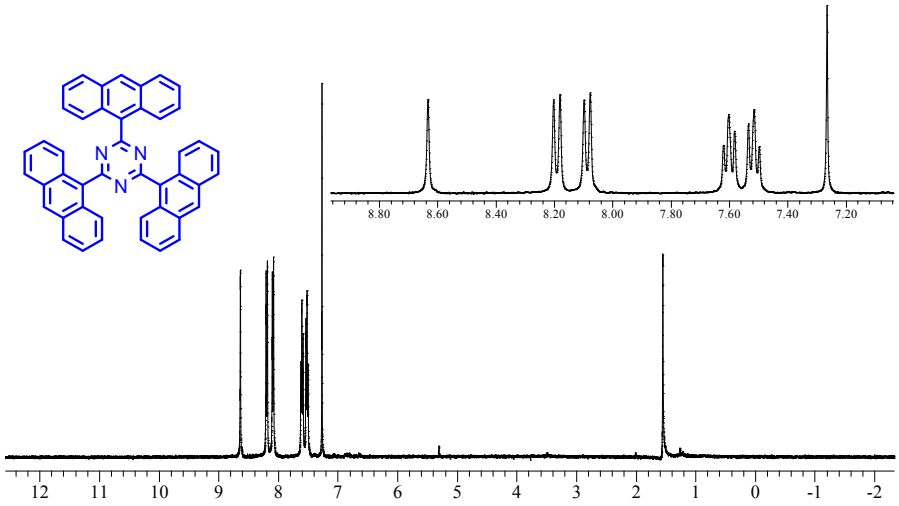
Micromass GCT (TOF MS EI^+). Melting point determination was taken on a Melt-Temp apparatus (X-6) from Beijing Fukai Instrument Plant and was uncorrected. Absorption spectra were recorded using a Lambdo 35 (Perk Elmer) spectrophotometer. Emission spectroscopy was carried out using a Fluoro SENS-9000 luminescence spectrometer. The fluoresence lifetimes were measured on a Combined Fluoresence Lifetime and Steady State Spectrometer (FLS920) with λ_{ex} = 367.4 nm and pulse widith of 875.8 ps. The concentrations of **TAT**, **3** and **4** are 1E-5 M in THF at room temperature. Suprasil quartz cells with a 10-mm optical path were employed in all these experiments. Low-temperature fluorescence experiments were performed using a quartz Dewar and 5-mm NMR quarts tubes. Fluoresence quantum yield was determined by the steady-state fluorescence using quinine sulfate as standard (Φ_f = 0.546 in 0.1 N sulphuric acid)[s2].

2. Experimental Section

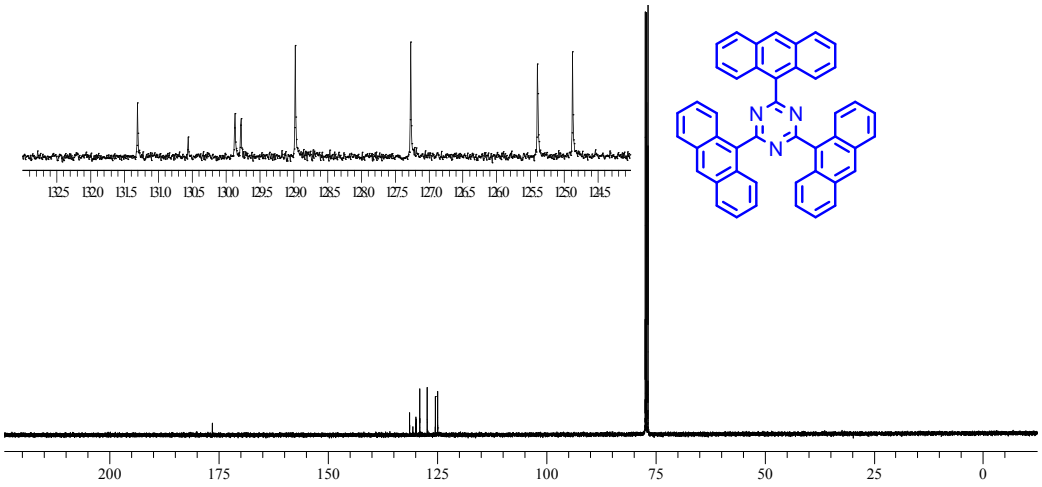
The synthetic work of Scheme 1 and 2 in manuscript has been carried out. The data are listed in Table 1 and Table 2. The following gives the synthetic procedure using $PdCl_2(dppf)_2$ as examples.

2.1 The synthesis of 2,4,6-tri(anthracen-9-yl)-1,3,5-triazine (TAT) from 1,3,5-trichlorotrizine with $PdCl_2(dppf)_2$ as example. (Entry 1, Table 1)

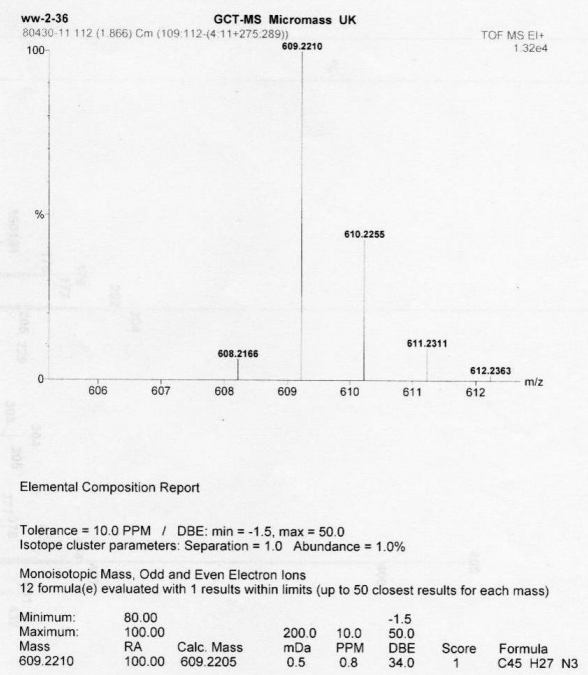
To a solution of 9-bromoanthracene (600 mg, 2.33 mmol, 3.3 equiv) in anhyd THF (30 mL), *t*-BuLi (1.5 M in pentane, 3.11 mL, 6.6 equiv) was added dropwise at –78 °C. The reaction mixture was kept at –78 °C for 2 h and warmed slowly to 0 °C. Then, 1,3,5-trichlorotrizine (130 mg, 0.71 mmol, 1 equiv), $PdCl_2$ (0.03 equiv) and dppf (0.06 equiv) were added under argon atmosphere. The reaction mixture was warmed slowly to ambient temperature first and then refluxed at 80 °C overnight. After the reaction mixture was quenched with water, the organic layer was separated, and the aqueous layer was extracted with $CHCl_3$ (3×50 mL). The combined organic layer was dried over $MgSO_4$ and purified by silica gel column chromatography with petroleum ether (60-90 ^oC)-$CHCl_3$ (1:1, v/v) as eluent to give 208 mg of **TAT** in 48% yield as yellow solid. From another reaction on 800 mg scale of **3**, 281 mg (49 %) of **TAT** was obtained. Mp > 300 °C; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.63 (3H, s), 8.19 (6H, d, *J* = 8.8 Hz), 8.08 (6H, d, *J* = 8.4 Hz), 7.60 (6H, t, *J* = 7.6 Hz), 7.51 (6H, t, *J* = 7.4 Hz); ^{13}C-NMR (100MHz, $CDCl_3$): δ 176.44, 131.28, 130.53, 129.84, 129.75, 128.95, 127.24, 125.37, 124.85; IR (KBr): 3051 (C-H) cm^{-1}. HRMS (TOF MS EI^+) m/z calcd for [$C_{45}H_{27}N_3$] 609.2205, found 609.2210.



^{1}H NMR (400 MHz, $CDCl_3$) of **TAT**



^{13}C NMR (100 MHz, $CDCl_3$) of **TAT**

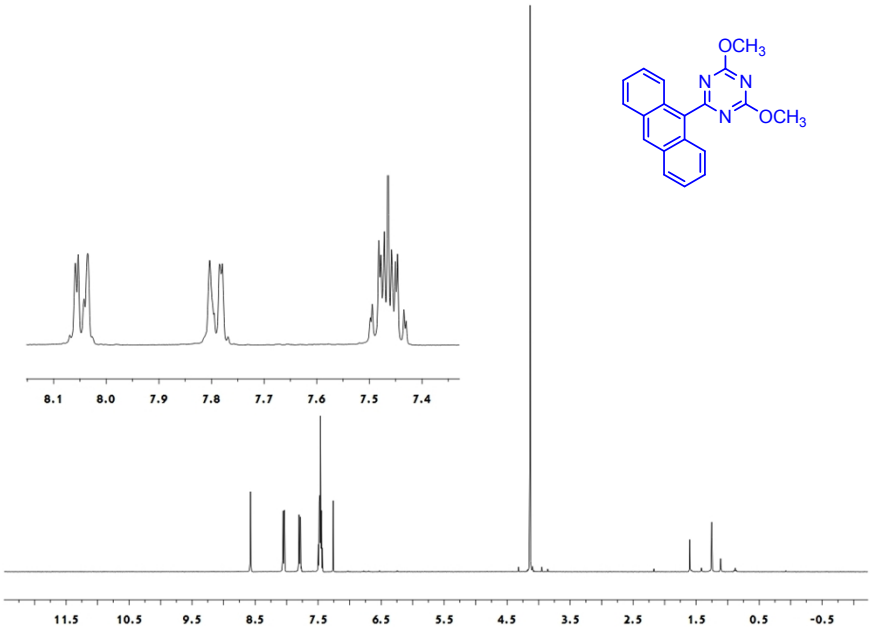


HRMS spectrum of **TAT**

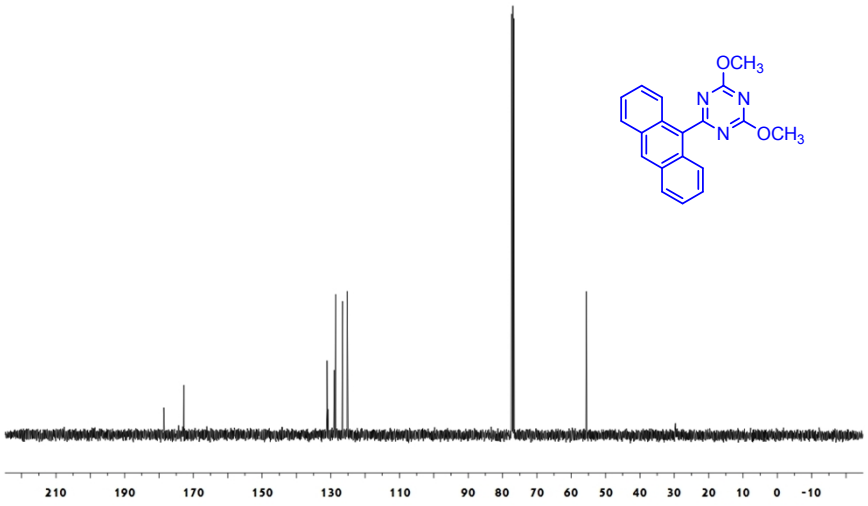
2.2 The synthesis of 2,4,6-tri(anthracen-9-yl)-1,3,5-triazine (TAT) from 2-chloro-4,6-dimethoxy-1,3,5-triazine and *1.0 equiv* 9-bromo-anthracene with $PdCl_2(dppf)_2$ as example (Entry 1, Table 2)

To a solution of 9-bromoanthracene (355.5 mg, 1.38 mmol, 1.0 equiv) in anhyd THF (50 mL), *t*-BuLi (1.67 M in pentane, 1.8 mL, 2.2 equiv) was added dropwise at –78 °C. The reaction mixture was kept at –78 °C for 2 h, then 2-chloro-4,6-dimethoxy-1,3,5-triazine (242.7 mg, 1.38 mmol, 1.0 equiv), $PdCl_2$ (0.01 equiv) and dppf (0.02 equiv) were added under argon atmosphere at –78 °C. The reaction mixture was warmed slowly to ambient temperature for 24 h. After the reaction mixture was quenched with water at 0 °C, the solvent was removed by rotary evaporator. The reaction mixture then were extracted with $CHCl_3$ (60 mL), washed by water (3×100 mL), dried over $MgSO_4$ and purified by silica gel column chromatography with petroleum ether (60-90 ^oC)-$CHCl_3$ (1:1, v/v) as eluent to give 145.6 mg (33 %) of **3** as light yellow solid. In addition, 90.7 mg (28 %) of **4** as yellow solid and 17.0 mg (6 %) of **TAT** were obtained at same time.

For **3**: Mp. 211-212 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.57 (1 H, s), 8.02-8.08 (2 H, m), 7.76-7.82 (2 H, m), 7.42-7.50 (4 H, m), 4.14 (6 H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.61, 172.78, 131.10, 130.84, 129.06, 128.97, 128.57, 126.56, 125.23, 125.11, 55.60; IR (KBr): 3045 (C-H) 1357, 1082 (C-O-C) cm^{-1}; HRMS (Tesla FTMS) m/z calcd for $[C_{19}H_{15}N_3O_2]$ 317.1164, found 318.1237 (M^++1).



^{1}H NMR (400 MHz, $CDCl_3$) of **3**



^{13}C NMR (100 MHz, $CDCl_3$) of **3**

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: IonSpec 4.7 Tesla FTMS

Card Serial Number : WI12 0251

Sample Serial Number: ZJJ-1-28-col3-col-R

Operator : HuaQin Date: 2012/01/11

Operation Mode: MALDI/DHB

Elemental Composition Search Report:

Target Mass:
Target m/z = 318.1233 ± 0.002
Charge = +1

Possible Elements:

Element	Exact Mass	Min:	Max:
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H	1.007825	0	100
N	14.003074	0	5
O	15.994915	0	5

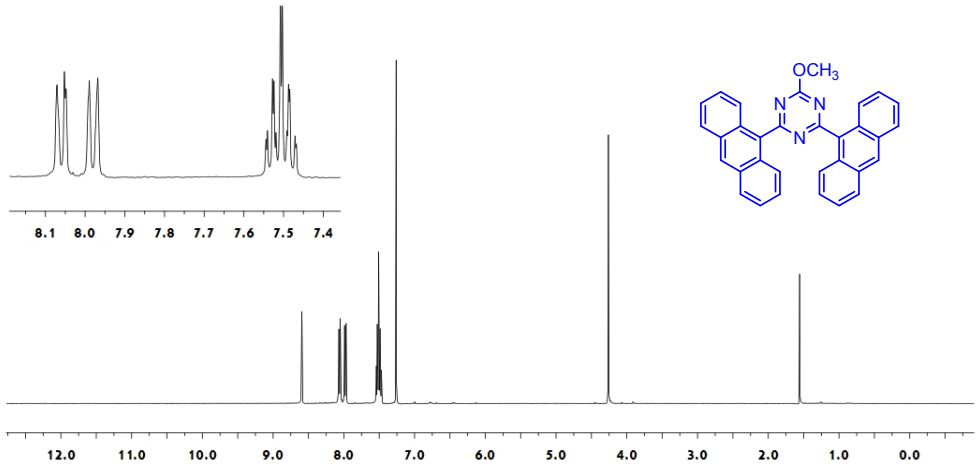
Additional Search Restrictions:
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

Search Results:
Number of Hits = 2

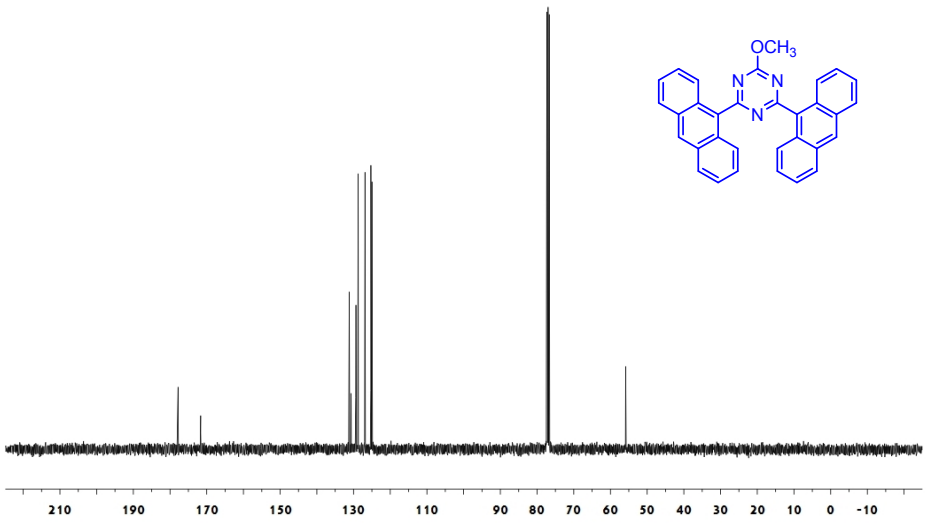
m/z	Delta m/z	DBE	Formula
318.12370	-0.00040	13.5	$C_{19}H_{16}N_3O_2^{+1}$
318.12505	-0.00175	13.0	$C_{21}H_{16}O_3^{+1}$

HRMS spectrum of **3**

For **4**: Mp. 261-262 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (2 H, s), 8.06 (4 H, d, J = 8.0 Hz), 7.78 (4 H, d, J = 8.4 Hz), 7.47-7.54 (8 H, m), 4.26 (3 H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.81, 171.66, 131.17, 130.67, 129.39, 129.34, 128.74, 126.87, 125.28, 124.98, 55.85; IR (KBr): 3049 (C-H), 1348, 1126 (C-O-C) cm^{-1}, HRMS (Tesla FTMS) m/z calcd for [$C_{32}H_{22}N_3O$] 464.1744, found 464.1757.



^{1}H NMR (400 MHz, $CDCl_3$) of **4**



^{13}C NMR (100 MHz, $CDCl_3$) of **4**

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: IonSpec 4.7 Tesla FTMS

Card Serial Number : WI12 0413

Sample Serial Number: zjj-1-36-col2-col2-c

Operator : HuaQin Date: 2012/03/22

Operation Mode: MALDI/DHB

Elemental Composition Search Report:

Target Mass:
Target m/z = 464.1744 ± 0.003
Charge = +1

Possible Elements:

Element	Exact Mass	Min.	Max.
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H	1.007825	0	100
N	14.003074	0	5
O	15.994915	0	5

Additional Search Restrictions:
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

Search Results:
Number of Hits = 4

m/z	Delta m/z	DBE	Formula
464.17574	-0.00134	23.5	$C_{39}H_{22}N_3O^{+1}$
464.17306	0.00134	19.0	$C_{29}H_{24}N_2O_4^{+1}$
464.17708	-0.00268	23.0	$C_{34}H_{24}O_2^{+1}$
464.17172	0.00268	19.5	$C_{27}H_{22}N_6O_3^{+1}$

HRMS data of **4**

2.3 The synthesis of 2,4,6-tri(anthracen-9-yl)-1,3,5-triazine (TAT) from 2-chloro-4,6-dimethoxy-1,3,5-triazine and *2.0 equiv* 9-bromo-anthracene with $PdCl_2(dppf)_2$ as example (Entry 2, Table 2)

Same procedure to the case of Entry 1, Table 2 was employed. The only difference is that 2.0 equiv 9-bromoanthracene and 4.4 equiv of *t*-BuLi were used for the reaction. On the scale of 44.9 mg (1.0 equiv) of 2-chloro-4,6-dimethoxy-1,3,5-triazine, 29.0 mg of **4** (28 %) and 13.6 mg of **TAT** (11 %) were obtained. In addition, a trace of **3** (2.0 mg, 1 %) was achieved at same time.

2.4 The synthesis of 2,4,6-tri(anthracen-9-yl)-1,3,5-triazine (TAT) from 2-chloro-4,6-

dimethoxy-1,3,5-triazine and *3.0 equiv* 9-bromo-anthracene with $PdCl_2(dppf)_2$ as example (Entry 3, Table 2)

Same procedure to the case of Entry 2, Table 2 was employed. The only difference is that 3.0 equiv 9-bromoanthracene and 6.6 equiv of *t*-BuLi were used for the reaction. On the scale of 57.6 mg (1.0 equiv) of 2-chloro-4,6-dimethoxy-1,3,5-triazine, 78.9 mg (40 %) of **TAT** was obtained.

3. Crystal Analysis of 3 and 4

Table 1. Crystal data and structure refinement for **3**.

Identification code	**3**
Empirical formula	C19 H15 N3 O2
Formula weight	317.34
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.2169(8) A alpha = 65.807(2) deg. b = 9.6220(9) A beta = 72.714(2) deg. c = 11.5715(11) A gamma = 89.496(2) deg.
Volume	790.10(13) A^3
Z, Calculated density	2, 1.334 Mg/m^3
Absorption coefficient	0.089 mm^-1
F(000)	332
Crystal size	0.52 x 0.42 x 0.37 mm
Theta range for data collection	2.04 to 25.00 deg.
Limiting indices	-8<=h<=9, -11<=k<=11, -13<=l<=13
Reflections collected / unique	3946 / 2752 [R(int) = 0.0096]
Completeness to theta = 25.00	98.9 %
Absorption correction	None
Max. and min. transmission	0.9678 and 0.9552
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2752 / 0 / 217
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.1062
R indices (all data)	R1 = 0.0578, wR2 = 0.1142
Largest diff. peak and hole	0.104 and -0.209 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for A. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)

N(1)	167(2)	1479(1)	5645(1)	48(1)
C(19)	2075(2)	-2348(2)	9334(1)	38(1)
C(7)	1614(2)	-3737(2)	8067(1)	38(1)
C(3)	-923(2)	224(2)	6511(1)	41(1)
O(2)	2836(1)	2651(1)	4880(1)	60(1)
N(3)	-584(1)	-1046(1)	7405(1)	40(1)
C(6)	1584(2)	-2399(2)	8287(1)	37(1)
C(14)	2629(2)	-3684(2)	10185(2)	43(1)
C(12)	2181(2)	-5058(2)	8927(1)	42(1)
O(1)	-2508(1)	309(1)	6439(1)	55(1)
N(2)	2283(2)	194(1)	6544(1)	43(1)
C(4)	1735(2)	1384(2)	5730(1)	43(1)
C(5)	1064(2)	-1001(2)	7361(1)	37(1)
C(8)	1147(2)	-3833(2)	7009(2)	46(1)
C(18)	2028(2)	-1033(2)	9608(2)	48(1)
C(13)	2665(2)	-4991(2)	9959(2)	48(1)
C(17)	2524(2)	-1034(2)	10624(2)	60(1)
C(9)	1228(2)	-5137(2)	6827(2)	56(1)
C(10)	1773(2)	-6430(2)	7678(2)	61(1)
C(16)	3085(2)	-2344(2)	11453(2)	67(1)
C(11)	2233(2)	-6401(2)	8691(2)	56(1)
C(15)	3130(2)	-3620(2)	11245(2)	59(1)
C(2)	4583(2)	2678(2)	4890(2)	77(1)
C(1)	-3785(2)	-990(2)	7342(2)	62(1)

Table 3. Bond lengths [A] and angles [deg] for A.

N(1)-C(4)	1.3204(19)
N(1)-C(3)	1.3265(19)
C(19)-C(6)	1.4052(19)
C(19)-C(18)	1.422(2)
C(19)-C(14)	1.431(2)
C(7)-C(6)	1.4096(19)
C(7)-C(8)	1.425(2)
C(7)-C(12)	1.433(2)
C(3)-N(3)	1.3304(18)
C(3)-O(1)	1.3290(17)
O(2)-C(4)	1.3339(17)
O(2)-C(2)	1.440(2)
N(3)-C(5)	1.3398(17)
C(6)-C(5)	1.4898(19)
C(14)-C(13)	1.385(2)

C(14)-C(15)	1.428(2)
C(12)-C(13)	1.389(2)
C(12)-C(11)	1.423(2)
O(1)-C(1)	1.4336(19)
N(2)-C(4)	1.3272(18)
N(2)-C(5)	1.3367(17)
C(8)-C(9)	1.353(2)
C(8)-H(8A)	0.9300
C(18)-C(17)	1.353(2)
C(18)-H(18A)	0.9300
C(13)-H(13A)	0.9300
C(17)-C(16)	1.408(2)
C(17)-H(17A)	0.9300
C(9)-C(10)	1.402(2)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.346(2)
C(10)-H(10A)	0.9300
C(16)-C(15)	1.343(2)
C(16)-H(16A)	0.9300
C(11)-H(11A)	0.9300
C(15)-H(15A)	0.9300
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(4)-N(1)-C(3)	113.08(12)
C(6)-C(19)-C(18)	123.20(13)
C(6)-C(19)-C(14)	118.95(13)
C(18)-C(19)-C(14)	117.85(13)
C(6)-C(7)-C(8)	123.22(13)
C(6)-C(7)-C(12)	118.70(13)
C(8)-C(7)-C(12)	118.06(13)
N(1)-C(3)-N(3)	127.07(13)
N(1)-C(3)-O(1)	113.62(13)
N(3)-C(3)-O(1)	119.31(13)
C(4)-O(2)-C(2)	118.39(13)
C(3)-N(3)-C(5)	113.57(12)
C(19)-C(6)-C(7)	121.38(13)
C(19)-C(6)-C(5)	119.70(12)
C(7)-C(6)-C(5)	118.90(12)
C(13)-C(14)-C(15)	122.12(14)
C(13)-C(14)-C(19)	119.33(13)

C(15)-C(14)-C(19)	118.55(14)
C(13)-C(12)-C(11)	122.17(14)
C(13)-C(12)-C(7)	119.30(13)
C(11)-C(12)-C(7)	118.53(14)
C(3)-O(1)-C(1)	117.84(12)
C(4)-N(2)-C(5)	113.93(12)
N(1)-C(4)-N(2)	127.10(14)
N(1)-C(4)-O(2)	113.63(13)
N(2)-C(4)-O(2)	119.27(13)
N(2)-C(5)-N(3)	125.22(13)
N(2)-C(5)-C(6)	117.29(12)
N(3)-C(5)-C(6)	117.48(12)
C(9)-C(8)-C(7)	120.88(15)
C(9)-C(8)-H(8A)	119.6
C(7)-C(8)-H(8A)	119.6
C(17)-C(18)-C(19)	121.15(15)
C(17)-C(18)-H(18A)	119.4
C(19)-C(18)-H(18A)	119.4
C(14)-C(13)-C(12)	122.34(14)
C(14)-C(13)-H(13A)	118.8
C(12)-C(13)-H(13A)	118.8
C(18)-C(17)-C(16)	120.96(16)
C(18)-C(17)-H(17A)	119.5
C(16)-C(17)-H(17A)	119.5
C(8)-C(9)-C(10)	120.81(16)
C(8)-C(9)-H(9A)	119.6
C(10)-C(9)-H(9A)	119.6
C(11)-C(10)-C(9)	120.74(15)
C(11)-C(10)-H(10A)	119.6
C(9)-C(10)-H(10A)	119.6
C(15)-C(16)-C(17)	120.12(16)
C(15)-C(16)-H(16A)	119.9
C(17)-C(16)-H(16A)	119.9
C(10)-C(11)-C(12)	120.98(15)
C(10)-C(11)-H(11A)	119.5
C(12)-C(11)-H(11A)	119.5
C(16)-C(15)-C(14)	121.36(16)
C(16)-C(15)-H(15A)	119.3
C(14)-C(15)-H(15A)	119.3
O(2)-C(2)-H(2A)	109.5
O(2)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
O(2)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5

H(2B)-C(2)-H(2C)	109.5
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for A. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	48(1)	46(1)	44(1)	-12(1)	-18(1)	10(1)
C(19)	32(1)	39(1)	41(1)	-16(1)	-12(1)	6(1)
C(7)	31(1)	40(1)	38(1)	-15(1)	-7(1)	4(1)
C(3)	41(1)	47(1)	42(1)	-22(1)	-17(1)	14(1)
O(2)	54(1)	48(1)	56(1)	-7(1)	-10(1)	-3(1)
N(3)	38(1)	41(1)	42(1)	-17(1)	-16(1)	9(1)
C(6)	30(1)	39(1)	39(1)	-15(1)	-10(1)	6(1)
C(14)	40(1)	46(1)	43(1)	-17(1)	-16(1)	10(1)
C(12)	39(1)	39(1)	44(1)	-16(1)	-9(1)	6(1)
O(1)	41(1)	61(1)	60(1)	-19(1)	-25(1)	14(1)
N(2)	39(1)	41(1)	43(1)	-15(1)	-12(1)	5(1)
C(4)	46(1)	41(1)	38(1)	-14(1)	-10(1)	5(1)
C(5)	38(1)	40(1)	38(1)	-20(1)	-13(1)	8(1)
C(8)	47(1)	48(1)	44(1)	-21(1)	-15(1)	6(1)
C(18)	53(1)	44(1)	50(1)	-22(1)	-18(1)	11(1)
C(13)	51(1)	43(1)	49(1)	-14(1)	-21(1)	15(1)
C(17)	72(1)	60(1)	63(1)	-36(1)	-28(1)	11(1)
C(9)	64(1)	59(1)	54(1)	-31(1)	-19(1)	5(1)
C(10)	77(1)	47(1)	65(1)	-34(1)	-15(1)	7(1)
C(16)	78(1)	80(1)	64(1)	-41(1)	-38(1)	16(1)
C(11)	65(1)	39(1)	57(1)	-19(1)	-15(1)	10(1)
C(15)	64(1)	66(1)	53(1)	-23(1)	-33(1)	18(1)
C(2)	52(1)	70(1)	85(1)	-19(1)	-7(1)	-12(1)
C(1)	40(1)	73(1)	71(1)	-26(1)	-22(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for

A.

	x	y	z	U(eq)
H(8A)	780	-2987	6435	55
H(18A)	1650	-159	9081	58
H(13A)	3025	-5856	10516	58
H(17A)	2494	-156	10777	72
H(9A)	919	-5176	6129	68
H(10A)	1816	-7318	7540	74
H(16A)	3425	-2325	12145	80
H(11A)	2590	-7270	9246	67
H(15A)	3495	-4481	11803	70
H(2A)	5225	3654	4238	115
H(2B)	5094	1875	4678	115
H(2C)	4596	2522	5762	115
H(1A)	-4865	-779	7190	93
H(1B)	-3901	-1184	8247	93
H(1C)	-3442	-1875	7194	93

Table 1. Crystal data and structure refinement for **4**.

Identification code	**4**
Empirical formula	C32 H21 N3 O
Formula weight	463.52
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.930(3) A alpha = 90 deg. b = 17.081(7) A beta = 100.949(8) deg. c = 17.894(7) A gamma = 90 deg.
Volume	2379.6(17) A^3
Z, Calculated density	4, 1.294 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	968
Crystal size	0.50 x 0.17 x 0.13 mm
Theta range for data collection	1.66 to 28.13 deg.
Limiting indices	-10<=h<=10, -12<=k<=22, -23<=l<=21
Reflections collected / unique	14365 / 5654 [R(int) = 0.0741]
Completeness to theta = 28.13	97.1 %
Absorption correction	None
Max. and min. transmission	0.9898 and 0.9614
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5654 / 0 / 325

Goodness-of-fit on F^2	0.926
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1171
R indices (all data)	R1 = 0.1587, wR2 = 0.1544
Largest diff. peak and hole	0.188 and -0.203 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for A. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O	8311(2)	1024(1)	1494(1)	53(1)
N(2)	9128(2)	1503(1)	415(1)	40(1)
C(19)	10058(3)	2072(1)	-687(1)	38(1)
C(3)	9269(3)	2158(1)	6(1)	37(1)
C(2)	8448(3)	1622(1)	1028(1)	39(1)
N(3)	8774(2)	2873(1)	180(1)	43(1)
C(20)	9167(3)	2368(1)	-1393(1)	40(1)
N(1)	7861(2)	2300(1)	1251(1)	46(1)
C(27)	12495(3)	1692(1)	-1282(1)	44(1)
C(4)	8065(3)	2909(1)	806(1)	40(1)
C(31)	12687(3)	1412(1)	70(1)	51(1)
C(5)	7457(3)	3685(1)	1029(1)	45(1)
C(32)	11711(3)	1722(1)	-620(1)	41(1)
C(25)	9972(3)	2316(1)	-2048(1)	44(1)
C(26)	11603(3)	1990(1)	-1972(1)	51(1)
C(18)	8616(4)	4168(1)	1525(1)	49(1)
C(28)	14156(3)	1349(2)	-1221(2)	58(1)
C(22)	6654(3)	2941(2)	-2198(1)	55(1)
C(24)	9063(4)	2594(2)	-2766(1)	55(1)
C(6)	5750(3)	3919(1)	765(1)	49(1)
C(13)	8030(4)	4899(2)	1777(2)	63(1)
C(11)	5168(4)	4656(2)	1013(2)	61(1)
C(29)	15019(3)	1058(2)	-554(2)	63(1)
C(21)	7479(3)	2693(1)	-1502(1)	49(1)
C(30)	14273(3)	1093(2)	103(2)	57(1)
C(23)	7466(4)	2890(2)	-2838(1)	59(1)
C(17)	10367(4)	3961(2)	1791(1)	60(1)
C(7)	4555(4)	3459(2)	246(2)	60(1)
C(14)	9217(6)	5382(2)	2282(2)	81(1)
C(12)	6325(5)	5115(2)	1517(2)	71(1)
C(1)	8940(4)	268(1)	1313(2)	67(1)
C(10)	3439(5)	4891(2)	722(2)	81(1)
C(15)	10860(6)	5146(2)	2519(2)	89(1)
C(16)	11453(4)	4435(2)	2275(2)	74(1)

C(9)	2357(4)	4433(2)	223(2)	83(1)
C(8)	2922(4)	3709(2)	-16(2)	77(1)

Table 3. Bond lengths [A] and angles [deg] for A.

O-C(2)	1.335(2)
O-C(1)	1.444(3)
N(2)-C(2)	1.328(3)
N(2)-C(3)	1.353(3)
C(19)-C(20)	1.418(3)
C(19)-C(32)	1.425(3)
C(19)-C(3)	1.499(3)
C(3)-N(3)	1.338(3)
C(2)-N(1)	1.337(3)
N(3)-C(4)	1.347(3)
C(20)-C(25)	1.440(3)
C(20)-C(21)	1.428(3)
N(1)-C(4)	1.338(3)
C(27)-C(26)	1.396(3)
C(27)-C(32)	1.440(3)
C(27)-C(28)	1.427(3)
C(4)-C(5)	1.491(3)
C(31)-C(30)	1.362(3)
C(31)-C(32)	1.429(3)
C(31)-H(31A)	0.9300
C(5)-C(6)	1.404(3)
C(5)-C(18)	1.414(3)
C(25)-C(26)	1.391(3)
C(25)-C(24)	1.430(3)
C(26)-H(26A)	0.9300
C(18)-C(17)	1.424(4)
C(18)-C(13)	1.436(3)
C(28)-C(29)	1.353(4)
C(28)-H(28A)	0.9300
C(22)-C(21)	1.359(3)
C(22)-C(23)	1.418(3)
C(22)-H(22A)	0.9300
C(24)-C(23)	1.347(3)
C(24)-H(24A)	0.9300
C(6)-C(7)	1.429(4)
C(6)-C(11)	1.440(3)
C(13)-C(12)	1.393(4)

C(13)-C(14)	1.435(4)
C(11)-C(12)	1.399(4)
C(11)-C(10)	1.429(4)
C(29)-C(30)	1.415(3)
C(29)-H(29A)	0.9300
C(21)-H(21A)	0.9300
C(30)-H(30A)	0.9300
C(23)-H(23A)	0.9300
C(17)-C(16)	1.365(4)
C(17)-H(17A)	0.9300
C(7)-C(8)	1.360(4)
C(7)-H(7A)	0.9300
C(14)-C(15)	1.353(5)
C(14)-H(14A)	0.9300
C(12)-H(12A)	0.9300
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(10)-C(9)	1.360(4)
C(10)-H(10A)	0.9300
C(15)-C(16)	1.402(4)
C(15)-H(15A)	0.9300
C(16)-H(16A)	0.9300
C(9)-C(8)	1.410(4)
C(9)-H(9A)	0.9300
C(8)-H(8A)	0.9300
C(2)-O-C(1)	118.17(18)
C(2)-N(2)-C(3)	114.13(19)
C(20)-C(19)-C(32)	121.29(19)
C(20)-C(19)-C(3)	119.1(2)
C(32)-C(19)-C(3)	119.6(2)
N(3)-C(3)-N(2)	124.85(19)
N(3)-C(3)-C(19)	118.0(2)
N(2)-C(3)-C(19)	117.17(19)
N(2)-C(2)-N(1)	126.7(2)
N(2)-C(2)-O	119.5(2)
N(1)-C(2)-O	113.72(19)
C(3)-N(3)-C(4)	114.98(19)
C(19)-C(20)-C(25)	118.7(2)
C(19)-C(20)-C(21)	123.8(2)
C(25)-C(20)-C(21)	117.5(2)
C(2)-N(1)-C(4)	114.09(18)
C(26)-C(27)-C(32)	119.3(2)
C(26)-C(27)-C(28)	121.5(2)

C(32)-C(27)-C(28)	119.2(2)
N(1)-C(4)-N(3)	125.2(2)
N(1)-C(4)-C(5)	116.80(18)
N(3)-C(4)-C(5)	118.0(2)
C(30)-C(31)-C(32)	122.0(2)
C(30)-C(31)-H(31A)	119.0
C(32)-C(31)-H(31A)	119.0
C(6)-C(5)-C(18)	121.1(2)
C(6)-C(5)-C(4)	120.2(2)
C(18)-C(5)-C(4)	118.8(2)
C(27)-C(32)-C(31)	116.8(2)
C(27)-C(32)-C(19)	118.7(2)
C(31)-C(32)-C(19)	124.6(2)
C(26)-C(25)-C(20)	119.5(2)
C(26)-C(25)-C(24)	121.4(2)
C(20)-C(25)-C(24)	119.0(2)
C(25)-C(26)-C(27)	122.5(2)
C(25)-C(26)-H(26A)	118.7
C(27)-C(26)-H(26A)	118.7
C(5)-C(18)-C(17)	122.8(2)
C(5)-C(18)-C(13)	119.6(3)
C(17)-C(18)-C(13)	117.6(3)
C(29)-C(28)-C(27)	121.6(2)
C(29)-C(28)-H(28A)	119.2
C(27)-C(28)-H(28A)	119.2
C(21)-C(22)-C(23)	120.4(2)
C(21)-C(22)-H(22A)	119.8
C(23)-C(22)-H(22A)	119.8
C(23)-C(24)-C(25)	121.0(2)
C(23)-C(24)-H(24A)	119.5
C(25)-C(24)-H(24A)	119.5
C(5)-C(6)-C(7)	122.7(2)
C(5)-C(6)-C(11)	119.3(3)
C(7)-C(6)-C(11)	118.0(3)
C(12)-C(13)-C(14)	122.5(3)
C(12)-C(13)-C(18)	118.5(3)
C(14)-C(13)-C(18)	119.0(3)
C(12)-C(11)-C(10)	123.0(3)
C(12)-C(11)-C(6)	118.7(3)
C(10)-C(11)-C(6)	118.3(3)
C(28)-C(29)-C(30)	119.8(3)
C(28)-C(29)-H(29A)	120.1
C(30)-C(29)-H(29A)	120.1
C(22)-C(21)-C(20)	121.5(2)

C(22)-C(21)-H(21A)	119.3
C(20)-C(21)-H(21A)	119.3
C(31)-C(30)-C(29)	120.6(3)
C(31)-C(30)-H(30A)	119.7
C(29)-C(30)-H(30A)	119.7
C(24)-C(23)-C(22)	120.6(2)
C(24)-C(23)-H(23A)	119.7
C(22)-C(23)-H(23A)	119.7
C(16)-C(17)-C(18)	121.5(3)
C(16)-C(17)-H(17A)	119.2
C(18)-C(17)-H(17A)	119.2
C(8)-C(7)-C(6)	121.5(3)
C(8)-C(7)-H(7A)	119.3
C(6)-C(7)-H(7A)	119.3
C(15)-C(14)-C(13)	120.3(3)
C(15)-C(14)-H(14A)	119.8
C(13)-C(14)-H(14A)	119.8
C(13)-C(12)-C(11)	122.9(3)
C(13)-C(12)-H(12A)	118.6
C(11)-C(12)-H(12A)	118.6
O-C(1)-H(1A)	109.5
O-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(9)-C(10)-C(11)	121.3(3)
C(9)-C(10)-H(10A)	119.3
C(11)-C(10)-H(10A)	119.3
C(14)-C(15)-C(16)	121.3(3)
C(14)-C(15)-H(15A)	119.3
C(16)-C(15)-H(15A)	119.3
C(17)-C(16)-C(15)	120.2(3)
C(17)-C(16)-H(16A)	119.9
C(15)-C(16)-H(16A)	119.9
C(10)-C(9)-C(8)	120.4(3)
C(10)-C(9)-H(9A)	119.8
C(8)-C(9)-H(9A)	119.8
C(7)-C(8)-C(9)	120.5(3)
C(7)-C(8)-H(8A)	119.7
C(9)-C(8)-H(8A)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for A. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12

	U11	U22	U33	U23	U13	U12
O	72(1)	44(1)	46(1)	10(1)	19(1)	0(1)
N(2)	43(1)	44(1)	32(1)	-1(1)	7(1)	1(1)
C(19)	43(2)	40(1)	31(1)	-4(1)	11(1)	-4(1)
C(3)	37(1)	43(1)	31(1)	-2(1)	6(1)	2(1)
C(2)	43(2)	42(1)	34(1)	2(1)	7(1)	-1(1)
N(3)	54(1)	44(1)	35(1)	1(1)	18(1)	5(1)
C(20)	47(2)	42(1)	33(1)	-4(1)	11(1)	-2(1)
N(1)	56(1)	45(1)	40(1)	2(1)	21(1)	0(1)
C(27)	44(2)	47(2)	43(2)	-8(1)	15(1)	-4(1)
C(4)	46(2)	43(1)	34(1)	-4(1)	12(1)	0(1)
C(31)	46(2)	59(2)	47(2)	-2(1)	11(1)	6(1)
C(5)	63(2)	41(1)	38(1)	2(1)	28(1)	6(1)
C(32)	44(2)	41(1)	38(1)	-4(1)	11(1)	0(1)
C(25)	52(2)	47(1)	33(1)	0(1)	14(1)	-4(1)
C(26)	57(2)	59(2)	41(2)	-6(1)	24(1)	-6(1)
C(18)	73(2)	39(1)	43(1)	1(1)	28(1)	3(1)
C(28)	51(2)	66(2)	63(2)	-9(2)	25(2)	1(2)
C(22)	52(2)	66(2)	45(2)	6(1)	4(1)	5(1)
C(24)	73(2)	61(2)	32(1)	-1(1)	15(1)	-6(2)
C(6)	60(2)	45(2)	50(2)	3(1)	28(1)	4(1)
C(13)	92(2)	49(2)	57(2)	-3(1)	38(2)	2(2)
C(11)	72(2)	52(2)	68(2)	9(2)	43(2)	17(2)
C(29)	41(2)	67(2)	83(2)	-10(2)	19(2)	3(1)
C(21)	51(2)	60(2)	38(1)	0(1)	13(1)	5(1)
C(30)	48(2)	64(2)	56(2)	-1(1)	-1(1)	6(1)
C(23)	70(2)	69(2)	37(2)	9(1)	3(1)	0(2)
C(17)	80(2)	52(2)	52(2)	-2(1)	26(2)	-4(2)
C(7)	59(2)	51(2)	77(2)	7(2)	28(2)	6(2)
C(14)	127(3)	53(2)	73(2)	-20(2)	41(2)	-12(2)
C(12)	108(3)	46(2)	72(2)	-5(2)	49(2)	11(2)
C(1)	86(2)	44(2)	72(2)	11(1)	14(2)	3(2)
C(10)	89(3)	68(2)	100(3)	17(2)	57(2)	29(2)
C(15)	118(3)	74(2)	76(2)	-18(2)	24(2)	-26(2)
C(16)	84(2)	74(2)	65(2)	-8(2)	17(2)	-18(2)
C(9)	62(2)	83(2)	113(3)	30(2)	37(2)	25(2)
C(8)	61(2)	68(2)	106(3)	18(2)	24(2)	8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

for

A.

	x	y	z	U(eq)
H(31A)	12225	1429	510	61
H(26A)	12118	1969	-2397	61
H(28A)	14658	1326	-1650	69
H(22A)	5549	3145	-2255	66
H(24A)	9581	2569	-3190	66
H(29A)	16099	835	-528	75
H(21A)	6932	2736	-1088	59
H(30A)	14871	896	562	69
H(23A)	6891	3064	-3310	71
H(17A)	10780	3492	1632	71
H(7A)	4902	2978	84	73
H(14A)	8856	5858	2447	98
H(12A)	5939	5585	1687	85
H(1A)	8765	-105	1693	101
H(1B)	10143	304	1304	101
H(1C)	8329	101	824	101
H(10A)	3045	5366	876	97
H(15A)	11612	5462	2850	106
H(16A)	12589	4285	2444	89
H(9A)	1238	4600	40	100
H(8A)	2171	3400	-356	93

4. Theoretical calculations of TAT at B3LYP/6-31G(d) level

Electronic structure calculations were carried out with the B3LYP functional and 6-31G(d) basis set for all atoms. For each stationary point, harmonic frequencies were computed at the fully optimized geometries, which allowed the assignment of the structures as minima. Absorption spectra were computed considering the fifty vertical excitations from the ground state by using time-dependent density functional linear response theory (TDDFT) in conjunction with a conductor-like polarizable continuum model (CPCM),[S3,S4] which has been proved to give the better results for common organic compounds. All these calculations were performed with Gaussian 03.[S5]

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