Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Cyclisation reactions of *N*-cinnamoyl-9-amino-anthracenes.

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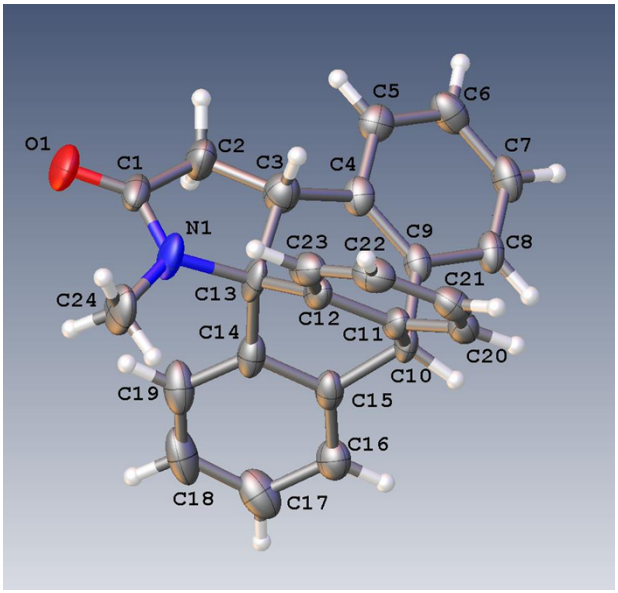
Table 1 Crystal data and structure refinement for 4b



Identification code	xstr0016
Empirical formula	$C_{24}H_{19}NO$
Formula weight	337.40
Temperature/K	150
Crystal system	monoclinic
Space group	Cc
a/Å	16.9504(14)
b/Å	11.2305(10)
c/Å	9.1731(9)
α/°	90
β/°	103.305(10)
γ/°	90
Volume/Å^3	1699.3(3)
Z	4
ρ_{calc}mg/mm^3	1.319
m/mm^{-1}	0.623
F(000)	712.0
Crystal size/mm^3	0.21 × 0.18 × 0.04
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection	9.528 to 149.326°
Index ranges	$-20 \le h \le 20$, $-12 \le k \le 13$, $-10 \le l \le 6$
Reflections collected	2772
Independent reflections	1846 [R_{int} = 0.0370, R_{sigma} = 0.0415]
Data/restraints/parameters	1846/2/236
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0582, wR_2 = 0.1438
Final R indexes [all data]	R_1 = 0.0603, wR_2 = 0.1464
Largest diff. peak/hole / e Å^{-3}	0.72/-0.24
Flack parameter	0.0(5)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for xstr0016. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	2942(2)	4770(4)	4164(5)	63.7(12)
N1	3720(2)	3180(4)	3975(5)	44(1)
C1	3522(2)	4324(4)	3796(5)	36.5(10)
C2	4126(3)	4927(4)	3051(7)	48.3(13)
C3	4818(3)	4092(4)	3305(6)	43.2(11)
C4	5445(2)	4183(4)	2349(4)	30.9(9)
C5	5745(3)	5306(4)	2217(5)	34.1(9)
C6	6386(3)	5511(4)	1533(5)	40.2(11)
C7	6733(2)	4549(5)	979(5)	39.5(11)
C8	6447(2)	3416(4)	1110(5)	32.3(9)
C9	5806(2)	3204(4)	1796(4)	28.7(8)
C10	5549(2)	1919(4)	1971(5)	29.2(9)
C11	5631(2)	1648(3)	3611(5)	29.6(9)
C12	5027(2)	2080(4)	4295(5)	32.5(9)
C13	4391(3)	2840(4)	3302(5)	38.2(11)
C14	4090(2)	2261(4)	1761(5)	36.7(10)
C15	4685(2)	1749(4)	1117(5)	33.0(9)
C16	4475(3)	1187(4)	-258(5)	39.1(10)
C17	3665(3)	1153(5)	-1022(6)	50.3(13)
C18	3083(3)	1723(6)	-404(7)	55.7(15)
C19	3299(3)	2257(5)	997(6)	47.9(13)
C20	6310(2)	1073(4)	4487(5)	32.0(9)
C21	6372(3)	898(4)	6005(5)	39(1)
C22	5766(3)	1315(4)	6674(6)	41.3(11)
C23	5101(3)	1905(4)	5824(5)	38.4(10)
C24	3192(3)	2318(5)	4465(7)	55.2(14)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for xstr0016. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	39(2)	70(2)	91(3)	-27(2)	34(2)	8.6(17)
N1	36(2)	46(2)	62(3)	7.1(19)	34(2)	11.6(17)
C1	25.2(19)	50(2)	33(2)	-13(2)	4.9(17)	6.2(18)
C2	36(2)	42(3)	74(4)	-4(3)	25(3)	5(2)
C3	42(2)	41(2)	51(3)	3(2)	20(2)	1(2)
C4	30(2)	41(2)	23.2(19)	6.5(17)	10.9(16)	0.9(17)
C5	36(2)	37(2)	30(2)	4.6(17)	7.3(18)	2.7(17)
C6	34(2)	42(2)	43(3)	15(2)	5(2)	-7.3(18)
C7	26(2)	57(3)	37(2)	11(2)	11.6(18)	-3.0(19)
C8	21.9(18)	51(2)	26(2)	4.2(18)	9.1(15)	2.7(17)
C9	21.6(18)	43(2)	22.7(19)	4.2(17)	7.2(15)	-0.7(16)
C10	21.7(18)	34.4(19)	35(2)	1.4(17)	14.3(16)	4.8(14)
C11	26.1(19)	27.5(18)	40(2)	-2.2(17)	17.3(17)	-2.6(15)
C12	27.8(19)	30.7(19)	45(2)	-4.7(18)	21.1(18)	-4.4(16)
C13	33(2)	39(2)	54(3)	10(2)	32(2)	9.8(18)
C14	29(2)	41(2)	45(3)	13(2)	18.6(19)	8.4(17)
C15	26.2(19)	33(2)	43(3)	9.4(18)	14.4(18)	3.0(15)
C16	35(2)	45(2)	41(3)	4(2)	15(2)	-1.9(18)
C17	40(3)	68(3)	39(3)	15(2)	2(2)	-9(2)
C18	26(2)	79(4)	60(4)	27(3)	6(2)	2(2)
C19	30(2)	70(3)	48(3)	20(3)	16(2)	8(2)
C20	27.4(19)	30.0(19)	40(2)	-0.1(18)	9.5(17)	-2.5(16)
C21	37(2)	38(2)	41(3)	1(2)	3.9(19)	-9.4(19)
C22	51(3)	42(2)	33(2)	-2(2)	14(2)	-11(2)
C23	42(2)	37(2)	42(3)	-6(2)	24(2)	-8.8(18)
C24	43(3)	60(3)	76(4)	6(3)	42(3)	1(2)

Table 4 Bond Lengths for xstr0016.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.220(5)	C10	C15	1.506(6)
N1	C1	1.329(6)	C11	C12	1.405(5)
N1	C13	1.464(5)	C11	C20	1.401(6)
N1	C24	1.457(6)	C12	C13	1.506(6)
C1	C2	1.515(7)	C12	C23	1.393(7)
C2	C3	1.478(7)	C13	C14	1.533(7)
C3	C4	1.528(6)	C14	C15	1.403(6)
C3	C13	1.582(6)	C14	C19	1.363(7)
C4	C5	1.376(6)	C15	C16	1.382(7)
C4	C9	1.408(6)	C16	C17	1.390(7)
C5	C6	1.394(6)	C17	C18	1.401(8)
C6	C7	1.382(7)	C18	C19	1.388(9)
C7	C8	1.377(7)	C20	C21	1.386(6)
C8	C9	1.397(5)	C21	C22	1.393(7)
C9	C10	1.526(6)	C22	C23	1.383(7)
C10	C11	1.510(6)			

Table 5 Bond Angles for xstr0016.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C13	113.5(4)	C20	C11	C12	119.3(4)
C1	N1	C24	121.7(4)	C11	C12	C13	114.8(4)
C24	N1	C13	123.3(4)	C23	C12	C11	119.6(4)
O1	C1	N1	124.0(5)	C23	C12	C13	125.1(4)
O1	C1	C2	127.8(5)	N1	C13	C3	99.6(3)
N1	C1	C2	108.1(3)	N1	C13	C12	114.2(4)
C3	C2	C1	103.8(4)	N1	C13	C14	112.0(4)
C2	C3	C4	119.9(4)	C12	C13	C3	103.8(4)
C2	C3	C13	102.5(4)	C12	C13	C14	110.9(3)
C4	C3	C13	115.9(4)	C14	C13	C3	115.7(4)
C5	C4	C3	115.6(4)	C15	C14	C13	116.3(4)
C5	C4	C9	118.9(4)	C19	C14	C13	123.7(4)
C9	C4	C3	124.8(4)	C19	C14	C15	119.9(5)
C4	C5	C6	122.3(4)	C14	C15	C10	115.9(4)
C7	C6	C5	118.6(4)	C16	C15	C10	123.2(4)
C8	C7	C6	120.1(4)	C16	C15	C14	120.8(4)
C7	C8	C9	121.6(4)	C15	C16	C17	119.4(5)
C4	C9	C10	122.9(3)	C16	C17	C18	119.3(5)
C8	C9	C4	118.5(4)	C19	C18	C17	120.8(5)
C8	C9	C10	118.6(4)	C14	C19	C18	119.7(5)
C11	C10	C9	109.4(3)	C21	C20	C11	120.2(4)
C15	C10	C9	109.4(3)	C20	C21	C22	120.2(4)
C15	C10	C11	110.4(3)	C23	C22	C21	120.0(4)
C12	C11	C10	117.8(4)	C22	C23	C12	120.6(4)
C20	C11	C10	122.7(4)				

Table 6 Torsion Angles for xstr0016.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	C3	162.7(5)	C10	C15	C16	C17	-174.9(4)
N1	C1	C2	C3	-18.3(6)	C11	C10	C15	C14	46.8(5)
N1	C13	C14	C15	-171.1(4)	C11	C10	C15	C16	-136.8(4)
N1	C13	C14	C19	10.9(6)	C11	C12	C13	N1	173.9(4)
C1	N1	C13	C3	24.4(5)	C11	C12	C13	C3	-78.7(4)
C1	N1	C13	C12	134.4(4)	C11	C12	C13	C14	46.2(5)
C1	N1	C13	C14	-98.5(5)	C11	C12	C23	C22	0.3(6)
C1	C2	C3	C4	161.9(4)	C11	C20	C21	C22	-1.3(6)
C1	C2	C3	C13	31.8(5)	C12	C11	C20	C21	2.1(6)
C2	C3	C4	C5	48.9(6)	C12	C13	C14	C15	-42.2(5)
C2	C3	C4	C9	-140.5(5)	C12	C13	C14	C19	139.8(4)
C2	C3	C13	N1	-33.7(5)	C13	N1	C1	O1	174.0(5)
C2	C3	C13	C12	-151.7(4)	C13	N1	C1	C2	-5.1(6)
C2	C3	C13	C14	86.5(5)	C13	C3	C4	C5	172.8(4)
C3	C4	C5	C6	172.3(4)	C13	C3	C4	C9	-16.6(6)
C3	C4	C9	C8	-171.4(4)	C13	C12	C23	C22	-171.7(4)
C3	C4	C9	C10	6.0(6)	C13	C14	C15	C10	-4.6(5)
C3	C13	C14	C15	75.7(5)	C13	C14	C15	C16	178.9(4)
C3	C13	C14	C19	-102.3(5)	C13	C14	C19	C18	179.2(4)
C4	C3	C13	N1	-166.2(4)	C14	C15	C16	C17	1.4(7)
C4	C3	C13	C12	75.8(5)	C15	C10	C11	C12	-42.8(5)
C4	C3	C13	C14	-46.0(5)	C15	C10	C11	C20	142.3(4)
C4	C5	C6	C7	-0.4(7)	C15	C14	C19	C18	1.3(8)
C4	C9	C10	C11	-56.8(5)	C15	C16	C17	C18	2.0(7)
C4	C9	C10	C15	64.2(5)	C16	C17	C18	C19	-3.8(8)
C5	C4	C9	C8	-1.1(6)	C17	C18	C19	C14	2.1(8)
C5	C4	C9	C10	176.3(4)	C19	C14	C15	C10	173.4(4)
C5	C6	C7	C8	-0.2(7)	C19	C14	C15	C16	-3.1(7)
C6	C7	C8	C9	0.1(6)	C20	C11	C12	C13	171.2(4)
C7	C8	C9	C4	0.5(6)	C20	C11	C12	C23	-1.6(6)
C7	C8	C9	C10	-177.0(4)	C20	C21	C22	C23	0.0(6)
C8	C9	C10	C11	120.6(4)	C21	C22	C23	C12	0.5(6)
C8	C9	C10	C15	-118.4(4)	C23	C12	C13	N1	-13.8(6)
C9	C4	C5	C6	1.1(6)	C23	C12	C13	C3	93.7(5)
C9	C10	C11	C12	77.5(4)	C23	C12	C13	C14	-141.4(4)
C9	C10	C11	C20	-97.3(4)	C24	N1	C1	O1	7.9(8)
C9	C10	C15	C14	-73.7(4)	C24	N1	C1	C2	-171.1(5)
C9	C10	C15	C16	102.7(5)	C24	N1	C13	C3	-169.9(5)
C10	C11	C12	C13	-3.8(5)	C24	N1	C13	C12	-59.9(7)
C10	C11	C12	C23	-176.6(4)	C24	N1	C13	C14	67.3(6)
C10	C11	C20	C21	176.8(4)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for xstr0016.

Atom	*x*	*y*	*z*	U(eq)
H2A	3895	5042	1967	58
H2B	4293	5710	3516	58
H3	5124	4228	4362	52
H5	5507	5964	2606	41
H6	6581	6295	1449	48
H7	7170	4670	506	47
H8	6692	2763	726	39
H10	5909	1371	1557	35
H16	4879	827	-676	47
H17	3509	749	-1953	60
H18	2534	1744	-949	67
H19	2897	2618	1421	57
H20	6730	801	4040	38
H21	6828	494	6590	47
H22	5810	1195	7715	50
H23	4692	2193	6287	46
H24A	3183	2475	5512	83
H24B	3397	1512	4376	83
H24C	2642	2389	3837	83

Experimental

Single crystals of $C_{24}H_{19}NO$ **[xstr0016]** were **[]**. A suitable crystal was selected and **[Nylon Loop]** on a **SuperNova, Dual, Cu at zero, Atlas** diffractometer. The crystal was kept at 150 K during data collection. Using Olex2 [1], the structure was solved with the Superflip [2] structure solution program using Charge Flipping and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Palatinus, L. & Chapuis, G. (2007). J. Appl. Cryst., 40, 786-790; Palatinus, L. & van der Lee, A. (2008). J. Appl. Cryst. 41, 975-984; Palatinus, L., Prathapa, S. J. & van Smaalen, S. (2012). J. Appl. Cryst. 45, 575-580
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122

Crystal structure determination of [xstr0016]

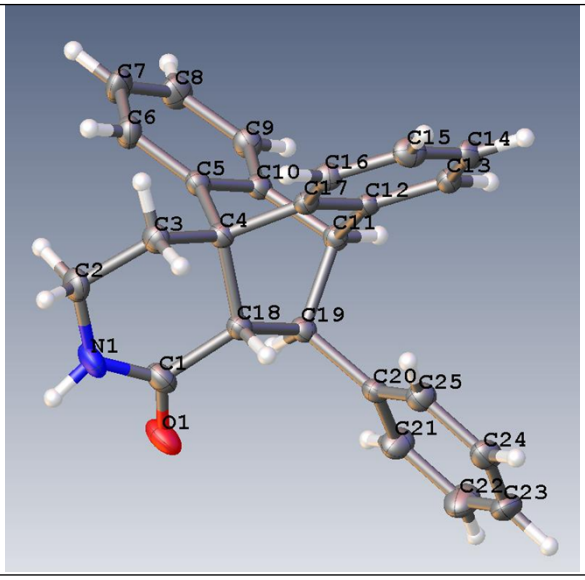
Crystal Data for $C_{24}H_{19}NO$ (M =337.40): monoclinic, space group Cc (no. 9), a = 16.9504(14) Å, b = 11.2305(10) Å, c = 9.1731(9) Å, β = 103.305(10)°, V = 1699.3(3) Å^3, Z = 4, T = 150 K, μ(CuKα) = 0.623 mm^{-1}, *Dcalc* = 1.319 g/mm^3, 2772 reflections measured ($9.528 \leq 2\Theta \leq 149.326$), 1846 unique ($R_{int}$ = 0.0370, R_{sigma} = 0.0415) which were used in all calculations. The final R_1 was 0.0582 ($I > 2\sigma(I)$) and wR_2 was 0.1464 (all data).

Refinement model description

Number of restraints - 2, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Ternary CH refined with riding coordinates:
 C3(H3), C10(H10)
2.b Secondary CH2 refined with riding coordinates:
 C2(H2A,H2B)
2.c Aromatic/amide H refined with riding coordinates:
 C5(H5), C6(H6), C7(H7), C8(H8), C16(H16), C17(H17), C18(H18), C19(H19),
 C20(H20), C21(H21), C22(H22), C23(H23)
2.d Idealised Me refined as rotating group:
 C24(H24A,H24B,H24C)

This report has been created with Olex2, compiled on 2013.12.10 svn.r2850 for OlexSys.

Table 7 Crystal data and structure refinement for **9**



Identification code	xstr0122
Empirical formula	$C_{28.5}H_{21}NO$
Formula weight	393.46
Temperature/K	150
Crystal system	triclinic
Space group	P-1
a/Å	8.9866(3)
b/Å	9.1620(3)
c/Å	13.9462(5)
α/°	93.732(3)
β/°	95.624(3)
γ/°	115.839(4)
Volume/Å^3	1021.00(7)
Z	2
ρ_{calc}mg/mm^3	1.280
m/mm^{-1}	0.598
F(000)	414.0
Crystal size/mm^3	0.28 × 0.26 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection	10.808 to 148.288°
Index ranges	$-11 \le h \le 11$, $-11 \le k \le 11$, $-16 \le l \le 17$
Reflections collected	15762
Independent reflections	4024 [R_{int} = 0.0305, R_{sigma} = 0.0228]
Data/restraints/parameters	4024/0/276
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0584, wR_2 = 0.1567
Final R indexes [all data]	R_1 = 0.0627, wR_2 = 0.1614
Largest diff. peak/hole / e Å^{-3}	0.62/-0.57

Table 8 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for xstr0122. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5113(2)	305.3(18)	3742.3(10)	38.7(4)
N1	3990(2)	1431(2)	4756.7(11)	33.8(4)
C1	4460(2)	1224(2)	3892.5(13)	28.4(4)
C2	2944(2)	2225(2)	4970.6(13)	29.7(4)
C3	2919(2)	3395(2)	4247.9(12)	24.2(4)
C4	2822.5(19)	2740.1(19)	3197.7(11)	19.8(3)
C5	1203(2)	1248.6(19)	2767.7(12)	20.7(3)
C6	-243(2)	540(2)	3187.8(13)	27.2(4)
C7	-1641(2)	-782(2)	2675.0(14)	31.7(4)
C8	-1583(2)	-1414(2)	1761.8(14)	29.1(4)
C9	-140(2)	-693(2)	1324.6(13)	24.5(4)
C10	1233(2)	659.4(19)	1818.0(12)	20.2(3)
C11	2825.7(19)	1664.7(19)	1417.0(11)	18.9(3)
C12	3105.3(18)	3423.7(19)	1536.0(11)	17.7(3)
C13	3409.7(19)	4449(2)	817.9(12)	21.3(3)
C14	3704(2)	6067(2)	1044.7(13)	25.7(4)
C15	3691(2)	6640(2)	1986.7(14)	27.2(4)
C16	3385(2)	5608(2)	2714.6(13)	23.4(4)
C17	3095.4(18)	4003.2(19)	2490.5(11)	18.4(3)
C18	4304(2)	2283(2)	3129.5(11)	20.5(3)
C19	4266(2)	1550.9(19)	2087.9(12)	19.8(3)
C20	5920(2)	2313(2)	1692.3(12)	21.2(3)
C21	6487(2)	1294(2)	1236.8(15)	31.2(4)
C22	7992(3)	1929(3)	871.7(17)	40.0(5)
C23	8969(2)	3601(3)	947.8(15)	35.2(5)
C24	8412(2)	4631(2)	1381.1(14)	30.0(4)
C25	6896(2)	3994(2)	1751.1(13)	25.8(4)
C31	947(5)	5808(6)	5747(3)	38.9(10)
C32	37(7)	5807(6)	4079(4)	58.8(12)
C33	1140(9)	6689(9)	5012(6)	79.6(17)
C34	1118(13)	7333(12)	4399(8)	62(2)
C41	459(9)	5958(8)	4534(6)	46.3(14)
C42	1349(10)	6776(10)	5470(7)	56.5(18)
C43	699(9)	5416(9)	5984(5)	43.4(17)
C44	608(14)	6989(13)	3556(8)	40(2)

Table 9 Anisotropic Displacement Parameters ($Å^2×10^3$) for xstr0122. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	56.1(9)	45.8(8)	29.6(7)	11.9(6)	2.3(6)	36.5(7)
N1	43.0(9)	44.5(9)	21.7(8)	14.6(7)	3.2(7)	25.4(8)
C1	30.4(9)	31.3(9)	24.5(9)	7.5(7)	-1.2(7)	15.1(8)
C2	32.2(9)	37.5(10)	18.8(8)	7.2(7)	4.4(7)	14.1(8)
C3	23.9(8)	27.8(8)	19.3(8)	3.0(6)	1.7(6)	10.2(7)
C4	19.0(7)	21.2(8)	18.8(8)	3.8(6)	1.7(6)	8.7(6)
C5	19.9(8)	20.2(8)	21.2(8)	6.1(6)	1.2(6)	8.0(6)
C6	25.8(9)	31.2(9)	21.5(8)	7.0(7)	5.2(7)	8.8(7)
C7	22.3(8)	33.2(10)	31.4(10)	12.2(8)	7.3(7)	3.0(7)
C8	22.5(8)	22.9(8)	31.7(9)	5.0(7)	-0.1(7)	1.4(7)
C9	24.5(8)	21.7(8)	23.7(8)	2.9(6)	0.8(7)	7.5(7)
C10	19.4(8)	19.5(7)	22.0(8)	5.5(6)	2.0(6)	8.8(6)
C11	18.3(7)	19.2(7)	17.9(7)	3.1(6)	1.3(6)	7.4(6)
C12	12.8(7)	19.3(7)	20.1(8)	4.5(6)	1.2(6)	6.2(6)
C13	16.7(7)	25.1(8)	21.0(8)	6.8(6)	2.8(6)	7.8(6)
C14	21.2(8)	22.8(8)	31.2(9)	13.8(7)	3.9(7)	6.7(7)
C15	25.5(8)	17.4(8)	37.7(10)	5.1(7)	2.6(7)	8.7(7)
C16	21.7(8)	21.9(8)	25.4(8)	1.1(6)	1.9(6)	9.2(6)
C17	13.9(7)	19.7(8)	20.1(8)	3.8(6)	1.4(6)	6.1(6)
C18	19.1(7)	22.1(8)	20.2(8)	5.1(6)	1.3(6)	8.8(6)
C19	20.4(8)	18.2(7)	21.7(8)	4.8(6)	2.2(6)	9.4(6)
C20	19.4(8)	24.4(8)	21.0(8)	6.1(6)	0.5(6)	10.9(6)
C21	30.9(9)	25.9(9)	42.7(11)	9.8(8)	11.0(8)	16.2(8)
C22	41.1(11)	42.2(11)	53.6(13)	16.8(10)	21.3(10)	29.8(10)
C23	22.4(9)	45.6(11)	44.3(11)	19.9(9)	11.6(8)	17.7(8)
C24	21.6(8)	28.9(9)	35.1(10)	9.6(7)	1.2(7)	7.1(7)
C25	22.9(8)	25.7(8)	27.8(9)	4.4(7)	3.1(7)	9.9(7)

Table 10 Bond Lengths for xstr0122.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.237(2)	C15	C16	1.397(2)
N1	C1	1.344(2)	C16	C17	1.385(2)
N1	C2	1.458(2)	C18	C19	1.551(2)
C1	C18	1.521(2)	C19	C20	1.518(2)
C2	C3	1.524(2)	C20	C21	1.392(2)
C3	C4	1.526(2)	C20	C25	1.393(2)
C4	C5	1.528(2)	C21	C22	1.384(3)
C4	C17	1.523(2)	C22	C23	1.385(3)
C4	C18	1.570(2)	C23	C24	1.379(3)
C5	C6	1.385(2)	C24	C25	1.395(3)
C5	C10	1.405(2)	C31	C32[1]	1.406(7)
C6	C7	1.393(3)	C31	C33	1.324(9)
C7	C8	1.379(3)	C32	C31[1]	1.407(7)
C8	C9	1.397(3)	C32	C33	1.497(9)
C9	C10	1.386(2)	C32	C34	1.322(11)
C10	C11	1.511(2)	C33	C34	1.073(12)
C11	C12	1.514(2)	C41	C42	1.432(11)
C11	C19	1.567(2)	C41	C43[1]	1.335(10)
C12	C13	1.383(2)	C41	C44	1.692(13)
C12	C17	1.403(2)	C42	C43	1.404(11)
C13	C14	1.396(2)	C43	C41[1]	1.335(10)
C14	C15	1.385(3)			

[1]-X,1-Y,1-Z

Table 11 Bond Angles for xstr0122.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C2	126.58(15)	C17	C16	C15	119.59(16)
O1	C1	N1	121.64(16)	C12	C17	C4	113.49(13)
O1	C1	C18	120.73(16)	C16	C17	C4	126.58(15)
N1	C1	C18	117.40(15)	C16	C17	C12	119.88(15)
N1	C2	C3	113.37(15)	C1	C18	C4	113.82(14)
C2	C3	C4	113.30(14)	C1	C18	C19	112.32(13)
C3	C4	C5	116.09(14)	C19	C18	C4	111.74(12)
C3	C4	C18	108.36(13)	C18	C19	C11	107.69(12)
C5	C4	C18	108.00(13)	C20	C19	C11	112.12(13)
C17	C4	C3	113.72(13)	C20	C19	C18	114.56(13)
C17	C4	C5	105.85(12)	C21	C20	C19	118.91(15)
C17	C4	C18	104.04(12)	C21	C20	C25	117.95(16)
C6	C5	C4	127.07(15)	C25	C20	C19	123.13(15)
C6	C5	C10	119.73(15)	C22	C21	C20	121.08(17)
C10	C5	C4	113.05(14)	C21	C22	C23	120.58(18)
C5	C6	C7	119.67(16)	C24	C23	C22	119.17(17)
C8	C7	C6	120.57(17)	C23	C24	C25	120.35(17)
C7	C8	C9	120.23(16)	C20	C25	C24	120.85(17)
C10	C9	C8	119.39(16)	C33	C31	C32[1]	137.7(5)
C5	C10	C11	113.75(14)	C31[1]	C32	C33	106.7(5)
C9	C10	C5	120.28(15)	C34	C32	C31[1]	150.5(7)
C9	C10	C11	125.93(15)	C34	C32	C33	44.2(5)
C10	C11	C12	107.40(13)	C31	C33	C32	115.6(6)
C10	C11	C19	106.15(12)	C34	C33	C31	172.3(9)
C12	C11	C19	107.84(12)	C34	C33	C32	59.2(7)
C13	C12	C11	126.22(15)	C33	C34	C32	76.6(8)
C13	C12	C17	120.32(14)	C42	C41	C44	121.4(7)
C17	C12	C11	113.43(13)	C43[1]	C41	C42	147.3(7)
C12	C13	C14	119.76(15)	C43[1]	C41	C44	91.0(8)
C15	C14	C13	119.96(15)	C43	C42	C41	97.1(6)
C14	C15	C16	120.49(15)	C41[1]	C43	C42	115.4(7)

[1]-X,1-Y,1-Z

Table 12Torsion Angles for xstr0122.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C18	C4	153.95(17)	C11	C12	C13	C14	-177.71(14)
O1	C1	C18	C19	25.7(2)	C11	C12	C17	C4	0.56(18)
N1	C1	C18	C4	-31.4(2)	C11	C12	C17	C16	178.11(14)
N1	C1	C18	C19	-159.69(16)	C11	C19	C20	C21	-103.16(17)
N1	C2	C3	C4	41.2(2)	C11	C19	C20	C25	75.97(19)
C1	N1	C2	C3	-22.1(3)	C12	C11	C19	C18	53.87(16)
C1	C18	C19	C11	134.55(14)	C12	C11	C19	C20	-73.04(16)
C1	C18	C19	C20	-99.97(16)	C12	C13	C14	C15	0.1(2)
C2	N1	C1	O1	-167.80(18)	C13	C12	C17	C4	-177.27(13)
C2	N1	C1	C18	17.7(3)	C13	C12	C17	C16	0.3(2)
C2	C3	C4	C5	66.70(19)	C13	C14	C15	C16	0.0(3)
C2	C3	C4	C17	-170.12(14)	C14	C15	C16	C17	0.1(3)
C2	C3	C4	C18	-54.97(18)	C15	C16	C17	C4	176.94(15)
C3	C4	C5	C6	7.5(2)	C15	C16	C17	C12	-0.3(2)
C3	C4	C5	C10	-176.86(13)	C17	C4	C5	C6	-119.65(18)
C3	C4	C17	C12	176.38(13)	C17	C4	C5	C10	55.95(17)
C3	C4	C17	C16	-1.0(2)	C17	C4	C18	C1	170.95(13)
C3	C4	C18	C1	49.63(18)	C17	C4	C18	C19	-60.51(16)
C3	C4	C18	C19	178.17(13)	C17	C12	C13	C14	-0.2(2)
C4	C5	C6	C7	177.21(16)	C18	C4	C5	C6	129.40(17)
C4	C5	C10	C9	179.84(14)	C18	C4	C5	C10	-55.00(17)
C4	C5	C10	C11	-2.30(19)	C18	C4	C17	C12	58.71(16)
C4	C18	C19	C11	5.22(17)	C18	C4	C17	C16	-118.65(17)
C4	C18	C19	C20	130.70(14)	C18	C19	C20	C21	133.71(16)
C5	C4	C17	C12	-55.01(17)	C18	C19	C20	C25	-47.2(2)
C5	C4	C17	C16	127.63(16)	C19	C11	C12	C13	117.50(16)
C5	C4	C18	C1	-76.88(17)	C19	C11	C12	C17	-60.18(17)
C5	C4	C18	C19	51.65(17)	C19	C20	C21	C22	-179.46(17)
C5	C6	C7	C8	1.5(3)	C19	C20	C25	C24	179.60(15)
C5	C10	C11	C12	-52.83(17)	C20	C21	C22	C23	-0.3(3)
C5	C10	C11	C19	62.31(16)	C21	C20	C25	C24	-1.3(3)
C6	C5	C10	C9	-4.2(2)	C21	C22	C23	C24	-0.9(3)
C6	C5	C10	C11	173.65(15)	C22	C23	C24	C25	1.0(3)
C6	C7	C8	C9	-2.5(3)	C23	C24	C25	C20	0.1(3)
C7	C8	C9	C10	0.2(3)	C25	C20	C21	C22	1.4(3)
C8	C9	C10	C5	3.2(2)	C31[1]	C32	C33	C31	-0.4(7)
C8	C9	C10	C11	-174.42(15)	C31[1]	C32	C33	C34	-174.0(8)
C9	C10	C11	C12	124.88(17)	C31[1]	C32	C34	C33	11.7(15)
C9	C10	C11	C19	-119.97(17)	C32[1]	C31	C33	C32	0.6(10)
C10	C5	C6	C7	1.9(3)	C34	C32	C33	C31	173.6(10)
C10	C11	C12	C13	-128.49(16)	C41	C42	C43	C41[1]	-3.5(9)
C10	C11	C12	C17	53.84(16)	C43[1]	C41	C42	C43	5.9(14)
C10	C11	C19	C18	-60.98(15)	C44	C41	C42	C43	176.3(7)
C10	C11	C19	C20	172.11(13)					

Table 13 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for xstr0122.

Atom	*x*	*y*	*z*	U(eq)
H1	4343	1056	5232	41
H2A	3346	2824	5616	36
H2B	1812	1393	4972	36
H3A	3921	4422	4413	29
H3B	1967	3615	4305	29
H6	-282	945	3809	33
H7	-2621	-1242	2951	38
H8	-2509	-2323	1436	35
H9	-101	-1116	708	29
H11	2773	1272	738	23
H13	3418	4063	186	26
H14	3908	6760	564	31
H15	3888	7718	2136	33
H16	3375	5997	3346	28
H18	5328	3315	3262	25
H19	3965	389	2106	24
H21	5845	168	1177	37
H22	8351	1226	573	48
H23	9987	4024	710	42
H24	9051	5757	1427	36
H25	6533	4701	2041	31

Table14 Atomic Occupancy for xstr0122.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
C31	0.6	C32	0.6	C33	0.6
C34	0.3	C41	0.4	C42	0.4
C43	0.4	C44	0.2		

Experimental

Single crystals of $C_{28.5}H_{21}NO$ **[xstr0122]** were crystallised from DCM/toluene. A suitable crystal was selected and **[Nylon Loop]** on a **SuperNova, Dual, Cu at zero, Atlas** diffractometer. The crystal was kept at 150 K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122

Crystal structure determination of [xstr0122]

Crystal Data for $C_{28.5}H_{21}NO$ (M =393.46): triclinic, space group P-1 (no. 2), a = 8.9866(3) Å, b = 9.1620(3) Å, c = 13.9462(5) Å, α = 93.732(3)°, β = 95.624(3)°, γ = 115.839(4)°, V = 1021.00(7) Å^3, Z = 2, T = 150 K, μ(CuKα) = 0.598 mm^{-1},*Dcalc* = 1.280 g/mm^3, 15762 reflections measured (10.808 ≤ 2Θ ≤ 148.288), 4024 unique (R_{int} = 0.0305, R_{sigma} = 0.0228) which were used in all calculations. The final R_1 was 0.0584 (I > 2σ(I)) and wR_2 was 0.1614 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
At 1.2 times of:
All C(H) groups, All C(H,H) groups, All N(H) groups
2. Others
Fixed Sof: C31(0.6) C32(0.6) C33(0.6) C34(0.3) C41(0.4) C42(0.4) C43(0.4) C44(0.2)
3.a Ternary CH refined with riding coordinates:
C11(H11), C18(H18), C19(H19)
3.b Secondary CH2 refined with riding coordinates:
C2(H2A,H2B), C3(H3A,H3B)
3.c Aromatic/amide H refined with riding coordinates:
N1(H1), C6(H6), C7(H7), C8(H8), C9(H9), C13(H13), C14(H14), C15(H15), C16(H16), C21(H21), C22(H22), C23(H23), C24(H24), C25(H25)