Electronic Supplementary Information (ESI)

The solution ESR spectra at room temperature, the time-profiles of TRESR, the spin density distribution of the ground states, the details of the synthetic procedures and X-ray crystallographic data of **1*m*** and **1*p*** are shown here.

S1. Conventional ESR spectra

The conventional solution ESR spectra of **1*m*** and **1*p*** were measured at room temperature using toluene as a solvent.

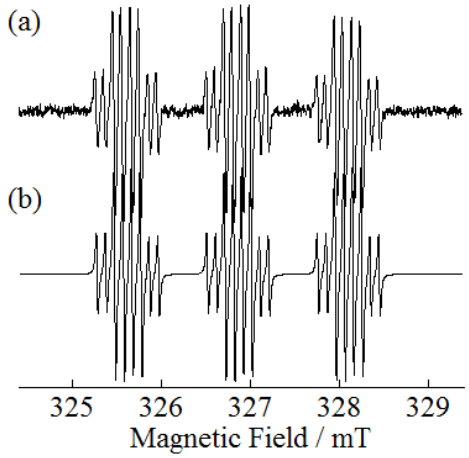

Fig.S1 Typical solution ESR spectrum of **1*m*** observed at room temperature. Toluene was used as the solvent. The microwave frequency is 9.3870 GHz.(a) Observed spectrum, (b) simulation. The *g* value and hyperfine coupling constants are shown in main text.

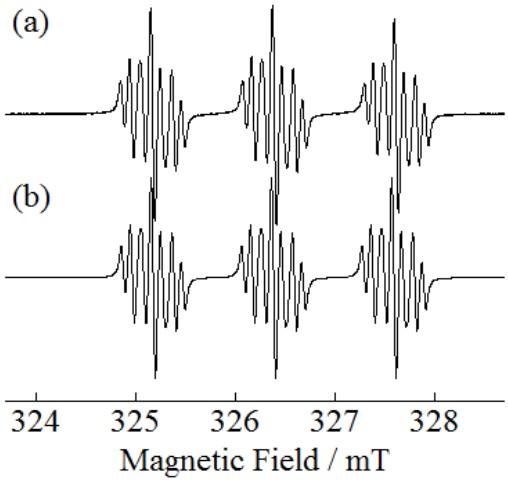

Fig.S2 Typical solution ESR spectrum of **1*p*** observed at room temperature. Toluene was used as the solvent. The microwave frequency is 9.16320 GHz GHz.(a) Observed spectrum, (b) simulation. The *g* value and hyperfine coupling constants are shown in main text.

S2. Another assignment of the TRESR spectrum of 1*p*.

Fig. S3 shows the energy level diagram calculated for $g = 2.005$, $D = 0.025$ cm^{-1}, and $E = 0.001$ cm^{-1} in eq. (1). In this case, the XY signals in Fig.4 split to X and Y signals. When the selective population (DEP) shown in this figure is assumed (Selective population of Ms = ±3/2 sublevels for H // X), only the signals arising from the external magnetic field being parallel to the X direction of the fine-structure tensor give *e*/*a* pattern, leading to the spectral pattern of Fig. S5(d) (*aae*/*aee*). This expected spectral pattern resembles to the observed TRESR in Fig. 4. However, at the moment, we cannot present the reasonable mechanism of such a dynamic electron spin polarization (DEP). The usual selective DEP originating from the (enhanced) intersystem crossing will give *aaa*/*eee* or *eee*/*aaa* pattern [S1] and the pattern through the quantum mixed state such as spin-separated triplet-radical pair leads to *aee*/*eaa* or *eaa*/*aee* pattern [S2].

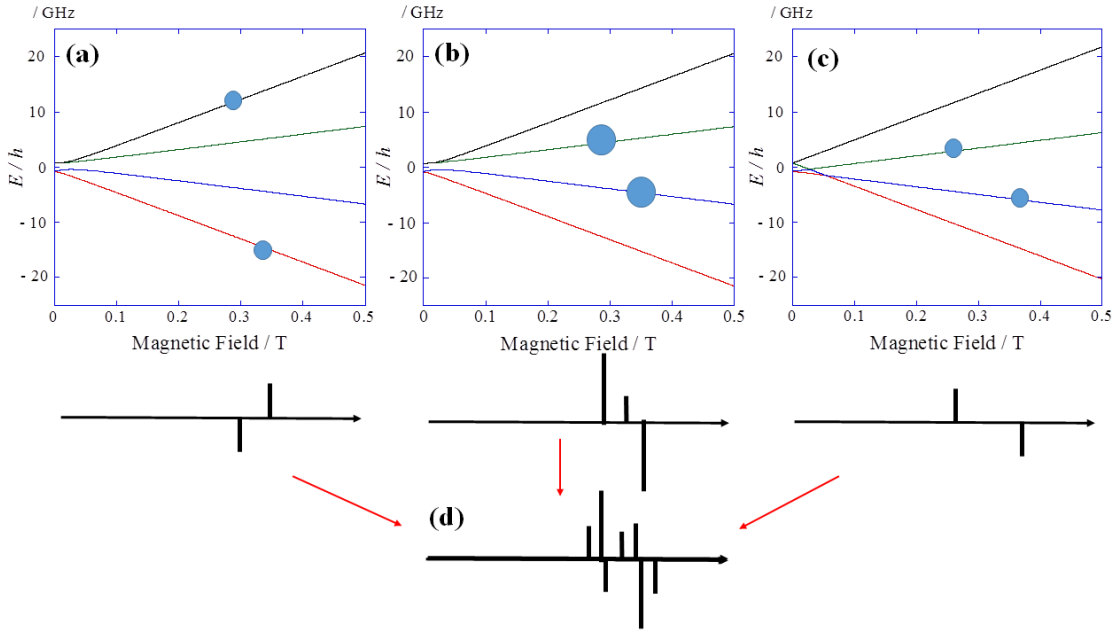

Fig. S3 Energy diagrams and possible DEP pattern of **1*m***. (a) H // X direction (there resonance fields are 299.78 (*e*), 321.41 (–), and 346.66 mT). (*a*). (b) H // Y direction (293.34 (*a*), 321.68 (*wa*), and 353.07 (*e*) mT)., (c) H // Z direction (269.78 (*a*), 323.20 (very weak *a*), and 376.64 (*e*) mT), and (d) Possible TRESR spectral pattern arising from the unique DEP shown in (a)-(c). Here, *a* and *e* are absorption and emission of the microwave, respecively.

[S1] (a)Y. Teki, S. Miyamoto, K. Iimura, M. Nakatsuji and Y. Miura, *J. Am. Chem. Soc*. 2000, **122**, 984. (b) Y. Teki, S. Miyamoto, K. Iimura, M. Nakatsuji and Y. Miura, *J. Am. Chem. Soc*. 2001, **123**, 294.

[S2] (a) Y. Teki, H. Tamekuni, J. Takeuchi and Y. Miura, *Angew. Chem. Int. Ed.*, 2006, **45**, 4666; (b) Y. Teki, H. Tamekuni, K. Haruta, J. Takeuchi and Y. Miura, *J. Mater. Chem*. 2008, **18,** 381.

S3. Comparison between cw-ESR and TRESR spectra of 1*p*.

Fig. S4 shows the comparison of the cw-SR spectrum at 30 K and the TRESR spectrum at 30 K of **1*p***. In order to compare both spectra, a spline interpolation was carried out for the TRESR as shown in Fig. S5(c). This comparison shows that the TRESR spectrum was broader than that of the integrated cw-ESR spectrum. The shoulder in cw-ESR at 323 mT was also clearly observed in the TRESR spectrum but higher-field shoulder of the cw-ESR at 327 mT was disappeared. These findings indicate the overlapping of the polarized doublet ground-state signal and the excited doublet signal with a little smaller g value in the TRESR spectrum.

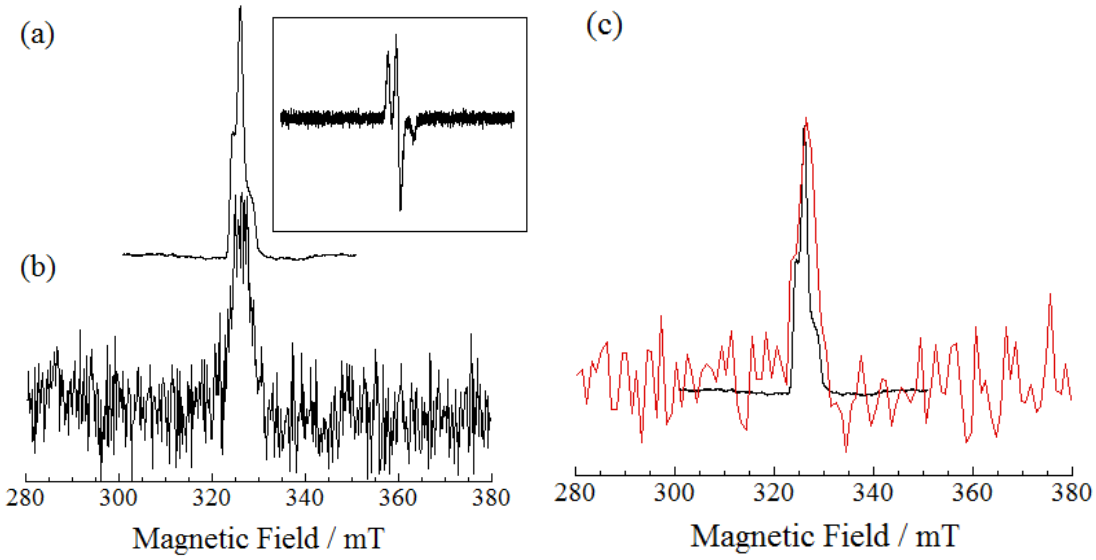

Fig. S4 Comparison between cw-ESR and TRESR spectra of **1*p***. (a) Integrated cw-ESR at 30 K. The cut shows the original cw-ESR spectrum. The microwave frequency is 9157.15 MHz. (b) TRESR at 30 K. The microwave frequency is 9157.1 MHz.. (c) Comparison between the integrated cw-ESR spectrum and spline-interpolated TRESR spectrum.

S4. Time variation of TRESR spectra

Fig. S5(a) and S5(b) show the time variation of the TRESR spectra of **1*m*** and **1*p***, respectively.

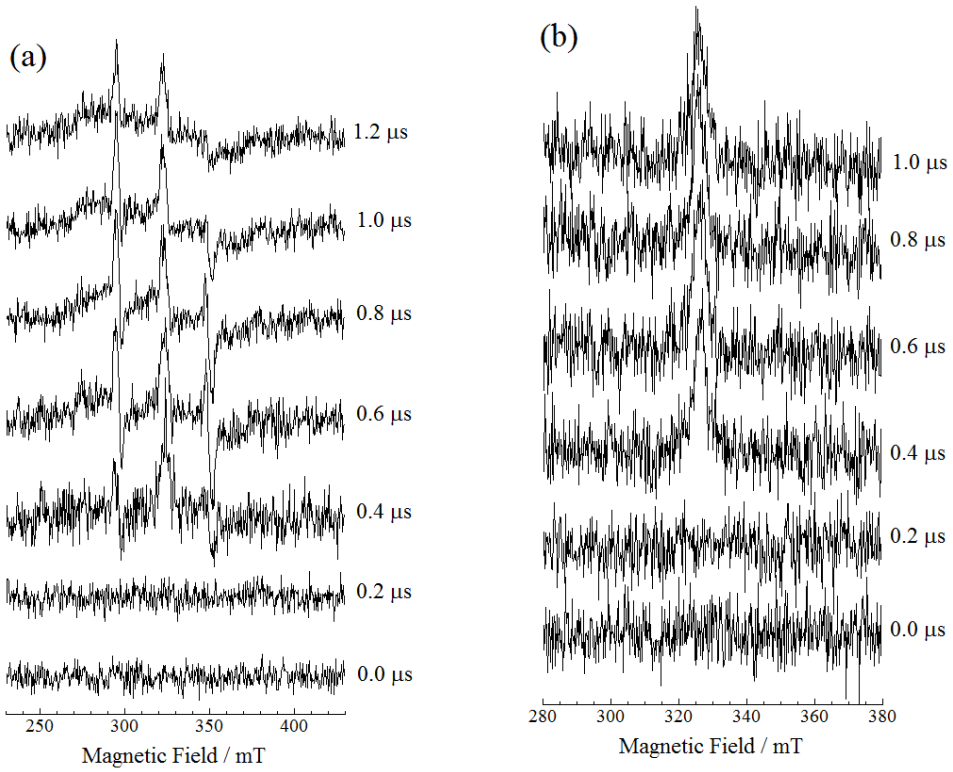

Fig.S5 Time variation of the TRESR spectra. (a) **1*m***, (b)**1*p***

S5. Time profiles of the TRESR spectra

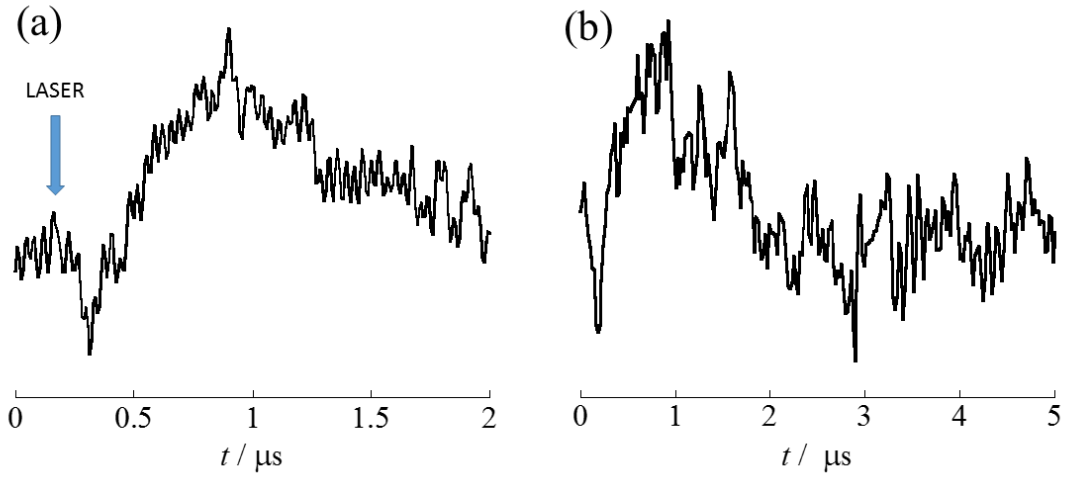

Fig.S6 Time profiles of the TRESR signals of **1*m*** and **1*p***. (a) Signal of **1*m*** at 295.23 mT, (b) Signal of **1*p***. at 325.82 mT. The time at LASER excitation in (a) is estimated from the raising position of the TRESR signal.

S6. Spin density distribution in the ground state

Fig. S7 shows the spin density distributions of the doublet ground states of **1*m*** and **1*p*** calculated by Gaussian 98W using the density functional theory (UBecke 3LYP) and the basis set 6-31G.

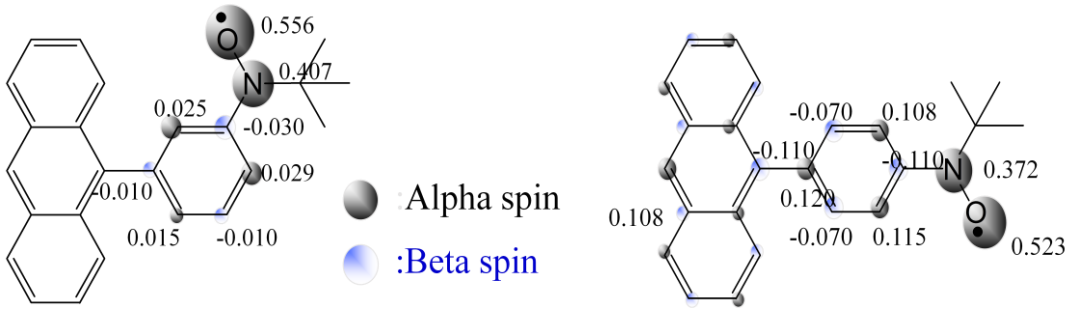

Fig.S7 Calculated spin density distributions of **1*m*** and **1*p***. in their electronic ground states ($S = 1/2$).

S7. Double exponential decay of the transient absorption signals

The formula describing the transient absorption decay of the thermally accessible doublet-quartet system is given by Asano et al. [S3] which is shown in Fig. S8. According to the formula, the double exponential decay is expected as shown in Figs.

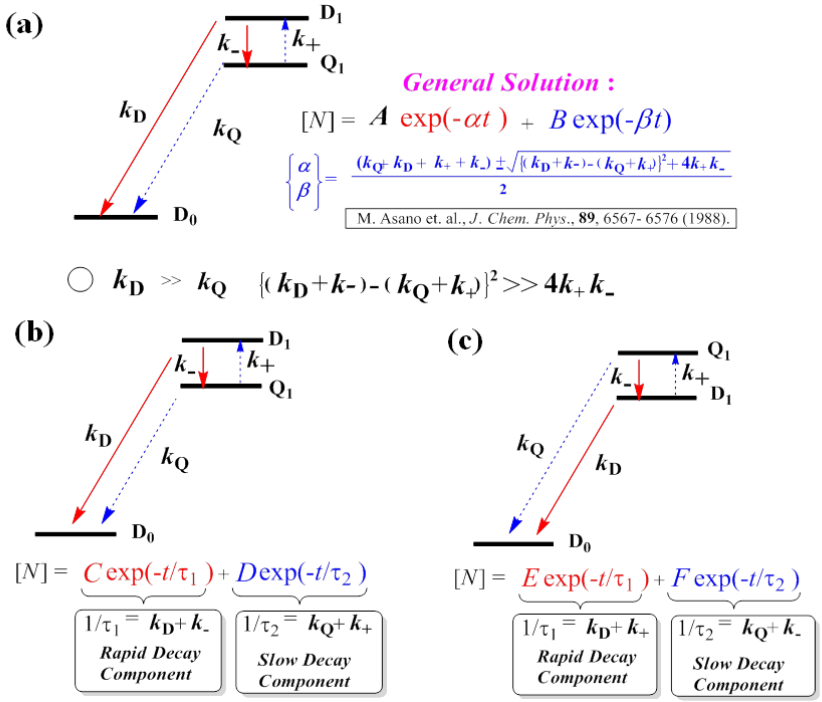

Fig. S8 Decay process of the transient absorption signal of the thermally accessible doublet-triplet system.

S8(b) and S8(c). in both cases ((b) the quartet is lower energy or (c) the doublet is lower energy). In both cases, the thermal process by k_{+a} and $\mathbf{k}_{-}$ produce no dynamic electron spin polarization, leading to very weak TRESR signal.

[S3] M. Asano, Y. Kaizu and H. Kobayashi, *J. Chem. Phys.*, 1988, **89**, 6567.

S8. Details of the syntheses

1*m* and **1*p*** were synthesized according to the procedures shown in Scheme 1(a) and 1(b) in the main text, respectively. THF was purified using benzophenonketyl and diluted. Other reagents were used as purchased. Column chromatography was performed on silica gel (Merk Silica 60) or alumina (Merk Alum. Ox. 60). ^{1}H NMR spectra were measured with a Varian λ-300 (300MHz) spectrometer; chemical shifts are expressed in ppm values (δ) using Me_4Si as an internal standard. HRMS spectra were recorded on a JEOL AccuTOF JMS-T100LP spectrometer.

N-(3-(1,3,2-dioxaborinan-2-yl)phenyl)-*N*-(*tert*-butyl)-*O*-(*tert*-butyldimethylsilyl)hydroxylamine (**3**)

N-(3-bromophenyl)-*N*-(*tert*-butyl)-*O*-(*tert*-butyldimethylsilyl)hydroxylamine was synthesized from 1,3-dibromobenzene by a similar procedures reported in the literature [S4]. To a solution of 17.87 g (49.9 mmol) of *N*-(3-bromophenyl)- *N*-(*tert*-butyl)-*O*-(*tert*-butyldimethylsilyl)hydroxylamine in 250 mL THF anhydrous was added dropwise *n*-Bu_4NF at -75 ºC under nitrogen. After warming the solution to -30 ºC, the solution was cooled again down to -75 ºC and to the solution was added dropwise trimethylborate. After warming the solution to room temperature, the reaction mixture was cooled again dawn to -40 ºC and to the solution was added NH_4Cl aq. The organic layer was extracted by ether, washed with brine, and dried with $MgSO_4$. To the oil product obtained by removing solvent was added 5 mL of 1,3-propylene glycol, 3g of $MgSO_4$ and 100 mL of $CHCl_3$ and stirred for 24 h. Adding THF, filtration, and evaporation gave 16.24g (46.5 mmol) of **3** (crude) as oil.

N-(3-(anthracen-9-yl)phenyl)-*N*-(*tert*-butyl)-*O*-(*tert*-buthyldimethylsilyl)hydroxylamine (**4**)

A mixture of 3.86 g (15 mmol) of 9-bromoanthracene, 8.18 g (22.5 mmol) of **3**, 0.52 g (0.45 mmol) of $Pd(PPh_3)_4$ and 8.3 g (60 mmol) of K_2CO_3 in benzene(100 mL)-EtOH(20 mL)-H2O(40 mL) was refluxed for 24 h under nitrogen. The organic layer was extracted

by benzene, washed with brine. Evaporation, column chromatography (silica gel, benzene) gave **4** (crude) of 8.6 g.

N-(3-(anthracen-9-yl)phenyl)-*N*-(*tert*-butyl)hydroxylamine (**5**)

To a solution of 8.64 g (19.0 mmol) of **4** in 75 mL THF anhydrous was added dropwise 25 mL (25 mmol) of 1M *n*-Bu_4NF at 0 ºC under nitrogen, stirred at 0 ºC for 15 min, and at room temperature for 15 min. The reaction mixture was neutralized by NH_4Cl aq. The organic layer was extracted by ether, washed with brine, and dried with $MgSO_4$. Evaporation, column chromatography (silica gel, CH_2Cl_2), after the first spot was removed the developing solvent was changed to THF. Evaporation, and recrystallization from hexane-benzene (1:1) gave **5** in 46% yield (3 g, 8.8 mmol) as white powder. ^1H NMR ($(CD_3)_2CO$): δ 1.21 (s, CH_3, 9H), 7.15 (d, J = 6.6 Hz, ArH, 1H), 7.41 (d, J = 8.8 Hz, ArH, 2H), 7.47-7.56 (m, ArH, 4H), 7.64 (s, CH_3, 1H), 7.65 (d, J = 8.8 Hz, ArH, 2H), 8.13 (d, J = 8.4 Hz, ArH, 2H), 8.62 (s, ArH, 1H). Anal. calcd for $C_{24}H_{23}NO$; C, 84.42; H, 6.79; N, 4.10. Found: C, 84.17; H, 6.68; N, 4.06.

N-(3-(anthracen-9-yl)phenyl)-(*N*-oxo-*N*-*tert*-butyl)amine (**1*m***)

To a mixture of 0.51 g (1.5 mmol) of **5** and 2 g (14.5 mmol) of K_2CO_3 in THF(10 mL)-$ClCH_2CH_2Cl$(10 mL) was added Ag_2O prepared freshly from 3.4 g (20 mmol) of $AgNO_3$, stirred at room temperature for 1 h. After the mixture was filtered, evaporation, column chromatography (basic alum., PH9, activity I, CH_2Cl_2), and recrystallization from EtOH gave **1*m*** of 43.1% yield (0.22 g, 0.65 mmol) as red crystals. HRMS(ESI+): m/z: calcd for [M+] $C_{24}H_{22}NO$: 340.17014; found 340.161936. Anal. Calcd for $C_{24}H_{22}NO$: C, 84.67; H, 6.51; N, 4.11 Found: C, 84.51; H, 6.86; N, 4.02.

p-Bromophenylanthracene (**6**)

To 4.72 g (20 mmol) of 1,4-dibromobenzene and 0.49 g (20 mmol) of Mg was added 13 mL of THF and stirred at 30 - 40 ºC. A solution was cooled in ice bath and 2.59 g (13.3 mmol) of anthrone in 16 mL THF was added to the mixture and stirred for overnight. The reaction mixture was cooled in ice bath, 20 mL of 6M HCl, and 20 mL of benzene were added. The organic layer extracted, washed with brine, and dried with $MgSO_4$. Evaporation, column chromatography (silica gel, benzene) and recrystallization gave **6** in 59.7% yield (2.65 g, 8.0 mmol).

N-(4-(anthracen-9-yl)phenyl)-*N*-(tert-butyl)hydroxylamine (**7**)

To a solution of 0.61 g (1.8 mmol) of **6** in 20 mL THF anhydrous was added dropwise

n-BuLi at -78 °C under nitrogen, stirred at -78 °C for 30 min. To the reaction mixture was added dropwise 0.22 g (2.6 mmol) of 2-methyl-2-nitrosopropane at -78 °C and stirred for 1h. After raising to room temperature, the reaction mixture was neutralized by NH_4Cl aq. The organic layer was extracted by ether, washed with brine, and dried with $MgSO_4$. Evaporation, column chromatography (silica gel, CH_2Cl_2), and recrystallization from EtOH gave **7** in 41% yield (0.25 g, 0.73 mmol) as white powder. ^1H NMR ($(CD_3)_2CO$): δ 1.29 (s, CH_3, 9H), 7.28-7.45 (m, ArH, 6H), 7.48 (d, J = 6.6 Hz, ArH, 2H), 7.67 (d, J = 8.8 Hz, ArH, 2H), 8.03 (d, J = 8.3 Hz, ArH, 2H), 8.47 (s, ArH, 1H).

N-(4-(anthracen-9-yl)phenyl)-(*N*-oxo-*N*-*tert*-butyl)amine (**1*p***)

To a mixture of 0.25 g (0.75 mmol) of **7** and 1 g (7.3 mmol) of K_2CO_3 in THF(10 mL)-$ClCH_2CH_2Cl$(10 mL) was added Ag_2O prepared freshly from 1.7 g (10 mmol) of $AgNO_3$, stirred at room temperature for 1 h. After the mixture was filtered, evaporation, column chromatography (basic alum., PH9, activity I, CH_2Cl_2), and recrystallization from EtOH gave **1*p*** of 82.2% yield (0.21 g, 0.62 mmol) as red needle crystals. HRMS(ESI+): m/z: calcd for [M+] $C_{24}H_{22}NO$: 341.1701; found 340.17041. Anal. Calcd for $C_{24}H_{22}NO$: C, 84.67; H, 6.51; N, 4.11 Found: C, 84.20; H, 6.52; N, 4.04.

[S4] T. Ishida and H. Iwamura, *J. Am. Chem. Soc.* 1991, **113**, 4238.

S9. X-ray crystallographic data of 1*m*

Diffraction data were collected on a Rigaku AFC-7/Mercury CCD area-detector diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.7107 Å). The CrystalClear software was used for the collection, processing and correction for Lorentzian and polarization effects. Absorption corrections were applied on comparison of multiple symmetry equivalent measurements. The structure was solved by the SIR2004 direct method [S5] and expanded using Fourier techniques and refined by full matrix least-squares against F^2 using SHELXL-97 [S6].

Crystal data for **1*m***: $C_{24}H_{22}NO$, M = 340.43, monoclinic, space group $C2/c$; a = 17.6732(11), b =7.1183(4), c = 29.6076(17) Å, β =100.828(2)°, V = 3658.4(4) Å^3, T = 150(2) K, Z = 8, D_c = 1.236 g cm^{-3}, μ = 0.075 mm^{-1}; 20604 reflections collected and 4130 independent reflections (R_{int} = 0.0342), final R indices [$I > 2\sigma(I)$] $R1$ = 0.0517, $wR2$ = 0.1307; R indices (all data) $R1$ = 0.0597, $wR2$ = 0.1374, GOF = 1.128. CCDC 1429645.

[S5] Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., Caro, L. De, Giacovazzo, C., Polidori, G., Spagna, R. SIR2004: an improved tool for crystal structure determination and refinement. *J. Appl. Crystallogr.* **2005**, *38*, 381-388

[S6] Sheldrick, G. M., A short history of SHELX. *Acta Crystallogr., Sect. A*: *Fundam. Crystallogr.* **2008**, *A64*, 112-122.

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for CrystalClear. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7331(1)	4470(2)	1491(1)	23(1)
C(2)	6873(1)	3505(2)	1758(1)	23(1)
C(3)	6068(1)	3875(2)	1727(1)	27(1)
C(4)	5645(1)	2945(2)	1997(1)	31(1)
C(5)	5996(1)	1579(2)	2319(1)	32(1)
C(6)	6753(1)	1165(2)	2354(1)	29(1)
C(7)	7217(1)	2079(2)	2075(1)	24(1)
C(8)	7997(1)	1667(2)	2114(1)	25(1)
C(9)	8456(1)	2624(2)	1857(1)	24(1)
C(10)	9267(1)	2298(2)	1920(1)	29(1)
C(11)	9719(1)	3292(2)	1680(1)	33(1)
C(12)	9381(1)	4648(2)	1351(1)	33(1)

C(13)	8612(1)	5006(2)	1281(1)	29(1)
C(14)	8119(1)	4040(2)	1535(1)	24(1)
C(15)	6962(1)	5986(2)	1175(1)	24(1)
C(16)	6774(1)	5660(2)	704(1)	25(1)
C(17)	6360(1)	7005(2)	411(1)	25(1)
C(18)	6151(1)	8697(2)	597(1)	27(1)
C(19)	6366(1)	9037(2)	1061(1)	29(1)
C(20)	6770(1)	7697(2)	1353(1)	28(1)
N(1)	6148(1)	6757(1)	-70(1)	31(1)
O(1)	5925(1)	8221(2)	-308(1)	67(1)
C(21)	6192(1)	4972(2)	-335(1)	29(1)
C(22)	7019(1)	4716(3)	-395(1)	51(1)
C(23)	5897(1)	3272(2)	-104(1)	36(1)
C(24)	5661(1)	5237(2)	-800(1)	54(1)

Table S2. Bond lengths [Å] and angles [°] for CrystalClear.

C(1)-C(14)	1.4091(18)
C(1)-C(2)	1.4107(17)
C(1)-C(15)	1.4952(16)
C(2)-C(3)	1.4328(18)
C(2)-C(7)	1.4370(16)
C(3)-C(4)	1.3632(19)
C(3)-H(3A)	1.005(15)
C(4)-C(5)	1.4203(19)
C(4)-H(4A)	1.013(17)
C(5)-C(6)	1.356(2)
C(5)-H(5A)	0.990(18)
C(6)-C(7)	1.4247(18)
C(6)-H(6A)	0.998(17)
C(7)-C(8)	1.3930(18)
C(8)-C(9)	1.3905(18)
C(8)-H(8A)	0.992(15)
C(9)-C(10)	1.4293(18)
C(9)-C(14)	1.4385(16)
C(10)-C(11)	1.361(2)
C(10)-H(10A)	0.988(15)
C(11)-C(12)	1.421(2)
C(11)-H(11A)	0.989(19)
C(12)-C(13)	1.361(2)
C(12)-H(12A)	1.001(16)
C(13)-C(14)	1.4280(18)
C(13)-H(13A)	0.974(16)
C(15)-C(16)	1.3910(17)
C(15)-C(20)	1.3937(17)
C(16)-C(17)	1.4024(17)
C(16)-H(16A)	1.008(15)
C(17)-C(18)	1.4023(17)
C(17)-N(1)	1.4129(16)
C(18)-C(19)	1.3778(19)
C(18)-H(18A)	0.946(16)

C(19)-C(20)	1.3903(17)
C(19)-H(19A)	0.983(16)
C(20)-H(20A)	0.995(15)
N(1)-O(1)	1.2780(14)
N(1)-C(21)	1.5037(16)
C(21)-C(22)	1.517(2)
C(21)-C(24)	1.523(2)
C(21)-C(23)	1.5305(18)
C(22)-H(22A)	0.993(19)
C(22)-H(22B)	1.02(2)
C(22)-H(22C)	1.02(2)
C(23)-H(23A)	1.01(2)
C(23)-H(23B)	0.97(2)
C(23)-H(23C)	0.99(2)
C(24)-H(24A)	0.96(2)
C(24)-H(24B)	1.04(3)
C(24)-H(24C)	1.02(2)
C(14)-C(1)-C(2)	120.29(11)
C(14)-C(1)-C(15)	121.39(11)
C(2)-C(1)-C(15)	118.29(11)
C(1)-C(2)-C(3)	122.80(11)
C(1)-C(2)-C(7)	119.53(11)
C(3)-C(2)-C(7)	117.67(11)
C(4)-C(3)-C(2)	121.34(12)
C(4)-C(3)-H(3A)	120.0(9)
C(2)-C(3)-H(3A)	118.7(9)
C(3)-C(4)-C(5)	120.55(13)
C(3)-C(4)-H(4A)	121.0(9)
C(5)-C(4)-H(4A)	118.4(9)
C(6)-C(5)-C(4)	119.96(13)
C(6)-C(5)-H(5A)	119.4(10)
C(4)-C(5)-H(5A)	120.7(10)
C(5)-C(6)-C(7)	121.59(12)
C(5)-C(6)-H(6A)	122.6(10)
C(7)-C(6)-H(6A)	115.8(10)
C(8)-C(7)-C(6)	121.52(11)

C(8)-C(7)-C(2)	119.60(11)
C(6)-C(7)-C(2)	118.84(11)
C(9)-C(8)-C(7)	121.42(11)
C(9)-C(8)-H(8A)	119.5(9)
C(7)-C(8)-H(8A)	119.1(9)
C(8)-C(9)-C(10)	121.56(11)
C(8)-C(9)-C(14)	119.68(11)
C(10)-C(9)-C(14)	118.70(12)
C(11)-C(10)-C(9)	121.27(12)
C(11)-C(10)-H(10A)	120.6(9)
C(9)-C(10)-H(10A)	118.1(9)
C(10)-C(11)-C(12)	119.96(13)
C(10)-C(11)-H(11A)	119.9(10)
C(12)-C(11)-H(11A)	120.2(10)
C(13)-C(12)-C(11)	120.66(13)
C(13)-C(12)-H(12A)	118.8(9)
C(11)-C(12)-H(12A)	120.5(9)
C(12)-C(13)-C(14)	121.37(12)
C(12)-C(13)-H(13A)	119.7(9)
C(14)-C(13)-H(13A)	118.9(9)
C(1)-C(14)-C(13)	122.51(11)
C(1)-C(14)-C(9)	119.46(11)
C(13)-C(14)-C(9)	117.99(11)
C(16)-C(15)-C(20)	119.69(11)
C(16)-C(15)-C(1)	120.06(10)
C(20)-C(15)-C(1)	120.17(11)
C(15)-C(16)-C(17)	120.36(11)
C(15)-C(16)-H(16A)	118.5(8)
C(17)-C(16)-H(16A)	121.1(8)
C(18)-C(17)-C(16)	119.22(11)
C(18)-C(17)-N(1)	117.59(11)
C(16)-C(17)-N(1)	123.18(11)
C(19)-C(18)-C(17)	119.96(12)
C(19)-C(18)-H(18A)	120.2(10)
C(17)-C(18)-H(18A)	119.8(10)
C(18)-C(19)-C(20)	120.83(12)

C(18)-C(19)-H(19A)	120.8(9)
C(20)-C(19)-H(19A)	118.3(9)
C(19)-C(20)-C(15)	119.86(12)
C(19)-C(20)-H(20A)	119.8(8)
C(15)-C(20)-H(20A)	120.4(8)
O(1)-N(1)-C(17)	116.67(11)
O(1)-N(1)-C(21)	116.21(10)
C(17)-N(1)-C(21)	127.04(10)
N(1)-C(21)-C(22)	107.97(12)
N(1)-C(21)-C(24)	106.49(12)
C(22)-C(21)-C(24)	110.68(15)
N(1)-C(21)-C(23)	112.21(11)
C(22)-C(21)-C(23)	111.97(12)
C(24)-C(21)-C(23)	107.40(12)
C(21)-C(22)-H(22A)	113.1(11)
C(21)-C(22)-H(22B)	108.4(13)
H(22A)-C(22)-H(22B)	105.6(17)
C(21)-C(22)-H(22C)	109.2(13)
H(22A)-C(22)-H(22C)	113.9(17)
H(22B)-C(22)-H(22C)	106.2(18)
C(21)-C(23)-H(23A)	114.5(11)
C(21)-C(23)-H(23B)	109.1(11)
H(23A)-C(23)-H(23B)	107.3(15)
C(21)-C(23)-H(23C)	111.4(13)
H(23A)-C(23)-H(23C)	103.6(16)
H(23B)-C(23)-H(23C)	110.8(17)
C(21)-C(24)-H(24A)	113.7(13)
C(21)-C(24)-H(24B)	112.2(16)
H(24A)-C(24)-H(24B)	108(2)
C(21)-C(24)-H(24C)	106.7(12)
H(24A)-C(24)-H(24C)	105.4(17)
H(24B)-C(24)-H(24C)	111(2)

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($Å^2$x 10^3)for CrystalClear. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(1)	22(1)	18(1)	-2(1)	1(1)	1(1)
C(2)	27(1)	21(1)	20(1)	-2(1)	0(1)	-1(1)
C(3)	26(1)	25(1)	27(1)	-1(1)	1(1)	1(1)
C(4)	27(1)	30(1)	37(1)	0(1)	5(1)	-1(1)
C(5)	32(1)	30(1)	36(1)	5(1)	10(1)	-3(1)
C(6)	34(1)	26(1)	28(1)	5(1)	5(1)	0(1)
C(7)	26(1)	22(1)	21(1)	-2(1)	2(1)	0(1)
C(8)	30(1)	24(1)	21(1)	1(1)	0(1)	3(1)
C(9)	27(1)	24(1)	20(1)	-4(1)	1(1)	2(1)
C(10)	29(1)	31(1)	26(1)	-4(1)	2(1)	6(1)
C(11)	28(1)	34(1)	36(1)	-7(1)	6(1)	2(1)
C(12)	32(1)	34(1)	35(1)	-4(1)	12(1)	-3(1)
C(13)	32(1)	28(1)	28(1)	1(1)	7(1)	1(1)
C(14)	28(1)	24(1)	20(1)	-3(1)	4(1)	1(1)
C(15)	25(1)	25(1)	22(1)	2(1)	4(1)	1(1)
C(16)	29(1)	23(1)	23(1)	0(1)	4(1)	2(1)
C(17)	29(1)	24(1)	22(1)	1(1)	4(1)	-2(1)
C(18)	28(1)	23(1)	30(1)	5(1)	4(1)	2(1)
C(19)	34(1)	23(1)	30(1)	-1(1)	7(1)	2(1)
C(20)	34(1)	26(1)	23(1)	-1(1)	5(1)	0(1)
N(1)	46(1)	24(1)	22(1)	4(1)	1(1)	2(1)
O(1)	133(1)	32(1)	28(1)	9(1)	-3(1)	22(1)
C(21)	37(1)	26(1)	24(1)	-1(1)	4(1)	-2(1)
C(22)	50(1)	47(1)	63(1)	4(1)	27(1)	3(1)
C(23)	43(1)	28(1)	37(1)	1(1)	5(1)	-6(1)
C(24)	87(2)	38(1)	29(1)	1(1)	-13(1)	-8(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CrystalClear.

	x	y	z	U(eq)
H(3A)	5815(9)	4840(20)	1500(5)	27(4)
H(4A)	5072(10)	3180(20)	1966(6)	39(4)
H(5A)	5692(10)	920(20)	2519(6)	42(4)
H(6A)	7022(10)	210(20)	2573(6)	41(4)
H(8A)	8232(9)	700(20)	2338(5)	30(4)
H(10A)	9497(9)	1360(20)	2153(5)	29(4)
H(11A)	10280(11)	3070(20)	1735(6)	45(5)
H(12A)	9704(9)	5340(20)	1161(5)	33(4)
H(13A)	8390(9)	5950(20)	1058(5)	34(4)
H(16A)	6945(9)	4450(20)	580(5)	27(4)
H(18A)	5861(9)	9600(20)	403(5)	33(4)
H(19A)	6237(9)	10230(20)	1195(5)	33(4)
H(20A)	6910(9)	7950(20)	1689(5)	29(4)
H(22A)	7380(11)	4490(30)	-101(7)	50(5)
H(22B)	7048(13)	3550(30)	-589(8)	73(6)
H(22C)	7171(13)	5810(30)	-579(8)	76(7)
H(23A)	6260(11)	2800(30)	177(7)	57(5)
H(23B)	5806(11)	2240(30)	-321(7)	55(5)
H(23C)	5422(14)	3580(30)	14(8)	73(7)
H(24A)	5819(12)	6230(30)	-981(7)	64(6)
H(24B)	5096(19)	5510(40)	-766(10)	114(10)
H(24C)	5697(13)	4030(30)	-983(7)	68(6)

Table S6. Torsion angles [°] for CrystalClear.

C(14)-C(1)-C(2)-C(3)	-179.67(11)
C(15)-C(1)-C(2)-C(3)	2.14(17)
C(14)-C(1)-C(2)-C(7)	0.03(17)
C(15)-C(1)-C(2)-C(7)	-178.16(10)
C(1)-C(2)-C(3)-C(4)	-178.59(12)
C(7)-C(2)-C(3)-C(4)	1.71(18)
C(2)-C(3)-C(4)-C(5)	0.2(2)
C(3)-C(4)-C(5)-C(6)	-1.3(2)
C(4)-C(5)-C(6)-C(7)	0.4(2)
C(5)-C(6)-C(7)-C(8)	179.28(12)
C(5)-C(6)-C(7)-C(2)	1.50(19)
C(1)-C(2)-C(7)-C(8)	-0.04(17)
C(3)-C(2)-C(7)-C(8)	179.67(11)
C(1)-C(2)-C(7)-C(6)	177.79(11)
C(3)-C(2)-C(7)-C(6)	-2.50(17)
C(6)-C(7)-C(8)-C(9)	-176.95(11)
C(2)-C(7)-C(8)-C(9)	0.82(18)
C(7)-C(8)-C(9)-C(10)	175.51(11)
C(7)-C(8)-C(9)-C(14)	-1.56(18)
C(8)-C(9)-C(10)-C(11)	-177.40(12)
C(14)-C(9)-C(10)-C(11)	-0.31(18)
C(9)-C(10)-C(11)-C(12)	-1.7(2)
C(10)-C(11)-C(12)-C(13)	1.8(2)
C(11)-C(12)-C(13)-C(14)	0.1(2)
C(2)-C(1)-C(14)-C(13)	-178.41(11)
C(15)-C(1)-C(14)-C(13)	-0.27(18)
C(2)-C(1)-C(14)-C(9)	-0.76(17)
C(15)-C(1)-C(14)-C(9)	177.38(10)
C(12)-C(13)-C(14)-C(1)	175.66(12)
C(12)-C(13)-C(14)-C(9)	-2.03(18)
C(8)-C(9)-C(14)-C(1)	1.51(17)
C(10)-C(9)-C(14)-C(1)	-175.64(11)
C(8)-C(9)-C(14)-C(13)	179.27(11)
C(10)-C(9)-C(14)-C(13)	2.12(17)

C(14)-C(1)-C(15)-C(16)	77.52(15)
C(2)-C(1)-C(15)-C(16)	-104.31(14)
C(14)-C(1)-C(15)-C(20)	-105.79(14)
C(2)-C(1)-C(15)-C(20)	72.38(15)
C(20)-C(15)-C(16)-C(17)	-3.06(19)
C(1)-C(15)-C(16)-C(17)	173.64(11)
C(15)-C(16)-C(17)-C(18)	1.21(19)
C(15)-C(16)-C(17)-N(1)	-179.69(12)
C(16)-C(17)-C(18)-C(19)	1.3(2)
N(1)-C(17)-C(18)-C(19)	-177.85(12)
C(17)-C(18)-C(19)-C(20)	-1.9(2)
C(18)-C(19)-C(20)-C(15)	0.1(2)
C(16)-C(15)-C(20)-C(19)	2.4(2)
C(1)-C(15)-C(20)-C(19)	-174.28(12)
C(18)-C(17)-N(1)-O(1)	13.9(2)
C(16)-C(17)-N(1)-O(1)	-165.18(14)
C(18)-C(17)-N(1)-C(21)	-169.33(12)
C(16)-C(17)-N(1)-C(21)	11.6(2)
O(1)-N(1)-C(21)-C(22)	96.80(16)
C(17)-N(1)-C(21)-C(22)	-79.95(17)
O(1)-N(1)-C(21)-C(24)	-22.09(19)
C(17)-N(1)-C(21)-C(24)	161.16(15)
O(1)-N(1)-C(21)-C(23)	-139.33(15)
C(17)-N(1)-C(21)-C(23)	43.92(19)

Symmetry transformations used to generate equivalent atoms:

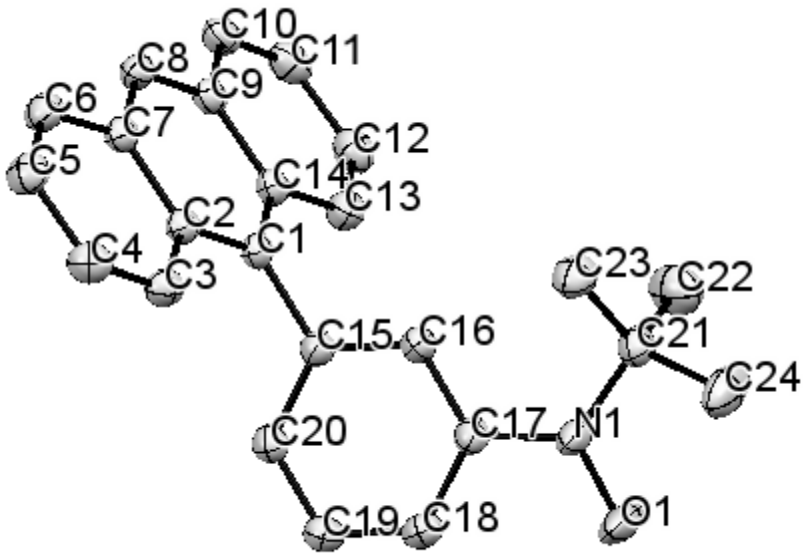

Fig. S9 ORTEP drawing of **1*m*.** H atoms are omitted.

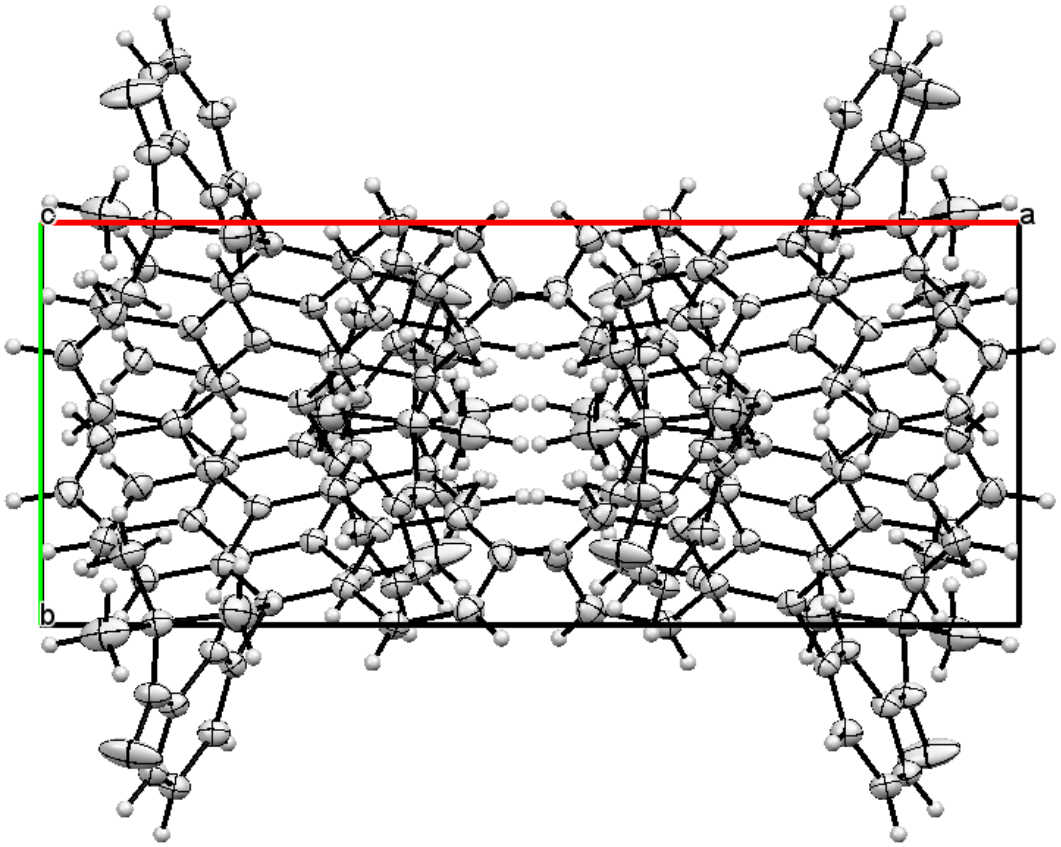

Fig. S10 *ab*-plane projection

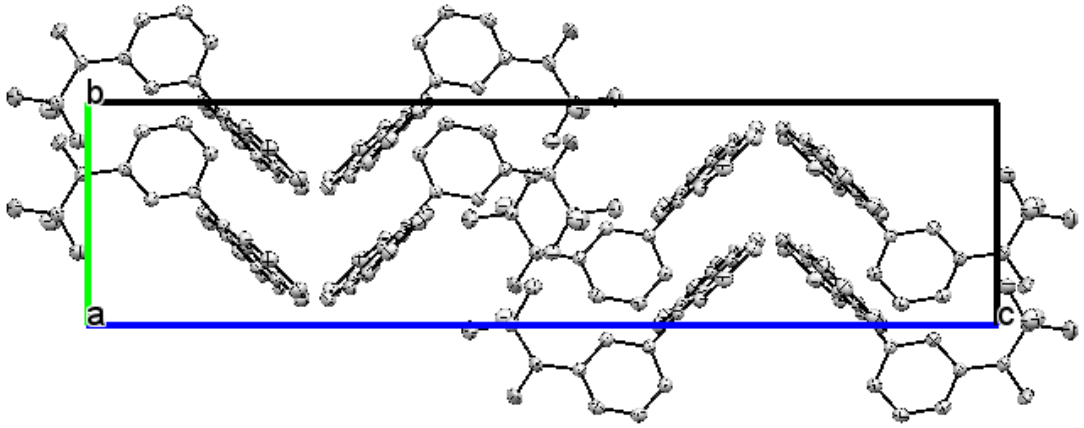

Fig. S11 *bc*-plane projection

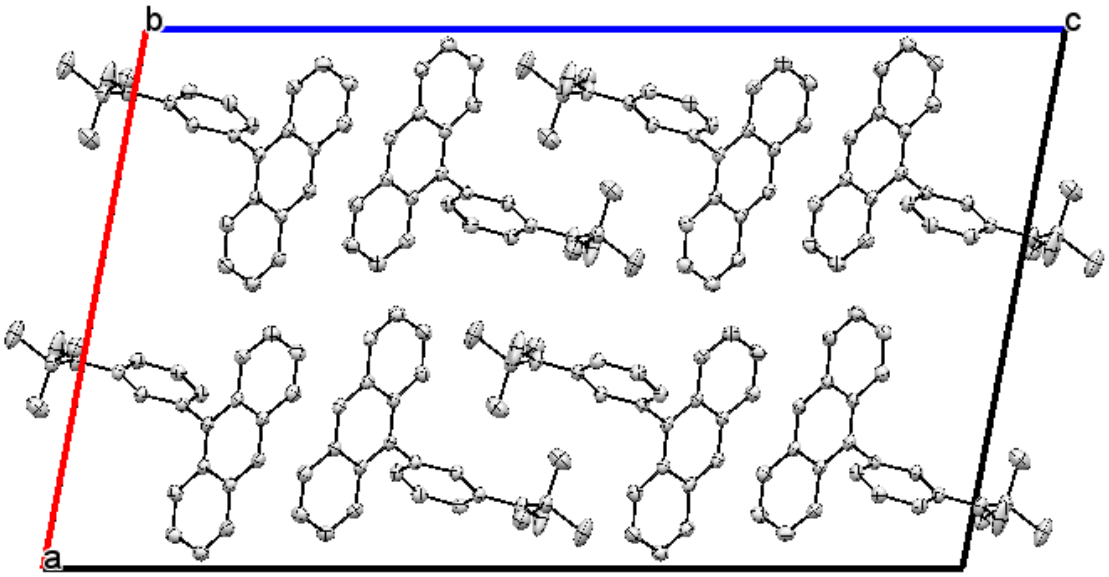

Fig. S12 *ac*-plane projection

S7. X-ray crystallographic data of 1*p*

Crystal data for **1*p***: $C_{24}H_{22}NO$, M = 340.43, monoclinic, space group $P21/c$; a = 8.7919(6), b =26.2294(18), c = 8.1257(7) Å, β =103.413(3)°, V = 1822.7(2) Å^3, T = 150(2) K, Z = 4, D_c = 1.241 g cm^{-3}, μ = 0.075 mm^{-1}; 20644 reflections collected and 4172 independent reflections (R_{int} = 0.0366), final R indices [$I > 2\sigma(I)$] $R1$ = 0.0467, $wR2$ = 0.1084; R indices (all data) $R1$ = 0.0580, $wR2$ = 0.1159, GOF = 1.079. CCDC 1429627.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for crystalclear. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4876(2)	1474(1)	-912(1)	22(1)
C(2)	6501(2)	1566(1)	-458(2)	24(1)
C(3)	7510(2)	1332(1)	984(2)	30(1)
C(4)	9080(2)	1419(1)	1378(2)	37(1)
C(5)	9765(2)	1751(1)	375(2)	41(1)
C(6)	8860(2)	1976(1)	-1010(2)	38(1)
C(7)	7213(2)	1890(1)	-1495(2)	28(1)
C(8)	6289(2)	2103(1)	-2957(2)	30(1)
C(9)	4689(2)	2010(1)	-3439(2)	26(1)
C(10)	3741(2)	2234(1)	-4932(2)	33(1)
C(11)	2179(2)	2155(1)	-5373(2)	36(1)
C(12)	1442(2)	1849(1)	-4340(2)	34(1)
C(13)	2299(2)	1624(1)	-2913(2)	27(1)
C(14)	3956(2)	1691(1)	-2405(1)	22(1)
C(15)	4141(1)	1152(1)	204(1)	22(1)
C(16)	4081(2)	1324(1)	1817(2)	24(1)
C(17)	3457(2)	1025(1)	2904(2)	23(1)
C(18)	2889(1)	538(1)	2406(1)	22(1)
C(19)	2894(2)	367(1)	774(2)	25(1)
C(20)	3511(2)	674(1)	-305(2)	25(1)
N(1)	2296(1)	245(1)	3590(1)	25(1)
O(1)	1859(1)	491(1)	4766(1)	42(1)
C(21)	2259(2)	-329(1)	3642(2)	25(1)
C(22)	787(2)	-522(1)	2409(2)	34(1)

C(23)	3753(2)	-548(1)	3260(2)	30(1)
C(24)	2196(2)	-485(1)	5440(2)	35(1)

Table S8. Bond lengths [Å] and angles [°] for crystalclear.

C(1)-C(2)	1.4109(18)
C(1)-C(14)	1.4131(17)
C(1)-C(15)	1.4912(16)
C(2)-C(3)	1.4333(18)
C(2)-C(7)	1.4379(17)
C(3)-C(4)	1.361(2)
C(3)-H(3A)	0.991(16)
C(4)-C(5)	1.419(2)
C(4)-H(4A)	0.983(18)
C(5)-C(6)	1.354(2)
C(5)-H(5A)	0.978(18)
C(6)-C(7)	1.428(2)
C(6)-H(6A)	0.972(17)
C(7)-C(8)	1.3921(19)
C(8)-C(9)	1.392(2)
C(8)-H(8A)	0.971(16)
C(9)-C(10)	1.4287(18)
C(9)-C(14)	1.4394(17)
C(10)-C(11)	1.352(2)
C(10)-H(10A)	1.000(18)
C(11)-C(12)	1.422(2)
C(11)-H(11A)	0.981(17)
C(12)-C(13)	1.3620(19)
C(12)-H(12A)	0.998(18)
C(13)-C(14)	1.4303(18)
C(13)-H(13A)	0.978(16)
C(15)-C(20)	1.3939(18)
C(15)-C(16)	1.3989(16)
C(16)-C(17)	1.3849(17)
C(16)-H(16A)	0.967(15)
C(17)-C(18)	1.3979(18)
C(17)-H(17A)	0.985(14)
C(18)-C(19)	1.4007(16)
C(18)-N(1)	1.4214(15)

C(19)-C(20)	1.3896(18)
C(19)-H(19A)	0.996(16)
C(20)-H(20A)	0.987(14)
N(1)-O(1)	1.2833(14)
N(1)-C(21)	1.5068(17)
C(21)-C(22)	1.5269(19)
C(21)-C(23)	1.5295(19)
C(21)-C(24)	1.5304(18)
C(22)-H(22A)	1.011(17)
C(22)-H(22B)	0.99(2)
C(22)-H(22C)	0.99(2)
C(23)-H(23A)	1.003(16)
C(23)-H(23B)	0.99(2)
C(23)-H(23C)	0.995(18)
C(24)-H(24A)	0.981(18)
C(24)-H(24B)	1.04(2)
C(24)-H(24C)	1.013(18)
C(2)-C(1)-C(14)	119.93(11)
C(2)-C(1)-C(15)	119.55(11)
C(14)-C(1)-C(15)	120.51(11)
C(1)-C(2)-C(3)	122.53(12)
C(1)-C(2)-C(7)	119.96(11)
C(3)-C(2)-C(7)	117.46(12)
C(4)-C(3)-C(2)	121.46(13)
C(4)-C(3)-H(3A)	120.2(9)
C(2)-C(3)-H(3A)	118.3(9)
C(3)-C(4)-C(5)	120.64(14)
C(3)-C(4)-H(4A)	120.7(10)
C(5)-C(4)-H(4A)	118.7(10)
C(6)-C(5)-C(4)	120.00(14)
C(6)-C(5)-H(5A)	119.6(10)
C(4)-C(5)-H(5A)	120.4(11)
C(5)-C(6)-C(7)	121.47(14)
C(5)-C(6)-H(6A)	121.4(10)
C(7)-C(6)-H(6A)	117.2(10)
C(8)-C(7)-C(6)	121.65(13)

C(8)-C(7)-C(2)	119.41(12)
C(6)-C(7)-C(2)	118.93(13)
C(9)-C(8)-C(7)	121.41(12)
C(9)-C(8)-H(8A)	119.6(9)
C(7)-C(8)-H(8A)	118.9(9)
C(8)-C(9)-C(10)	121.26(12)
C(8)-C(9)-C(14)	119.86(12)
C(10)-C(9)-C(14)	118.87(13)
C(11)-C(10)-C(9)	121.21(13)
C(11)-C(10)-H(10A)	121.7(10)
C(9)-C(10)-H(10A)	117.1(10)
C(10)-C(11)-C(12)	120.27(13)
C(10)-C(11)-H(11A)	120.6(10)
C(12)-C(11)-H(11A)	119.1(10)
C(13)-C(12)-C(11)	120.64(14)
C(13)-C(12)-H(12A)	119.5(10)
C(11)-C(12)-H(12A)	119.9(10)
C(12)-C(13)-C(14)	121.13(13)
C(12)-C(13)-H(13A)	119.7(9)
C(14)-C(13)-H(13A)	119.2(9)
C(1)-C(14)-C(13)	122.68(11)
C(1)-C(14)-C(9)	119.41(12)
C(13)-C(14)-C(9)	117.87(11)
C(20)-C(15)-C(16)	117.95(11)
C(20)-C(15)-C(1)	121.85(10)
C(16)-C(15)-C(1)	120.20(11)
C(17)-C(16)-C(15)	121.46(12)
C(17)-C(16)-H(16A)	119.3(8)
C(15)-C(16)-H(16A)	119.2(8)
C(16)-C(17)-C(18)	120.04(11)
C(16)-C(17)-H(17A)	120.5(9)
C(18)-C(17)-H(17A)	119.5(8)
C(17)-C(18)-C(19)	119.11(11)
C(17)-C(18)-N(1)	117.51(10)
C(19)-C(18)-N(1)	123.36(11)
C(20)-C(19)-C(18)	119.98(12)

C(20)-C(19)-H(19A)	119.6(8)
C(18)-C(19)-H(19A)	120.4(8)
C(19)-C(20)-C(15)	121.35(11)
C(19)-C(20)-H(20A)	118.8(9)
C(15)-C(20)-H(20A)	119.9(9)
O(1)-N(1)-C(18)	116.87(11)
O(1)-N(1)-C(21)	117.98(10)
C(18)-N(1)-C(21)	124.98(10)
N(1)-C(21)-C(22)	109.40(11)
N(1)-C(21)-C(23)	110.12(10)
C(22)-C(21)-C(23)	112.33(12)
N(1)-C(21)-C(24)	107.45(11)
C(22)-C(21)-C(24)	108.99(11)
C(23)-C(21)-C(24)	108.42(11)
C(21)-C(22)-H(22A)	110.3(10)
C(21)-C(22)-H(22B)	108.8(10)
H(22A)-C(22)-H(22B)	108.8(14)
C(21)-C(22)-H(22C)	108.7(11)
H(22A)-C(22)-H(22C)	112.3(15)
H(22B)-C(22)-H(22C)	107.8(15)
C(21)-C(23)-H(23A)	113.7(9)
C(21)-C(23)-H(23B)	107.9(11)
H(23A)-C(23)-H(23B)	108.7(13)
C(21)-C(23)-H(23C)	109.5(10)
H(23A)-C(23)-H(23C)	108.4(13)
H(23B)-C(23)-H(23C)	108.5(14)
C(21)-C(24)-H(24A)	111.4(10)
C(21)-C(24)-H(24B)	104.2(10)
H(24A)-C(24)-H(24B)	108.2(15)
C(21)-C(24)-H(24C)	110.5(9)
H(24A)-C(24)-H(24C)	109.3(14)
H(24B)-C(24)-H(24C)	113.2(14)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for crystalclear. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(1)	20(1)	21(1)	-2(1)	9(1)	-1(1)
C(2)	27(1)	25(1)	22(1)	-3(1)	8(1)	-4(1)
C(3)	29(1)	37(1)	25(1)	-1(1)	7(1)	-3(1)
C(4)	28(1)	52(1)	30(1)	-4(1)	4(1)	-3(1)
C(5)	26(1)	58(1)	39(1)	-11(1)	9(1)	-13(1)
C(6)	36(1)	43(1)	38(1)	-8(1)	17(1)	-17(1)
C(7)	32(1)	28(1)	28(1)	-5(1)	13(1)	-8(1)
C(8)	42(1)	24(1)	28(1)	-1(1)	17(1)	-8(1)
C(9)	38(1)	20(1)	22(1)	-1(1)	11(1)	1(1)
C(10)	52(1)	23(1)	26(1)	3(1)	15(1)	8(1)
C(11)	50(1)	33(1)	25(1)	2(1)	8(1)	18(1)
C(12)	33(1)	38(1)	28(1)	-2(1)	5(1)	12(1)
C(13)	29(1)	27(1)	26(1)	-2(1)	8(1)	3(1)
C(14)	29(1)	19(1)	22(1)	-3(1)	9(1)	1(1)
C(15)	20(1)	24(1)	22(1)	2(1)	6(1)	0(1)
C(16)	26(1)	21(1)	25(1)	-1(1)	8(1)	-2(1)
C(17)	24(1)	24(1)	22(1)	-1(1)	8(1)	2(1)
C(18)	19(1)	23(1)	24(1)	3(1)	8(1)	1(1)
C(19)	25(1)	24(1)	26(1)	-3(1)	8(1)	-3(1)
C(20)	25(1)	29(1)	22(1)	-3(1)	7(1)	-3(1)
N(1)	26(1)	25(1)	27(1)	-1(1)	13(1)	-1(1)
O(1)	61(1)	31(1)	48(1)	-6(1)	41(1)	-4(1)
C(21)	25(1)	22(1)	28(1)	2(1)	8(1)	-3(1)
C(22)	28(1)	36(1)	38(1)	-1(1)	8(1)	-9(1)
C(23)	28(1)	27(1)	35(1)	-1(1)	10(1)	3(1)
C(24)	42(1)	33(1)	31(1)	7(1)	13(1)	-1(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for crystalclear.

	x	y	z	U(eq)
H(3A)	7042(18)	1096(6)	1681(18)	31(4)
H(4A)	9760(20)	1248(7)	2350(20)	47(5)
H(5A)	10890(20)	1812(7)	660(20)	47(5)
H(6A)	9310(20)	2198(7)	-1730(20)	44(5)
H(8A)	6782(18)	2313(6)	-3668(18)	34(4)
H(10A)	4290(20)	2443(7)	-5650(20)	44(5)
H(11A)	1540(20)	2312(7)	-6400(20)	47(5)
H(12A)	280(20)	1802(7)	-4650(20)	43(5)
H(13A)	1774(18)	1413(6)	-2218(19)	33(4)
H(16A)	4508(17)	1655(6)	2190(17)	25(4)
H(17A)	3415(17)	1153(6)	4032(18)	25(4)
H(19A)	2477(18)	24(6)	389(18)	31(4)
H(20A)	3484(17)	550(6)	-1458(18)	27(4)
H(22A)	780(20)	-411(7)	1220(20)	41(4)
H(22B)	770(20)	-899(8)	2450(20)	48(5)
H(22C)	-140(20)	-395(7)	2790(20)	54(5)
H(23A)	3820(19)	-502(6)	2050(20)	36(4)
H(23B)	3790(20)	-917(8)	3520(20)	50(5)
H(23C)	4680(20)	-383(7)	4000(20)	46(5)
H(24A)	1230(20)	-364(7)	5730(20)	38(4)
H(24B)	2160(20)	-881(8)	5400(20)	58(5)
H(24C)	3130(20)	-346(7)	6290(20)	41(4)

Table S11. Torsion angles [°] for crystalclear.

C(14)-C(1)-C(2)-C(3)	-176.21(12)
C(15)-C(1)-C(2)-C(3)	4.53(19)
C(14)-C(1)-C(2)-C(7)	1.40(18)
C(15)-C(1)-C(2)-C(7)	-177.86(11)
C(1)-C(2)-C(3)-C(4)	178.71(13)
C(7)-C(2)-C(3)-C(4)	1.0(2)
C(2)-C(3)-C(4)-C(5)	0.7(2)
C(3)-C(4)-C(5)-C(6)	-1.4(2)
C(4)-C(5)-C(6)-C(7)	0.2(2)
C(5)-C(6)-C(7)-C(8)	-177.16(14)
C(5)-C(6)-C(7)-C(2)	1.6(2)
C(1)-C(2)-C(7)-C(8)	-1.10(19)
C(3)-C(2)-C(7)-C(8)	176.63(12)
C(1)-C(2)-C(7)-C(6)	-179.91(12)
C(3)-C(2)-C(7)-C(6)	-2.18(19)
C(6)-C(7)-C(8)-C(9)	178.83(13)
C(2)-C(7)-C(8)-C(9)	0.0(2)
C(7)-C(8)-C(9)-C(10)	179.35(12)
C(7)-C(8)-C(9)-C(14)	0.7(2)
C(8)-C(9)-C(10)-C(11)	-178.04(13)
C(14)-C(9)-C(10)-C(11)	0.65(19)
C(9)-C(10)-C(11)-C(12)	0.6(2)
C(10)-C(11)-C(12)-C(13)	-1.1(2)
C(11)-C(12)-C(13)-C(14)	0.4(2)
C(2)-C(1)-C(14)-C(13)	-178.36(12)
C(15)-C(1)-C(14)-C(13)	0.90(18)
C(2)-C(1)-C(14)-C(9)	-0.68(17)
C(15)-C(1)-C(14)-C(9)	178.58(11)
C(12)-C(13)-C(14)-C(1)	178.45(12)
C(12)-C(13)-C(14)-C(9)	0.74(19)
C(8)-C(9)-C(14)-C(1)	-0.36(18)
C(10)-C(9)-C(14)-C(1)	-179.07(11)
C(8)-C(9)-C(14)-C(13)	177.43(12)
C(10)-C(9)-C(14)-C(13)	-1.28(17)

C(2)-C(1)-C(15)-C(20)	-112.24(14)
C(14)-C(1)-C(15)-C(20)	68.50(17)
C(2)-C(1)-C(15)-C(16)	67.16(16)
C(14)-C(1)-C(15)-C(16)	-112.10(14)
C(20)-C(15)-C(16)-C(17)	1.82(19)
C(1)-C(15)-C(16)-C(17)	-177.60(12)
C(15)-C(16)-C(17)-C(18)	0.82(19)
C(16)-C(17)-C(18)-C(19)	-2.91(19)
C(16)-C(17)-C(18)-N(1)	178.57(11)
C(17)-C(18)-C(19)-C(20)	2.34(19)
N(1)-C(18)-C(19)-C(20)	-179.23(12)
C(18)-C(19)-C(20)-C(15)	0.3(2)
C(16)-C(15)-C(20)-C(19)	-2.40(19)
C(1)-C(15)-C(20)-C(19)	177.01(12)
C(17)-C(18)-N(1)-O(1)	21.77(17)
C(19)-C(18)-N(1)-O(1)	-156.69(12)
C(17)-C(18)-N(1)-C(21)	-153.37(12)
C(19)-C(18)-N(1)-C(21)	28.18(18)
O(1)-N(1)-C(21)-C(22)	99.95(13)
C(18)-N(1)-C(21)-C(22)	-84.96(14)
O(1)-N(1)-C(21)-C(23)	-136.13(12)
C(18)-N(1)-C(21)-C(23)	38.96(16)
O(1)-N(1)-C(21)-C(24)	-18.23(16)
C(18)-N(1)-C(21)-C(24)	156.86(12)

Symmetry transformations used to generate equivalent atoms:

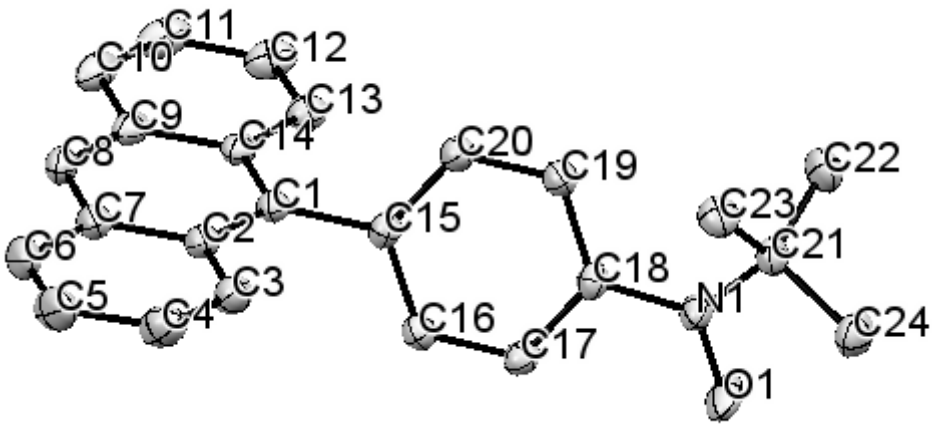

Fig. S13. ORTEP drawing of **1*p***. H atoms are omitted.

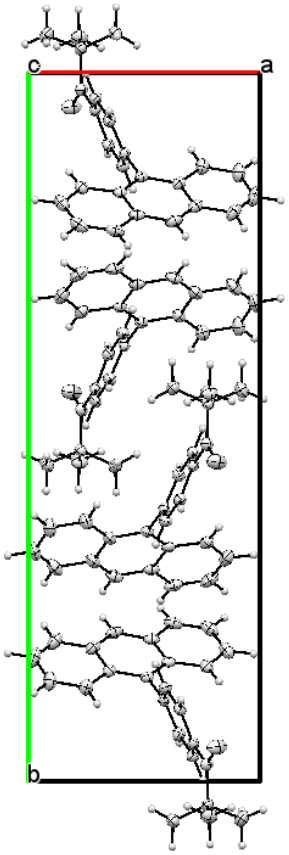

Fig. S14. *ab*-plane projection

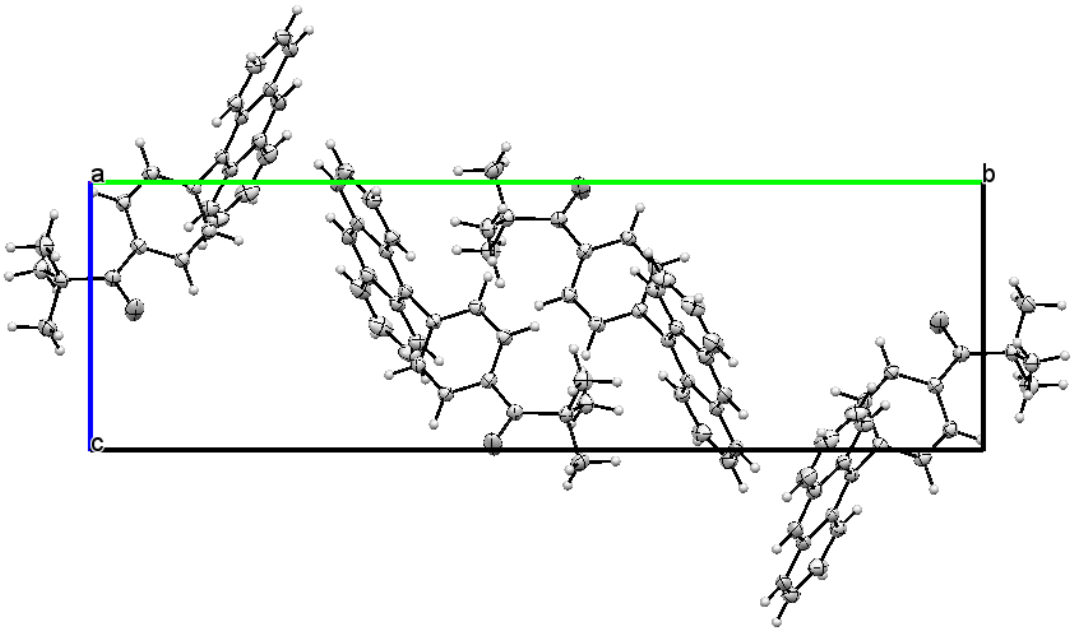

Fig. S15. *bc*-plane projection

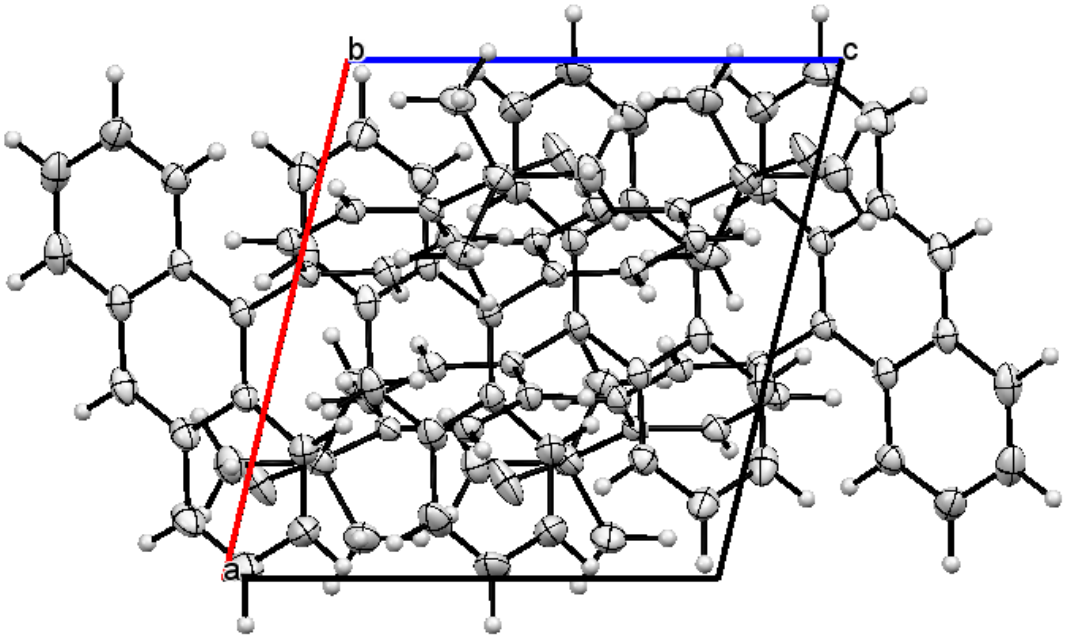

Fig. S16. *ac*-plane projection