Supplementary Material for Organic & Biomolecular Chemistry

Dichotomies in microwave-assisted propargyl–isomerization–Claisen domino sequences dependent on base strengths

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Supporting Information

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6-Benzhydrylidene-8-(4-nitro-phenyl)-tricyclo[3.2.1.0^{2,7}]oct-3-en-1-yl]-phenyl-methanone (2a)

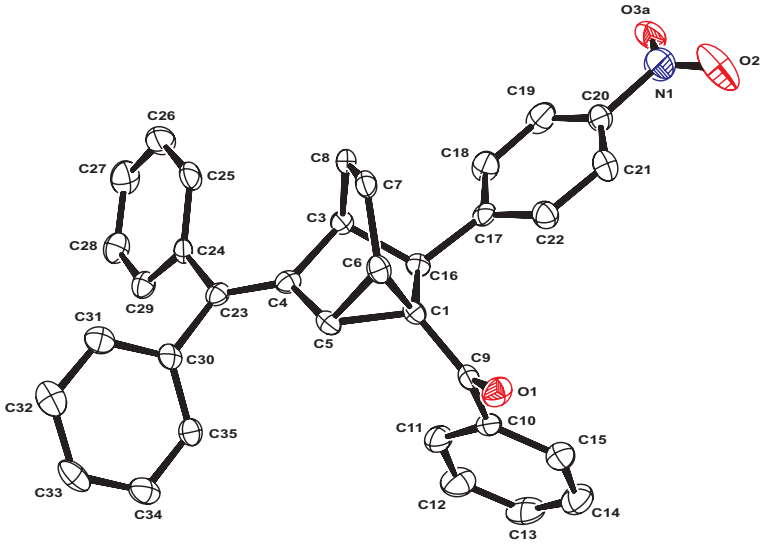


Table 1: Crystal data and structure refinement for **2a**.

Empirical formula	$C_{37}H_{31}NO_4$	
Formula weight	553.63	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Z	4	
Unit cell dimensions	a = 15.348(2) Å	α = 90.0 deg.
	b = 8.806(1) Å	β =109.831(3) deg.
	c = 22.612(4) Å	γ = 90.0 deg.
Volume	2874.9(7) Å^3	
Density (calculated)	1.28 g/cm^3	
Absorption coefficient	0.08 mm^{-1}	
Crystal shape	irregular	
Crystal size	0.43 x 0.065 x 0.04 mm^3	
Theta range for data collection	2.5 to 22.0 deg.	
Index ranges	-16≤h≤16, -9≤k≤9, -23≤l≤23	
Reflections collected	16360	
Independent reflections	3488 (R(int) = 0.0536)	
Observed reflections	2697 (I >2σ(I))	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.99 and 0.98	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3488 / 0 / 509	
Goodness-of-fit on F^2	1.04	
Final R indices (I>2σ(I))	R1 = 0.048, wR2 = 0.107	
Largest diff. peak and hole	0.54 and -0.59 eÅ^{-3}	

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

Atom	x	y	z	U_{eq}

O1	0.0267(1)	0.2994(2)	0.5058(1)	0.0258(5)
O2	0.3837(2)	-0.2924(3)	0.6161(2)	0.0610(8)
O3	0.4813(5)	-0.2290(7)	0.6948(3)	0.0525(16)
O3A	0.5199(4)	-0.1722(6)	0.6778(3)	0.0353(13)
N1	0.4250(2)	-0.1875(4)	0.6488(2)	0.0536(9)
C1	0.1420(2)	0.3945(3)	0.5974(1)	0.0175(6)
C3	0.2564(2)	0.4570(3)	0.6971(1)	0.0178(7)
C4	0.1821(2)	0.5802(3)	0.6813(1)	0.0188(7)
C5	0.1035(2)	0.5152(3)	0.6310(1)	0.0196(7)
C6	0.0884(2)	0.3450(3)	0.6399(1)	0.0196(7)
C7	0.1415(2)	0.2787(3)	0.7014(1)	0.0197(7)
C8	0.2248(2)	0.3341(3)	0.7317(1)	0.0193(7)
C9	0.0973(2)	0.3745(3)	0.5279(1)	0.0199(7)
C10	0.1408(2)	0.4484(3)	0.4857(1)	0.0204(7)
C11	0.1847(2)	0.5886(3)	0.4998(2)	0.0291(8)
C12	0.2206(2)	0.6568(4)	0.4579(2)	0.0378(9)
C13	0.2145(2)	0.5853(4)	0.4024(2)	0.0396(9)
C14	0.1716(2)	0.4462(4)	0.3876(2)	0.0352(8)
C15	0.1345(2)	0.3776(4)	0.4290(1)	0.0274(8)
C16	0.2464(2)	0.3928(3)	0.6301(1)	0.0179(7)
C17	0.2930(2)	0.2399(3)	0.6322(1)	0.0186(7)
C18	0.3857(2)	0.2228(4)	0.6681(1)	0.0285(8)
C19	0.4299(2)	0.0843(4)	0.6742(2)	0.0345(9)
C20	0.3799(2)	-0.0377(4)	0.6414(1)	0.0309(8)
C21	0.2891(2)	-0.0256(4)	0.6041(2)	0.0297(8)
C22	0.2453(2)	0.1140(3)	0.5999(1)	0.0240(7)
C23	0.1846(2)	0.7164(3)	0.7090(1)	0.0182(7)
C24	0.2657(2)	0.7723(3)	0.7617(1)	0.0187(7)
C25	0.3165(2)	0.6786(4)	0.8112(1)	0.0262(7)
C26	0.3931(2)	0.7325(4)	0.8590(2)	0.0356(9)
C27	0.4213(2)	0.8815(4)	0.8580(2)	0.0362(9)
C28	0.3715(2)	0.9769(4)	0.8101(1)	0.0295(8)
C29	0.2942(2)	0.9237(3)	0.7630(1)	0.0237(7)
C30	0.1027(2)	0.8224(3)	0.6874(1)	0.0180(7)
C31	0.0576(2)	0.8647(3)	0.7291(2)	0.0239(7)
C32	-0.0182(2)	0.9610(3)	0.7107(2)	0.0281(8)
C33	-0.0495(2)	1.0190(3)	0.6502(2)	0.0280(8)
C34	-0.0052(2)	0.9798(3)	0.6084(2)	0.0277(8)
C35	0.0696(2)	0.8822(3)	0.6268(1)	0.0225(7)
O50	0.5830(5)	0.8589(7)	0.6076(3)	0.092(2)
C50	0.6140(6)	0.8271(8)	0.5646(5)	0.0449(19)
C51	0.6943(7)	0.9148(11)	0.5623(5)	0.072(2)
O50A	0.4930(5)	0.9416(7)	0.5343(3)	0.085(2)
C50A	0.5503(8)	0.8594(10)	0.5298(4)	0.055(2)
C51A	0.6291(7)	0.9211(11)	0.5177(5)	0.072(2)
C52	0.5653(4)	0.6986(5)	0.5273(2)	0.126(3)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **2a**.

Atom	x	y	z	U_{eq}
H3	0.3186(18)	0.494(3)	0.7201(11)	0.010(6)
H5	0.0496(18)	0.573(3)	0.6091(12)	0.012(7)
H6	0.029(2)	0.311(3)	0.6168(12)	0.019(7)
H7	0.1174(19)	0.200(3)	0.7195(13)	0.026(8)
H8	0.2646(18)	0.300(3)	0.7733(13)	0.020(7)
H11	0.1908(18)	0.640(3)	0.5382(14)	0.023(8)
H12	0.252(2)	0.755(4)	0.4688(15)	0.043(9)
H13	0.238(2)	0.632(3)	0.3720(15)	0.038(9)

H14	0.168(2)	0.388(3)	0.3455(15)	0.038(8)
H15	0.103(2)	0.282(3)	0.4202(13)	0.029(8)
H16	0.2751(16)	0.466(3)	0.6118(11)	0.004(6)
H18	0.420(2)	0.305(3)	0.6897(13)	0.026(8)
H19	0.492(2)	0.071(3)	0.7000(15)	0.041(9)
H21	0.258(2)	-0.114(4)	0.5813(14)	0.032(8)
H22	0.178(2)	0.122(3)	0.5748(14)	0.032(8)
H25	0.2955(18)	0.581(3)	0.8122(12)	0.022(8)
H26	0.427(2)	0.669(3)	0.8926(14)	0.028(8)
H27	0.476(2)	0.917(4)	0.8905(15)	0.041(9)
H28	0.3909(19)	1.085(3)	0.8089(13)	0.028(8)
H29	0.2569(19)	0.992(3)	0.7287(13)	0.022(7)
H31	0.0793(18)	0.822(3)	0.7710(14)	0.026(8)
H32	-0.050(2)	0.984(3)	0.7395(14)	0.033(9)
H33	-0.1021(19)	1.087(3)	0.6371(12)	0.019(7)
H34	-0.027(2)	1.023(3)	0.5659(16)	0.040(9)
H35	0.0974(19)	0.849(3)	0.5974(13)	0.024(8)
H51A	0.7123	0.8794	0.5270	0.109
H51B	0.7462	0.9008	0.6016	0.109
H51C	0.6780	1.0227	0.5566	0.109
H51D	0.6268	1.0322	0.5189	0.109
H51E	0.6282	0.8881	0.4761	0.109
H51F	0.6860	0.8851	0.5498	0.109
H52A	0.5160	0.6650	0.5428	0.189
H52B	0.6090	0.6150	0.5308	0.189
H52C	0.5381	0.7292	0.4831	0.189

Table 4: Anisotropic displacement parameters ($Å^2$) for **2a**. 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	Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0257(12)	0.0261(12)	0.0224(11)	-0.0030(9)	0.0038(9)	-0.0063(10)	
O2	0.0543(17)	0.0283(15)	0.106(2)	0.0049(16)	0.0342(16)	0.0115(13)	
O3	0.062(4)	0.053(4)	0.030(3)	0.001(3)	-0.001(3)	0.035(3)	
O3A	0.033(3)	0.029(3)	0.039(3)	0.004(2)	0.006(3)	0.012(2)	
N1	0.066(2)	0.052(2)	0.037(2)	-0.0002(17)	0.0101(18)	0.040(2)	
C1	0.0189(15)	0.0132(15)	0.0205(16)	0.0007(12)	0.0070(13)	-0.0001(12)	
C3	0.0161(16)	0.0175(16)	0.0186(16)	-0.0011(13)	0.0042(13)	-0.0008(13)	
C4	0.0208(16)	0.0179(17)	0.0175(16)	0.0018(13)	0.0060(13)	-0.0038(13)	
C5	0.0207(17)	0.0154(16)	0.0230(17)	0.0024(13)	0.0077(14)	0.0029(13)	
C6	0.0193(17)	0.0155(16)	0.0241(17)	-0.0027(13)	0.0075(14)	-0.0027(13)	
C7	0.0269(18)	0.0135(16)	0.0229(17)	-0.0014(14)	0.0138(15)	-0.0001(14)	
C8	0.0245(18)	0.0175(16)	0.0167(17)	-0.0019(13)	0.0083(14)	0.0042(13)	
C9	0.0222(17)	0.0148(15)	0.0218(17)	-0.0022(13)	0.0061(13)	0.0038(14)	
C10	0.0216(16)	0.0205(17)	0.0172(16)	0.0018(13)	0.0040(13)	0.0012(13)	
C11	0.040(2)	0.0234(19)	0.0221(18)	0.0004(15)	0.0078(15)	-0.0042(15)	
C12	0.049(2)	0.030(2)	0.033(2)	0.0080(17)	0.0122(17)	-0.0096(17)	
C13	0.042(2)	0.052(2)	0.029(2)	0.0169(19)	0.0172(17)	0.0022(18)	
C14	0.037(2)	0.045(2)	0.026(2)	0.0009(17)	0.0136(16)	0.0019(17)	
C15	0.0270(17)	0.0281(19)	0.0253(19)	-0.0001(15)	0.0067(14)	0.0002(15)	
C16	0.0211(16)	0.0142(16)	0.0201(16)	0.0019(13)	0.0094(13)	-0.0035(13)	
C17	0.0201(16)	0.0235(17)	0.0150(15)	0.0007(13)	0.0098(13)	0.0012(13)	
C18	0.0220(18)	0.034(2)	0.0281(18)	-0.0048(16)	0.0074(15)	0.0017(17)	
C19	0.0237(19)	0.054(2)	0.0243(18)	-0.0038(17)	0.0058(15)	0.0142(18)	
C20	0.038(2)	0.031(2)	0.0246(18)	0.0005(15)	0.0123(16)	0.0188(16)	
C21	0.034(2)	0.0230(19)	0.0329(19)	-0.0032(15)	0.0128(16)	0.0062(16)	
C22	0.0228(18)	0.0234(18)	0.0258(17)	-0.0006(14)	0.0083(15)	0.0023(14)	
C23	0.0214(16)	0.0184(16)	0.0159(16)	0.0009(13)	0.0079(12)	-0.0029(13)	

C24	0.0210(16)	0.0174(16)	0.0191(16)	-0.0043(13)	0.0086(13)	0.0017(13)
C25	0.0315(18)	0.0164(18)	0.0274(19)	-0.0067(15)	0.0054(15)	0.0018(15)
C26	0.034(2)	0.034(2)	0.028(2)	-0.0038(17)	-0.0034(16)	0.0072(17)
C27	0.0269(19)	0.040(2)	0.035(2)	-0.0123(18)	0.0020(17)	-0.0034(17)
C28	0.0309(19)	0.029(2)	0.0297(19)	-0.0065(16)	0.0124(16)	-0.0071(16)
C29	0.0268(17)	0.0226(18)	0.0226(18)	-0.0040(15)	0.0096(15)	-0.0032(14)
C30	0.0206(16)	0.0102(15)	0.0220(17)	-0.0023(13)	0.0055(13)	-0.0051(12)
C31	0.0264(18)	0.0176(17)	0.0282(19)	0.0035(15)	0.0100(15)	-0.0039(14)
C32	0.0264(18)	0.0206(18)	0.043(2)	0.0010(16)	0.0195(17)	-0.0031(15)
C33	0.0207(17)	0.0142(16)	0.045(2)	-0.0009(15)	0.0053(16)	0.0006(14)
C34	0.0296(19)	0.0158(17)	0.029(2)	-0.0010(15)	-0.0016(16)	-0.0016(15)
C35	0.0271(18)	0.0157(16)	0.0236(18)	-0.0038(14)	0.0073(15)	-0.0019(14)
O50	0.123(6)	0.078(5)	0.093(5)	-0.020(4)	0.062(5)	-0.047(4)
C50	0.057(6)	0.033(5)	0.049(5)	-0.003(4)	0.025(5)	-0.007(4)
C51	0.099(7)	0.062(4)	0.071(6)	-0.004(5)	0.050(4)	0.000(5)
O50A	0.088(5)	0.054(4)	0.099(5)	-0.022(3)	0.015(4)	0.016(4)
C50A	0.084(7)	0.043(6)	0.034(5)	0.001(4)	0.013(5)	-0.008(5)
C51A	0.099(7)	0.062(4)	0.071(6)	-0.004(5)	0.050(4)	0.000(5)
C52	0.173(6)	0.056(3)	0.087(4)	-0.008(3)	-0.038(4)	0.034(4)

Table 5: Bond lengths (Å) and angles (deg) for **2a**.

O1-C9	1.222(3)	C18-H18	0.93(3)
O2-N1	1.218(4)	C19-C20	1.381(5)
O3-O3A	0.952(6)	C19-H19	0.95(3)
O3-N1	1.164(6)	C20-C21	1.366(4)
O3A-N1	1.387(6)	C21-C22	1.389(4)
N1-C20	1.473(4)	C21-H21	0.96(3)
C1-C9	1.497(4)	C22-H22	1.00(3)
C1-C16	1.520(4)	C23-C24	1.485(4)
C1-C6	1.525(4)	C23-C30	1.507(4)
C1-C5	1.538(4)	C24-C25	1.395(4)
C3-C8	1.509(4)	C24-C29	1.400(4)
C3-C4	1.526(4)	C25-C26	1.385(4)
C3-C16	1.575(4)	C25-H25	0.92(3)
C3-H3	0.97(3)	C26-C27	1.385(5)
C4-C23	1.348(4)	C26-H26	0.95(3)
C4-C5	1.466(4)	C27-C28	1.378(5)
C5-C6	1.541(4)	C27-H27	0.96(3)
C5-H5	0.95(3)	C28-C29	1.380(4)
C6-C7	1.475(4)	C28-H28	1.00(3)
C6-H6	0.93(3)	C29-H29	1.00(3)
C7-C8	1.321(4)	C30-C35	1.394(4)
C7-H7	0.94(3)	C30-C31	1.396(4)
C8-H8	0.98(3)	C31-C32	1.384(4)
C9-C10	1.487(4)	C31-H31	0.97(3)
C10-C11	1.391(4)	C32-C33	1.385(4)
C10-C15	1.398(4)	C32-H32	0.95(3)
C11-C12	1.384(4)	C33-C34	1.382(5)
C11-H11	0.96(3)	C33-H33	0.97(3)
C12-C13	1.378(5)	C34-C35	1.381(4)
C12-H12	0.98(3)	C34-H34	0.98(3)
C13-C14	1.378(5)	C35-H35	0.95(3)
C13-H13	0.96(3)	O50-C50	1.250(9)
C14-C15	1.387(4)	C50-C52	1.458(9)
C14-H14	1.06(3)	C50-C51	1.471(12)
C15-H15	0.96(3)	C51-H51A	0.9800
C16-C17	1.517(4)	C51-H51B	0.9800
C16-H16	0.95(2)	C51-H51C	0.9800
C17-C18	1.386(4)	O50A-C50A	1.170(11)
C17-C22	1.391(4)	C50A-C52	1.439(10)
C18-C19	1.380(4)	C50A-C51A	1.434(13)

C51A-H51D	0.9800
C51A-H51E	0.9800
C51A-H51F	0.9800
C52-H52A	0.9800
C52-H52B	0.9800
C52-H52C	0.9800
O3A-O3-N1	81.3(6)
O3-O3A-N1	56.0(5)
O3-N1-O2	112.3(5)
O3-N1-O3A	42.7(3)
O2-N1-O3A	127.4(3)
O3-N1-C20	124.1(4)
O2-N1-C20	118.8(3)
O3A-N1-C20	110.2(4)
C9-C1-C16	122.8(2)
C9-C1-C6	118.3(2)
C16-C1-C6	113.3(2)
C9-C1-C5	119.0(2)
C16-C1-C5	106.6(2)
C6-C1-C5	60.39(18)
C8-C3-C4	106.5(2)
C8-C3-C16	107.3(2)
C4-C3-C16	102.1(2)
C8-C3-H3	113.1(14)
C4-C3-H3	113.9(14)
C16-C3-H3	113.1(14)
C23-C4-C5	126.4(3)
C23-C4-C3	128.6(2)
C5-C4-C3	104.9(2)
C4-C5-C1	107.4(2)
C4-C5-C6	113.5(2)
C1-C5-C6	59.41(18)
C4-C5-H5	122.3(15)
C1-C5-H5	121.6(15)
C6-C5-H5	116.5(15)
C7-C6-C1	117.7(2)
C7-C6-C5	116.7(2)
C1-C6-C5	60.20(18)
C7-C6-H6	121.7(17)
C1-C6-H6	111.7(16)
C5-C6-H6	113.6(17)
C8-C7-C6	118.1(3)
C8-C7-H7	120.0(17)
C6-C7-H7	121.9(17)
C7-C8-C3	114.9(3)
C7-C8-H8	124.3(16)
C3-C8-H8	120.7(16)
O1-C9-C10	120.2(2)
O1-C9-C1	121.3(2)
C10-C9-C1	118.5(2)
C11-C10-C15	118.9(3)
C11-C10-C9	121.9(3)
C15-C10-C9	119.1(3)
C12-C11-C10	120.2(3)
C12-C11-H11	118.4(16)
C10-C11-H11	121.4(16)
C13-C12-C11	120.3(3)
C13-C12-H12	120.5(19)
C11-C12-H12	119.1(19)
C14-C13-C12	120.4(3)
C14-C13-H13	117.7(18)
C12-C13-H13	121.9(19)
C13-C14-C15	119.7(3)
C13-C14-H14	121.2(16)
C15-C14-H14	119.0(16)
C14-C15-C10	120.5(3)
C14-C15-H15	122.5(17)
C10-C15-H15	117.0(17)
C17-C16-C1	115.6(2)
C17-C16-C3	113.4(2)
C1-C16-C3	101.9(2)
C17-C16-H16	109.4(14)
C1-C16-H16	110.5(14)
C3-C16-H16	105.5(14)
C18-C17-C22	118.3(3)
C18-C17-C16	119.6(3)
C22-C17-C16	122.2(2)
C19-C18-C17	121.8(3)
C19-C18-H18	117.5(17)
C17-C18-H18	120.7(17)
C18-C19-C20	117.9(3)
C18-C19-H19	122.2(19)
C20-C19-H19	119.9(19)
C21-C20-C19	122.4(3)
C21-C20-N1	118.8(3)
C19-C20-N1	118.8(3)
C20-C21-C22	118.7(3)
C20-C21-H21	118.8(18)
C22-C21-H21	122.4(18)
C21-C22-C17	120.8(3)
C21-C22-H22	119.2(17)
C17-C22-H22	119.9(16)
C4-C23-C24	123.4(2)
C4-C23-C30	120.8(2)
C24-C23-C30	115.8(2)
C25-C24-C29	117.4(3)
C25-C24-C23	122.4(3)
C29-C24-C23	120.2(2)
C26-C25-C24	121.3(3)
C26-C25-H25	120.8(17)
C24-C25-H25	117.8(17)
C25-C26-C27	119.9(3)
C25-C26-H26	121.0(18)
C27-C26-H26	119.1(18)
C28-C27-C26	119.9(3)
C28-C27-H27	120.8(19)
C26-C27-H27	119.3(19)
C29-C28-C27	120.1(3)
C29-C28-H28	119.2(16)
C27-C28-H28	120.7(16)
C28-C29-C24	121.3(3)
C28-C29-H29	120.8(16)
C24-C29-H29	117.9(16)
C35-C30-C31	117.7(3)
C35-C30-C23	122.6(2)
C31-C30-C23	119.8(2)
C32-C31-C30	121.3(3)
C32-C31-H31	120.3(16)
C30-C31-H31	118.3(16)
C31-C32-C33	119.8(3)
C31-C32-H32	119.6(18)
C33-C32-H32	120.6(18)
C34-C33-C32	119.9(3)
C34-C33-H33	119.8(16)
C32-C33-H33	120.3(16)
C35-C34-C33	120.1(3)
C35-C34-H34	120.9(18)
C33-C34-H34	119.1(18)
C34-C35-C30	121.3(3)

C34-C35-H35	120.5(17)
C30-C35-H35	118.0(17)
O50-C50-C52	111.6(7)
O50-C50-C51	117.1(8)
C52-C50-C51	131.2(8)
C50-C51-H51A	109.5
C50-C51-H51B	109.5
H51A-C51-H51B	109.5
C50-C51-H51C	109.5
H51A-C51-H51C	109.5
H51B-C51-H51C	109.5
O50A-C50A-C52	138.3(9)
O50A-C50A-C51A	119.3(8)
C52-C50A-C51A	102.1(9)
C50A-C51A-H51D	109.5
C50A-C51A-H51E	109.5
H51D-C51A-H51E	109.5
C50A-C51A-H51F	109.5
H51D-C51A-H51F	109.5
H51E-C51A-H51F	109.5
C50A-C52-C50	43.1(4)
C50A-C52-H52A	97.5
C50-C52-H52A	109.5
C50A-C52-H52B	148.2
C50-C52-H52B	109.5
H52A-C52-H52B	109.5
C50A-C52-H52C	75.5
C50-C52-H52C	109.5
H52A-C52-H52C	109.5
H52B-C52-H52C	109.5

(4-8-Benzhydrylidene-7-benzoyl-tricyclo[3.2.1.0^{2,7}]oct-3-en-6-yl)-benzonitrile (2c)

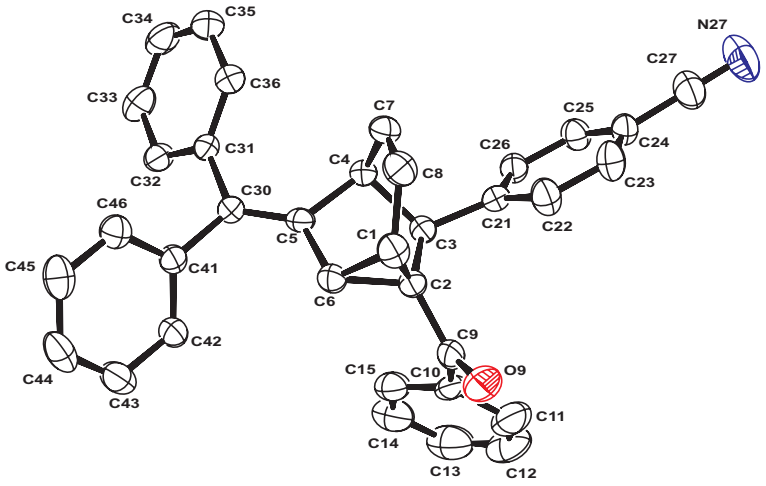


Table 1: Crystal data and structure refinement for **2c**.

Empirical formula	$C_{35}H_{25}NO$	
Formula weight	475.56	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	6	
Unit cell dimensions	a = 12.1762(2) Å	α = 80.239(1) deg.
	b = 17.4387(2) Å	β = 73.766(1) deg.
	c = 20.1060(1) Å	γ = 73.137(1) deg.
Volume	3904.56(8) Å^3	
Density (calculated)	1.21 g/cm^3	
Absorption coefficient	0.07 mm^{-1}	
Crystal shape	plate	
Crystal size	0.40 x 0.24 x 0.08 mm^3	
Crystal colour	colourless	
Theta range for data collection	1.7 to 22.7 deg.	
Index ranges	$-13\le h\le 13$, $-18\le k\le 18$, $-21\le l\le 21$	
Reflections collected	26587	
Independent reflections	10487 (R(int) = 0.0491)	
Observed reflections	7415 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.99 and 0.97	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	10487 / 0 / 1000	
Goodness-of-fit on F^2	1.03	
Final R indices ($I>2\sigma(I)$)	R1 = 0.049, wR2 = 0.107	
Largest diff. peak and hole	0.37 and -0.23 eÅ^{-3}	

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

Atom	x	y	z	U_{eq}
O9	-0.1767(2)	0.2384(1)	0.2153(1)	0.0562(5)
N27	-0.0174(3)	-0.2500(2)	0.2083(1)	0.0716(8)
C1	0.0773(2)	0.1871(1)	0.2075(1)	0.0358(6)

C2	0.0197(2)	0.1906(1)	0.1489(1)	0.0310(6)
C3	0.0826(2)	0.1250(1)	0.0997(1)	0.0286(6)
C4	0.2165(2)	0.1186(1)	0.0945(1)	0.0290(6)
C5	0.2163(2)	0.2069(1)	0.0914(1)	0.0271(6)
C6	0.1052(2)	0.2431(1)	0.1409(1)	0.0323(6)
C7	0.2430(2)	0.0800(1)	0.1630(1)	0.0347(6)
C8	0.1726(2)	0.1152(2)	0.2185(1)	0.0381(6)
C9	-0.1104(2)	0.2263(1)	0.1581(2)	0.0383(7)
C10	-0.1556(2)	0.2453(2)	0.0934(2)	0.0409(7)
C11	-0.2619(3)	0.2285(2)	0.0945(2)	0.0649(9)
C12	-0.3007(3)	0.2447(2)	0.0324(2)	0.0700(10)
C13	-0.2378(3)	0.2791(2)	-0.0267(2)	0.0726(10)
C14	-0.1362(3)	0.2972(2)	-0.0277(2)	0.0581(8)
C15	-0.0947(2)	0.2790(2)	0.0324(2)	0.0439(7)
C21	0.0486(2)	0.0460(1)	0.1221(1)	0.0290(6)
C22	-0.0018(2)	0.0238(2)	0.1910(1)	0.0417(7)
C23	-0.0205(2)	-0.0519(2)	0.2119(1)	0.0435(7)
C24	0.0085(2)	-0.1065(2)	0.1632(1)	0.0370(6)
C25	0.0542(2)	-0.0842(1)	0.0935(1)	0.0374(6)
C26	0.0738(2)	-0.0086(1)	0.0737(1)	0.0330(6)
C27	-0.0060(3)	-0.1866(2)	0.1870(2)	0.0493(7)
C30	0.3019(2)	0.2428(1)	0.0559(1)	0.0282(6)
C31	0.4161(2)	0.1982(1)	0.0117(1)	0.0299(6)
C32	0.4627(2)	0.2328(2)	-0.0541(1)	0.0354(6)
C33	0.5659(2)	0.1914(2)	-0.0964(1)	0.0461(7)
C34	0.6263(2)	0.1164(2)	-0.0736(2)	0.0516(8)
C35	0.5837(2)	0.0826(2)	-0.0081(2)	0.0536(8)
C36	0.4795(2)	0.1232(2)	0.0341(2)	0.0413(7)
C41	0.2913(2)	0.3292(1)	0.0620(1)	0.0288(6)
C42	0.1983(2)	0.3917(1)	0.0466(1)	0.0340(6)
C43	0.1915(2)	0.4703(2)	0.0544(1)	0.0448(7)
C44	0.2758(3)	0.4881(2)	0.0785(1)	0.0493(8)
C45	0.3681(3)	0.4267(2)	0.0944(1)	0.0496(8)
C46	0.3761(2)	0.3484(2)	0.0857(1)	0.0393(7)
O9A	0.9091(2)	0.4184(1)	0.1198(1)	0.0436(5)
N27A	0.7858(2)	0.8995(1)	0.0808(1)	0.0552(7)
C1A	0.6591(2)	0.4665(1)	0.1244(1)	0.0315(6)
C2A	0.7125(2)	0.4698(1)	0.1832(1)	0.0273(6)
C3A	0.6480(2)	0.5414(1)	0.2253(1)	0.0272(6)
C4A	0.5149(2)	0.5481(1)	0.2288(1)	0.0305(6)
C5A	0.5136(2)	0.4596(1)	0.2410(1)	0.0286(6)
C6A	0.6253(2)	0.4177(1)	0.1951(1)	0.0299(6)
C7A	0.5681(2)	0.5379(1)	0.1061(1)	0.0354(6)
C8A	0.4945(2)	0.5791(1)	0.1577(1)	0.0351(6)
C9A	0.8417(2)	0.4330(1)	0.1764(1)	0.0301(6)
C10A	0.8872(2)	0.4160(1)	0.2398(1)	0.0343(6)
C11A	0.9958(2)	0.4300(2)	0.2364(2)	0.0525(8)
C12A	1.0407(3)	0.4141(2)	0.2945(2)	0.0739(10)
C13A	0.9787(4)	0.3816(2)	0.3558(2)	0.0820(12)
C14A	0.8727(3)	0.3663(2)	0.3599(2)	0.0675(10)
C15A	0.8259(3)	0.3844(2)	0.3024(1)	0.0460(7)
C21A	0.6863(2)	0.6184(1)	0.1963(1)	0.0280(6)
C22A	0.7688(2)	0.6240(1)	0.1333(1)	0.0335(6)
C23A	0.7975(2)	0.6962(2)	0.1064(1)	0.0366(6)
C24A	0.7436(2)	0.7640(1)	0.1415(1)	0.0328(6)
C25A	0.6637(2)	0.7591(2)	0.2056(1)	0.0385(6)
C26A	0.6367(2)	0.6865(1)	0.2324(1)	0.0354(6)
C27A	0.7677(2)	0.8398(2)	0.1088(1)	0.0400(7)
C30A	0.4303(2)	0.4263(1)	0.2837(1)	0.0311(6)
C31A	0.3157(2)	0.4739(1)	0.3240(1)	0.0335(6)
C32A	0.2717(2)	0.4498(2)	0.3938(1)	0.0454(7)
C33A	0.1651(3)	0.4937(2)	0.4313(2)	0.0568(8)
C34A	0.0996(3)	0.5608(2)	0.3995(2)	0.0600(9)
C35A	0.1409(2)	0.5846(2)	0.3309(2)	0.0567(8)
C36A	0.2478(2)	0.5416(2)	0.2933(2)	0.0434(7)

C41A	0.4475(2)	0.3370(1)	0.2918(1)	0.0398(7)
C42A	0.5266(3)	0.2868(2)	0.3284(2)	0.0691(10)
C43A	0.5422(3)	0.2035(2)	0.3348(3)	0.1006(16)
C44A	0.4798(4)	0.1715(2)	0.3052(2)	0.0952(16)
C45A	0.4011(4)	0.2200(2)	0.2688(2)	0.0837(13)
C46A	0.3841(3)	0.3032(2)	0.2631(2)	0.0579(8)
O9B	0.4744(2)	0.9280(1)	0.4747(1)	0.0514(5)
N27B	0.5836(3)	0.4542(2)	0.4224(2)	0.0955(12)
C1B	0.6946(2)	0.8608(1)	0.5149(1)	0.0334(6)
C2B	0.6805(2)	0.8680(1)	0.4417(1)	0.0301(6)
C3B	0.7630(2)	0.7993(1)	0.3994(1)	0.0301(6)
C4B	0.8786(2)	0.7827(1)	0.4252(1)	0.0321(6)
C5B	0.8857(2)	0.8681(1)	0.4270(1)	0.0305(6)
C6B	0.7615(2)	0.9122(1)	0.4571(1)	0.0315(6)
C7B	0.7627(2)	0.7836(2)	0.5429(1)	0.0378(6)
C8B	0.8555(2)	0.7436(2)	0.4986(1)	0.0363(6)
C9B	0.5632(2)	0.9126(1)	0.4273(1)	0.0352(6)
C10B	0.5566(2)	0.9365(1)	0.3539(1)	0.0368(6)
C11B	0.6495(2)	0.9571(1)	0.3026(1)	0.0421(7)
C12B	0.6393(3)	0.9798(2)	0.2343(2)	0.0516(8)
C13B	0.5357(3)	0.9803(2)	0.2180(2)	0.0617(9)
C14B	0.4439(3)	0.9597(2)	0.2684(2)	0.0679(9)
C15B	0.4531(3)	0.9386(2)	0.3356(2)	0.0518(8)
C21B	0.7196(2)	0.7252(1)	0.4055(1)	0.0296(6)
C22B	0.6148(2)	0.7155(2)	0.4515(1)	0.0396(7)
C23B	0.5788(2)	0.6458(2)	0.4569(1)	0.0447(7)
C24B	0.6487(2)	0.5844(2)	0.4163(1)	0.0418(7)
C25B	0.7541(2)	0.5931(2)	0.3702(1)	0.0420(7)
C26B	0.7875(2)	0.6633(1)	0.3645(1)	0.0357(6)
C27B	0.6116(3)	0.5119(2)	0.4211(2)	0.0610(9)
C30B	0.9850(2)	0.8941(1)	0.4056(1)	0.0330(6)
C31B	1.1029(2)	0.8337(2)	0.3892(1)	0.0388(7)
C32B	1.1344(2)	0.7704(2)	0.4380(2)	0.0485(7)
C33B	1.2426(3)	0.7145(2)	0.4254(2)	0.0624(9)
C34B	1.3223(3)	0.7212(2)	0.3633(2)	0.0701(10)
C35B	1.2956(3)	0.7831(2)	0.3137(2)	0.0706(10)
C36B	1.1856(3)	0.8402(2)	0.3264(2)	0.0567(8)
C41B	0.9876(2)	0.9794(2)	0.4009(1)	0.0362(6)
C42B	1.0796(3)	0.9981(2)	0.4185(1)	0.0456(7)
C43B	1.0850(3)	1.0769(2)	0.4142(1)	0.0562(9)
C44B	0.9991(3)	1.1389(2)	0.3925(2)	0.0620(9)
C45B	0.9079(3)	1.1221(2)	0.3739(1)	0.0549(8)
C46B	0.9030(2)	1.0428(2)	0.3778(1)	0.0432(7)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **2c**.

Atom	x	y	z	U_{eq}
H1	0.0254	0.2134	0.2499	0.043
H3	0.0663	0.1459	0.0530	0.034
H4	0.2722	0.0910	0.0536	0.035
H6	0.0753	0.3029	0.1413	0.039
H7	0.3061	0.0334	0.1662	0.042
H8	0.1831	0.0950	0.2638	0.046
H11	-0.3069	0.2066	0.1361	0.078
H12	-0.3709	0.2317	0.0317	0.084
H13	-0.2658	0.2904	-0.0679	0.087
H14	-0.0940	0.3219	-0.0688	0.070
H15	-0.0223	0.2902	0.0314	0.053
H22	-0.0239	0.0615	0.2245	0.050
H23	-0.0532	-0.0665	0.2595	0.052
H25	0.0718	-0.1208	0.0596	0.045

H26	0.1051	0.0064	0.0260	0.040
H32	0.4231	0.2853	-0.0699	0.042
H33	0.5953	0.2150	-0.1417	0.055
H34	0.6970	0.0881	-0.1030	0.062
H35	0.6259	0.0312	0.0083	0.064
H36	0.4509	0.0991	0.0793	0.050
H42	0.1389	0.3804	0.0306	0.041
H43	0.1281	0.5125	0.0431	0.054
H44	0.2703	0.5422	0.0841	0.059
H45	0.4263	0.4384	0.1114	0.059
H46	0.4408	0.3067	0.0961	0.047
H1A	0.7128	0.4351	0.0852	0.038
H3A	0.6602	0.5264	0.2734	0.033
H4A	0.4579	0.5808	0.2663	0.037
H6A	0.6533	0.3576	0.1999	0.036
H7A	0.5627	0.5535	0.0593	0.042
H8A	0.4329	0.6252	0.1502	0.042
H11A	1.0393	0.4507	0.1936	0.063
H12A	1.1135	0.4254	0.2923	0.089
H13A	1.0100	0.3696	0.3957	0.098
H14A	0.8314	0.3433	0.4024	0.081
H15A	0.7514	0.3752	0.3056	0.055
H22A	0.8060	0.5779	0.1084	0.040
H23A	0.8546	0.6990	0.0634	0.044
H25A	0.6280	0.8051	0.2308	0.046
H26A	0.5829	0.6830	0.2767	0.042
H32A	0.3153	0.4029	0.4158	0.054
H33A	0.1369	0.4776	0.4791	0.068
H34A	0.0260	0.5905	0.4254	0.072
H35A	0.0958	0.6307	0.3089	0.068
H36A	0.2754	0.5585	0.2456	0.052
H42A	0.5702	0.3090	0.3492	0.083
H43A	0.5965	0.1691	0.3598	0.121
H44A	0.4908	0.1148	0.3098	0.114
H45A	0.3587	0.1972	0.2478	0.100
H46A	0.3281	0.3371	0.2390	0.070
H1B	0.6255	0.8911	0.5490	0.040
H3B	0.7802	0.8207	0.3492	0.036
H4B	0.9498	0.7506	0.3936	0.039
H6B	0.7385	0.9722	0.4561	0.038
H7B	0.7409	0.7636	0.5903	0.045
H8B	0.9043	0.6935	0.5123	0.044
H11B	0.7206	0.9557	0.3142	0.050
H12B	0.7024	0.9947	0.1995	0.062
H13B	0.5283	0.9950	0.1714	0.074
H14B	0.3735	0.9603	0.2565	0.082
H15B	0.3886	0.9251	0.3702	0.062
H22B	0.5669	0.7573	0.4797	0.048
H23B	0.5065	0.6401	0.4883	0.054
H25B	0.8028	0.5508	0.3428	0.050
H26B	0.8585	0.6696	0.3318	0.043
H32B	1.0795	0.7655	0.4816	0.058
H33B	1.2614	0.6717	0.4598	0.075
H34B	1.3968	0.6827	0.3543	0.084
H35B	1.3518	0.7874	0.2706	0.085
H36B	1.1678	0.8833	0.2920	0.068
H42B	1.1394	0.9559	0.4336	0.055
H43B	1.1482	1.0883	0.4263	0.067
H44B	1.0024	1.1930	0.3904	0.074
H45B	0.8488	1.1647	0.3585	0.066
H46B	0.8406	1.0317	0.3645	0.052

Table 4: Anisotropic displacement parameters ($Å^2$) for **2c**. 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}
O9	0.0401(12)	0.0525(12)	0.0574(13)	-0.0075(10)	0.0117(11)	-0.0052(9)
N27	0.096(2)	0.0478(17)	0.080(2)	0.0130(15)	-0.0294(17)	-0.0368(16)
C1	0.0410(16)	0.0351(15)	0.0294(14)	-0.0055(11)	-0.0022(12)	-0.0114(12)
C2	0.0280(14)	0.0264(13)	0.0334(14)	-0.0035(11)	-0.0004(12)	-0.0055(11)
C3	0.0292(14)	0.0246(13)	0.0305(14)	-0.0009(11)	-0.0056(11)	-0.0072(11)
C4	0.0254(13)	0.0251(13)	0.0336(14)	-0.0023(11)	-0.0047(11)	-0.0049(10)
C5	0.0254(14)	0.0242(13)	0.0304(14)	-0.0021(11)	-0.0098(11)	-0.0017(11)
C6	0.0308(14)	0.0270(14)	0.0357(15)	-0.0049(11)	-0.0029(12)	-0.0063(11)
C7	0.0333(15)	0.0285(14)	0.0423(16)	0.0021(12)	-0.0155(13)	-0.0053(11)
C8	0.0448(17)	0.0376(15)	0.0315(15)	0.0012(12)	-0.0104(13)	-0.0114(13)
C9	0.0327(16)	0.0249(14)	0.0498(18)	-0.0077(13)	0.0052(15)	-0.0083(12)
C10	0.0221(14)	0.0312(15)	0.069(2)	-0.0207(14)	-0.0087(14)	-0.0005(11)
C11	0.0361(18)	0.059(2)	0.099(3)	-0.0344(19)	-0.0062(19)	-0.0061(15)
C12	0.041(2)	0.074(2)	0.111(3)	-0.040(2)	-0.036(2)	-0.0054(17)
C13	0.068(3)	0.060(2)	0.099(3)	-0.025(2)	-0.042(2)	0.0015(19)
C14	0.062(2)	0.0472(18)	0.069(2)	-0.0128(16)	-0.0314(18)	-0.0024(16)
C15	0.0387(16)	0.0383(16)	0.0573(19)	-0.0101(14)	-0.0202(15)	-0.0028(13)
C21	0.0236(13)	0.0292(14)	0.0328(15)	-0.0027(11)	-0.0068(11)	-0.0048(11)
C22	0.0496(17)	0.0355(16)	0.0383(16)	-0.0069(13)	0.0004(14)	-0.0171(13)
C23	0.0504(18)	0.0451(17)	0.0360(16)	0.0019(14)	-0.0031(14)	-0.0243(14)
C24	0.0342(15)	0.0338(15)	0.0462(17)	0.0042(13)	-0.0127(13)	-0.0151(12)
C25	0.0417(16)	0.0319(15)	0.0407(17)	-0.0061(12)	-0.0100(13)	-0.0114(12)
C26	0.0332(15)	0.0330(15)	0.0334(15)	-0.0008(12)	-0.0080(12)	-0.0110(11)
C27	0.058(2)	0.0426(19)	0.0535(19)	0.0048(15)	-0.0188(15)	-0.0224(15)
C30	0.0258(14)	0.0272(13)	0.0319(14)	-0.0010(11)	-0.0081(12)	-0.0072(11)
C31	0.0237(14)	0.0265(14)	0.0408(16)	-0.0052(12)	-0.0087(12)	-0.0067(11)
C32	0.0284(15)	0.0363(15)	0.0410(16)	-0.0057(13)	-0.0089(13)	-0.0061(12)
C33	0.0337(16)	0.060(2)	0.0441(17)	-0.0117(15)	-0.0026(14)	-0.0141(15)
C34	0.0280(16)	0.052(2)	0.072(2)	-0.0289(17)	-0.0018(16)	-0.0040(14)
C35	0.0336(17)	0.0335(16)	0.086(2)	-0.0086(16)	-0.0071(17)	-0.0028(13)
C36	0.0299(15)	0.0333(15)	0.0555(18)	0.0004(13)	-0.0065(14)	-0.0068(12)
C41	0.0281(14)	0.0276(14)	0.0282(14)	-0.0050(11)	-0.0008(11)	-0.0077(11)
C42	0.0336(15)	0.0284(15)	0.0386(15)	-0.0050(12)	-0.0050(12)	-0.0084(12)
C43	0.0503(18)	0.0294(16)	0.0465(17)	-0.0033(13)	-0.0042(15)	-0.0055(13)
C44	0.067(2)	0.0299(16)	0.0509(18)	-0.0073(13)	-0.0055(16)	-0.0195(15)
C45	0.060(2)	0.0487(19)	0.0525(18)	-0.0089(15)	-0.0153(16)	-0.0285(16)
C46	0.0393(16)	0.0374(16)	0.0444(17)	-0.0034(13)	-0.0135(13)	-0.0117(13)
O9A	0.0308(10)	0.0500(11)	0.0411(11)	-0.0117(9)	0.0012(9)	-0.0025(8)
N27A	0.0770(19)	0.0477(16)	0.0451(15)	0.0024(12)	-0.0082(13)	-0.0327(14)
C1A	0.0285(14)	0.0349(15)	0.0305(14)	-0.0051(11)	-0.0018(12)	-0.0115(11)
C2A	0.0266(14)	0.0252(13)	0.0288(14)	-0.0035(11)	-0.0038(11)	-0.0069(11)
C3A	0.0261(13)	0.0264(13)	0.0280(13)	-0.0027(11)	-0.0049(11)	-0.0069(10)
C4A	0.0250(14)	0.0267(13)	0.0356(15)	-0.0033(11)	-0.0004(11)	-0.0068(10)
C5A	0.0259(14)	0.0255(13)	0.0332(14)	-0.0053(11)	-0.0037(12)	-0.0066(11)
C6A	0.0275(14)	0.0248(13)	0.0356(14)	-0.0011(11)	-0.0047(12)	-0.0080(11)
C7A	0.0354(15)	0.0386(15)	0.0365(15)	0.0056(13)	-0.0127(13)	-0.0177(13)
C8A	0.0269(14)	0.0294(14)	0.0476(17)	0.0057(13)	-0.0104(13)	-0.0091(11)
C9A	0.0294(14)	0.0237(13)	0.0357(16)	-0.0052(11)	-0.0022(13)	-0.0084(11)
C10A	0.0315(15)	0.0252(14)	0.0437(17)	-0.0100(12)	-0.0097(13)	0.0008(11)
C11A	0.0397(18)	0.0489(18)	0.072(2)	-0.0160(16)	-0.0189(16)	-0.0055(14)
C12A	0.062(2)	0.075(2)	0.102(3)	-0.019(2)	-0.047(2)	-0.0109(19)
C13A	0.105(3)	0.070(2)	0.086(3)	-0.010(2)	-0.068(3)	-0.001(2)
C14A	0.099(3)	0.052(2)	0.052(2)	0.0032(16)	-0.035(2)	-0.0098(19)
C15A	0.0531(18)	0.0375(16)	0.0463(18)	-0.0006(13)	-0.0163(16)	-0.0080(14)
C21A	0.0248(13)	0.0294(14)	0.0302(14)	-0.0040(11)	-0.0065(12)	-0.0072(11)
C22A	0.0328(15)	0.0298(14)	0.0359(15)	-0.0065(12)	-0.0019(12)	-0.0092(11)
C23A	0.0359(15)	0.0418(16)	0.0321(15)	-0.0021(13)	-0.0006(12)	-0.0182(13)
C24A	0.0353(15)	0.0304(15)	0.0368(15)	-0.0002(12)	-0.0105(13)	-0.0145(12)

C25A	0.0435(16)	0.0311(15)	0.0395(16)	-0.0066(12)	-0.0052(14)	-0.0101(12)
C26A	0.0360(15)	0.0318(15)	0.0333(15)	-0.0027(12)	0.0001(12)	-0.0096(12)
C27A	0.0469(17)	0.0394(17)	0.0380(16)	-0.0025(14)	-0.0101(13)	-0.0183(14)
C30A	0.0278(14)	0.0272(14)	0.0350(14)	0.0001(11)	-0.0045(12)	-0.0069(11)
C31A	0.0278(14)	0.0306(14)	0.0405(16)	-0.0021(12)	-0.0017(12)	-0.0121(12)
C32A	0.0407(17)	0.0405(16)	0.0466(18)	-0.0026(13)	-0.0009(14)	-0.0080(13)
C33A	0.0478(19)	0.059(2)	0.0506(19)	-0.0094(16)	0.0120(16)	-0.0151(16)
C34A	0.0392(18)	0.0436(19)	0.081(2)	-0.0165(17)	0.0119(18)	-0.0056(15)
C35A	0.0361(18)	0.0401(17)	0.079(2)	0.0027(16)	-0.0005(17)	-0.0049(14)
C36A	0.0285(15)	0.0402(16)	0.0526(18)	0.0011(14)	-0.0001(14)	-0.0077(13)
C41A	0.0354(16)	0.0263(14)	0.0449(17)	-0.0013(13)	0.0103(13)	-0.0089(12)
C42A	0.0413(18)	0.0394(19)	0.110(3)	0.0245(18)	-0.0111(19)	-0.0109(14)
C43A	0.049(2)	0.049(2)	0.155(4)	0.036(3)	0.010(3)	0.0013(18)
C44A	0.094(3)	0.035(2)	0.109(4)	-0.008(2)	0.048(3)	-0.013(2)
C45A	0.135(4)	0.056(2)	0.055(2)	-0.0176(19)	0.021(2)	-0.054(3)
C46A	0.084(2)	0.0442(19)	0.0455(18)	-0.0061(14)	-0.0009(17)	-0.0303(17)
O9B	0.0346(11)	0.0597(13)	0.0528(12)	-0.0106(10)	-0.0050(10)	-0.0039(9)
N27B	0.131(3)	0.082(2)	0.074(2)	-0.0353(17)	0.0409(19)	-0.077(2)
C1B	0.0316(14)	0.0359(15)	0.0310(14)	-0.0048(12)	-0.0027(12)	-0.0099(12)
C2B	0.0291(14)	0.0289(14)	0.0326(15)	-0.0006(11)	-0.0083(12)	-0.0087(11)
C3B	0.0318(14)	0.0270(13)	0.0312(14)	-0.0013(11)	-0.0069(12)	-0.0087(11)
C4B	0.0261(14)	0.0327(14)	0.0372(15)	-0.0056(12)	-0.0075(12)	-0.0061(11)
C5B	0.0334(15)	0.0314(14)	0.0284(14)	-0.0047(11)	-0.0100(12)	-0.0077(12)
C6B	0.0338(15)	0.0292(14)	0.0333(14)	-0.0038(11)	-0.0077(12)	-0.0107(11)
C7B	0.0412(16)	0.0441(16)	0.0294(15)	0.0002(13)	-0.0099(13)	-0.0136(13)
C8B	0.0377(16)	0.0343(15)	0.0383(16)	0.0013(12)	-0.0146(13)	-0.0089(12)
C9B	0.0322(16)	0.0256(14)	0.0481(17)	-0.0059(12)	-0.0076(14)	-0.0084(11)
C10B	0.0358(16)	0.0261(14)	0.0462(17)	-0.0018(12)	-0.0142(14)	-0.0013(12)
C11B	0.0452(17)	0.0305(15)	0.0493(18)	-0.0009(13)	-0.0160(15)	-0.0054(13)
C12B	0.062(2)	0.0321(16)	0.050(2)	0.0003(14)	-0.0111(16)	-0.0010(14)
C13B	0.076(2)	0.053(2)	0.053(2)	0.0070(16)	-0.037(2)	0.0018(17)
C14B	0.058(2)	0.076(2)	0.074(3)	0.0116(19)	-0.039(2)	-0.0116(18)
C15B	0.0438(18)	0.0477(18)	0.064(2)	0.0067(15)	-0.0259(16)	-0.0061(14)
C21B	0.0302(14)	0.0306(14)	0.0291(14)	-0.0002(11)	-0.0108(12)	-0.0076(11)
C22B	0.0431(17)	0.0329(15)	0.0406(16)	-0.0081(12)	-0.0030(14)	-0.0106(13)
C23B	0.0460(17)	0.0426(17)	0.0455(17)	-0.0044(14)	0.0011(14)	-0.0233(14)
C24B	0.0553(18)	0.0374(16)	0.0365(16)	-0.0026(13)	-0.0043(14)	-0.0247(14)
C25B	0.0508(18)	0.0363(16)	0.0414(16)	-0.0099(13)	-0.0064(14)	-0.0159(13)
C26B	0.0320(15)	0.0358(15)	0.0389(16)	-0.0045(12)	-0.0049(12)	-0.0113(12)
C27B	0.082(2)	0.057(2)	0.0433(18)	-0.0144(15)	0.0162(17)	-0.0425(19)
C30B	0.0348(15)	0.0412(16)	0.0271(14)	-0.0045(12)	-0.0063(12)	-0.0167(12)
C31B	0.0309(15)	0.0538(18)	0.0370(16)	-0.0141(14)	-0.0031(13)	-0.0185(13)
C32B	0.0319(16)	0.0586(19)	0.0495(18)	-0.0115(16)	-0.0019(14)	-0.0076(14)
C33B	0.0386(19)	0.073(2)	0.067(2)	-0.0103(18)	-0.0044(17)	-0.0055(16)
C34B	0.047(2)	0.086(3)	0.070(2)	-0.021(2)	-0.010(2)	-0.0021(18)
C35B	0.038(2)	0.115(3)	0.051(2)	-0.028(2)	0.0104(16)	-0.017(2)
C36B	0.0428(19)	0.083(2)	0.0441(18)	-0.0111(16)	-0.0021(15)	-0.0208(17)
C41B	0.0428(16)	0.0436(16)	0.0262(14)	-0.0033(12)	-0.0032(13)	-0.0223(14)
C42B	0.0555(19)	0.0580(19)	0.0318(15)	-0.0026(13)	-0.0062(14)	-0.0328(15)
C43B	0.080(2)	0.071(2)	0.0336(17)	-0.0080(16)	-0.0052(17)	-0.050(2)
C44B	0.099(3)	0.053(2)	0.0398(18)	-0.0104(16)	0.0039(19)	-0.045(2)
C45B	0.073(2)	0.0459(19)	0.0412(18)	-0.0025(14)	0.0009(16)	-0.0233(16)
C46B	0.0534(18)	0.0436(18)	0.0352(16)	-0.0058(13)	-0.0029(14)	-0.0228(15)

Table 5: Bond lengths (Å) and angles (deg) for **2c**.

O9-C9	1.217(3)	C2-C3	1.525(3)
N27-C27	1.148(3)	C2-C6	1.536(3)
C1-C8	1.473(3)	C3-C21	1.512(3)
C1-C2	1.516(3)	C3-C4	1.576(3)
C1-C6	1.535(3)	C3-H3	1.0000
C1-H1	1.0000	C4-C7	1.504(3)
C2-C9	1.495(3)	C4-C5	1.531(3)

C4-H4	1.0000	C3A-H3A	1.0000
C5-C30	1.341(3)	C4A-C8A	1.502(3)
C5-C6	1.477(3)	C4A-C5A	1.524(3)
C6-H6	1.0000	C4A-H4A	1.0000
C7-C8	1.323(3)	C5A-C30A	1.339(3)
C7-H7	0.9500	C5A-C6A	1.478(3)
C8-H8	0.9500	C6A-H6A	1.0000
C9-C10	1.501(4)	C7A-C8A	1.325(3)
C10-C15	1.379(4)	C7A-H7A	0.9500
C10-C11	1.401(4)	C8A-H8A	0.9500
C11-C12	1.411(5)	C9A-C10A	1.480(3)
C11-H11	0.9500	C10A-C15A	1.386(3)
C12-C13	1.370(5)	C10A-C11A	1.394(4)
C12-H12	0.9500	C11A-C12A	1.378(4)
C13-C14	1.358(4)	C11A-H11A	0.9500
C13-H13	0.9500	C12A-C13A	1.378(5)
C14-C15	1.390(4)	C12A-H12A	0.9500
C14-H14	0.9500	C13A-C14A	1.370(5)
C15-H15	0.9500	C13A-H13A	0.9500
C21-C26	1.387(3)	C14A-C15A	1.380(4)
C21-C22	1.389(3)	C14A-H14A	0.9500
C22-C23	1.381(3)	C15A-H15A	0.9500
C22-H22	0.9500	C21A-C22A	1.387(3)
C23-C24	1.383(4)	C21A-C26A	1.391(3)
C23-H23	0.9500	C22A-C23A	1.385(3)
C24-C25	1.390(3)	C22A-H22A	0.9500
C24-C27	1.442(4)	C23A-C24A	1.379(3)
C25-C26	1.381(3)	C23A-H23A	0.9500
C25-H25	0.9500	C24A-C25A	1.386(3)
C26-H26	0.9500	C24A-C27A	1.445(3)
C30-C31	1.497(3)	C25A-C26A	1.384(3)
C30-C41	1.497(3)	C25A-H25A	0.9500
C31-C36	1.385(3)	C26A-H26A	0.9500
C31-C32	1.394(3)	C30A-C31A	1.488(3)
C32-C33	1.381(3)	C30A-C41A	1.497(3)
C32-H32	0.9500	C31A-C36A	1.389(3)
C33-C34	1.374(4)	C31A-C32A	1.394(3)
C33-H33	0.9500	C32A-C33A	1.382(4)
C34-C35	1.372(4)	C32A-H32A	0.9500
C34-H34	0.9500	C33A-C34A	1.379(4)
C35-C36	1.382(4)	C33A-H33A	0.9500
C35-H35	0.9500	C34A-C35A	1.368(4)
C36-H36	0.9500	C34A-H34A	0.9500
C41-C42	1.390(3)	C35A-C36A	1.379(4)
C41-C46	1.391(3)	C35A-H35A	0.9500
C42-C43	1.382(3)	C36A-H36A	0.9500
C42-H42	0.9500	C41A-C46A	1.381(4)
C43-C44	1.376(4)	C41A-C42A	1.388(4)
C43-H43	0.9500	C42A-C43A	1.397(5)
C44-C45	1.378(4)	C42A-H42A	0.9500
C44-H44	0.9500	C43A-C44A	1.362(6)
C45-C46	1.379(3)	C43A-H43A	0.9500
C45-H45	0.9500	C44A-C45A	1.371(6)
C46-H46	0.9500	C44A-H44A	0.9500
O9A-C9A	1.220(3)	C45A-C46A	1.394(4)
N27A-C27A	1.147(3)	C45A-H45A	0.9500
C1A-C7A	1.478(3)	C46A-H46A	0.9500
C1A-C2A	1.517(3)	O9B-C9B	1.222(3)
C1A-C6A	1.543(3)	N27B-C27B	1.147(3)
C1A-H1A	1.0000	C1B-C7B	1.475(3)
C2A-C9A	1.494(3)	C1B-C2B	1.510(3)
C2A-C3A	1.520(3)	C1B-C6B	1.535(3)
C2A-C6A	1.533(3)	C1B-H1B	1.0000
C3A-C21A	1.518(3)	C2B-C9B	1.496(3)
C3A-C4A	1.573(3)	C2B-C3B	1.528(3)

C2B-C6B	1.536(3)	C6-C1-H1	116.6
C3B-C21B	1.507(3)	C9-C2-C1	120.2(2)
C3B-C4B	1.567(3)	C9-C2-C3	119.1(2)
C3B-H3B	1.0000	C1-C2-C3	114.6(2)
C4B-C8B	1.503(3)	C9-C2-C6	121.65(19)
C4B-C5B	1.523(3)	C1-C2-C6	60.38(15)
C4B-H4B	1.0000	C3-C2-C6	106.84(18)
C5B-C30B	1.346(3)	C21-C3-C2	115.71(19)
C5B-C6B	1.489(3)	C21-C3-C4	114.13(18)
C6B-H6B	1.0000	C2-C3-C4	101.53(18)
C7B-C8B	1.321(3)	C21-C3-H3	108.4
C7B-H7B	0.9500	C2-C3-H3	108.4
C8B-H8B	0.9500	C4-C3-H3	108.4
C9B-C10B	1.482(4)	C7-C4-C5	105.56(19)
C10B-C11B	1.389(3)	C7-C4-C3	107.95(18)
C10B-C15B	1.398(4)	C5-C4-C3	102.13(17)
C11B-C12B	1.392(4)	C7-C4-H4	113.4
C11B-H11B	0.9500	C5-C4-H4	113.4
C12B-C13B	1.387(4)	C3-C4-H4	113.4
C12B-H12B	0.9500	C30-C5-C6	127.0(2)
C13B-C14B	1.372(4)	C30-C5-C4	127.9(2)
C13B-H13B	0.9500	C6-C5-C4	104.98(18)
C14B-C15B	1.366(4)	C5-C6-C1	112.7(2)
C14B-H14B	0.9500	C5-C6-C2	107.22(19)
C15B-H15B	0.9500	C1-C6-C2	59.15(15)
C21B-C22B	1.387(3)	C5-C6-H6	120.7
C21B-C26B	1.390(3)	C1-C6-H6	120.7
C22B-C23B	1.385(3)	C2-C6-H6	120.7
C22B-H22B	0.9500	C8-C7-C4	115.5(2)
C23B-C24B	1.384(4)	C8-C7-H7	122.2
C23B-H23B	0.9500	C4-C7-H7	122.2
C24B-C25B	1.389(4)	C7-C8-C1	117.6(2)
C24B-C27B	1.441(4)	C7-C8-H8	121.2
C25B-C26B	1.376(3)	C1-C8-H8	121.2
C25B-H25B	0.9500	O9-C9-C2	121.8(3)
C26B-H26B	0.9500	O9-C9-C10	121.6(2)
C30B-C41B	1.485(3)	C2-C9-C10	116.6(2)
C30B-C31B	1.502(3)	C15-C10-C11	118.8(3)
C31B-C32B	1.387(4)	C15-C10-C9	121.4(2)
C31B-C36B	1.390(4)	C11-C10-C9	119.7(3)
C32B-C33B	1.379(4)	C10-C11-C12	118.7(3)
C32B-H32B	0.9500	C10-C11-H11	120.7
C33B-C34B	1.362(4)	C12-C11-H11	120.7
C33B-H33B	0.9500	C13-C12-C11	120.4(3)
C34B-C35B	1.370(4)	C13-C12-H12	119.8
C34B-H34B	0.9500	C11-C12-H12	119.8
C35B-C36B	1.404(4)	C14-C13-C12	121.2(3)
C35B-H35B	0.9500	C14-C13-H13	119.4
C36B-H36B	0.9500	C12-C13-H13	119.4
C41B-C46B	1.390(4)	C13-C14-C15	119.1(3)
C41B-C42B	1.399(4)	C13-C14-H14	120.5
C42B-C43B	1.381(4)	C15-C14-H14	120.5
C42B-H42B	0.9500	C10-C15-C14	121.8(3)
C43B-C44B	1.375(4)	C10-C15-H15	119.1
C43B-H43B	0.9500	C14-C15-H15	119.1
C44B-C45B	1.385(4)	C26-C21-C22	118.1(2)
C44B-H44B	0.9500	C26-C21-C3	119.9(2)
C45B-C46B	1.389(4)	C22-C21-C3	121.9(2)
C45B-H45B	0.9500	C23-C22-C21	121.2(2)
C46B-H46B	0.9500	C23-C22-H22	119.4
C8-C1-C2	118.0(2)	C21-C22-H22	119.4
C8-C1-C6	116.6(2)	C22-C23-C24	119.9(2)
C2-C1-C6	60.47(15)	C22-C23-H23	120.1
C8-C1-H1	116.6	C24-C23-H23	120.1
C2-C1-H1	116.6	C23-C24-C25	119.8(2)

C23-C24-C27	118.6(2)
C25-C24-C27	121.6(2)
C26-C25-C24	119.6(2)
C26-C25-H25	120.2
C24-C25-H25	120.2
C25-C26-C21	121.4(2)
C25-C26-H26	119.3
C21-C26-H26	119.3
N27-C27-C24	177.6(3)
C5-C30-C31	122.5(2)
C5-C30-C41	121.3(2)
C31-C30-C41	116.09(19)
C36-C31-C32	117.8(2)
C36-C31-C30	122.4(2)
C32-C31-C30	119.8(2)
C33-C32-C31	120.6(2)
C33-C32-H32	119.7
C31-C32-H32	119.7
C34-C33-C32	120.6(3)
C34-C33-H33	119.7
C32-C33-H33	119.7
C35-C34-C33	119.6(3)
C35-C34-H34	120.2
C33-C34-H34	120.2
C34-C35-C36	120.1(3)
C34-C35-H35	120.0
C36-C35-H35	120.0
C35-C36-C31	121.3(3)
C35-C36-H36	119.3
C31-C36-H36	119.3
C42-C41-C46	117.8(2)
C42-C41-C30	122.9(2)
C46-C41-C30	119.2(2)
C43-C42-C41	120.6(2)
C43-C42-H42	119.7
C41-C42-H42	119.7
C44-C43-C42	120.7(3)
C44-C43-H43	119.7
C42-C43-H43	119.7
C43-C44-C45	119.5(2)
C43-C44-H44	120.3
C45-C44-H44	120.3
C44-C45-C46	120.0(3)
C44-C45-H45	120.0
C46-C45-H45	120.0
C45-C46-C41	121.4(2)
C45-C46-H46	119.3
C41-C46-H46	119.3
C7A-C1A-C2A	118.1(2)
C7A-C1A-C6A	117.3(2)
C2A-C1A-C6A	60.15(15)
C7A-C1A-H1A	116.5
C2A-C1A-H1A	116.5
C6A-C1A-H1A	116.5
C9A-C2A-C1A	118.9(2)
C9A-C2A-C3A	120.6(2)
C1A-C2A-C3A	114.00(19)
C9A-C2A-C6A	121.51(19)
C1A-C2A-C6A	60.79(15)
C3A-C2A-C6A	106.46(18)
C21A-C3A-C2A	115.36(18)
C21A-C3A-C4A	114.14(18)
C2A-C3A-C4A	101.95(18)
C21A-C3A-H3A	108.3
C2A-C3A-H3A	108.3
C4A-C3A-H3A	108.3
C8A-C4A-C5A	107.46(19)
C8A-C4A-C3A	107.86(18)
C5A-C4A-C3A	101.15(17)
C8A-C4A-H4A	113.2
C5A-C4A-H4A	113.2
C3A-C4A-H4A	113.2
C30A-C5A-C6A	127.0(2)
C30A-C5A-C4A	128.1(2)
C6A-C5A-C4A	104.99(18)
C5A-C6A-C2A	106.83(19)
C5A-C6A-C1A	113.07(19)
C2A-C6A-C1A	59.06(14)
C5A-C6A-H6A	120.7
C2A-C6A-H6A	120.7
C1A-C6A-H6A	120.7
C8A-C7A-C1A	117.3(2)
C8A-C7A-H7A	121.4
C1A-C7A-H7A	121.4
C7A-C8A-C4A	115.4(2)
C7A-C8A-H8A	122.3
C4A-C8A-H8A	122.3
O9A-C9A-C10A	120.4(2)
O9A-C9A-C2A	121.0(2)
C10A-C9A-C2A	118.6(2)
C15A-C10A-C11A	118.9(3)
C15A-C10A-C9A	121.6(2)
C11A-C10A-C9A	119.5(2)
C12A-C11A-C10A	120.7(3)
C12A-C11A-H11A	119.6
C10A-C11A-H11A	119.6
C11A-C12A-C13A	119.2(3)
C11A-C12A-H12A	120.4
C13A-C12A-H12A	120.4
C14A-C13A-C12A	121.0(3)
C14A-C13A-H13A	119.5
C12A-C13A-H13A	119.5
C13A-C14A-C15A	119.8(3)
C13A-C14A-H14A	120.1
C15A-C14A-H14A	120.1
C14A-C15A-C10A	120.4(3)
C14A-C15A-H15A	119.8
C10A-C15A-H15A	119.8
C22A-C21A-C26A	118.0(2)
C22A-C21A-C3A	122.0(2)
C26A-C21A-C3A	120.0(2)
C23A-C22A-C21A	120.8(2)
C23A-C22A-H22A	119.6
C21A-C22A-H22A	119.6
C24A-C23A-C22A	120.4(2)
C24A-C23A-H23A	119.8
C22A-C23A-H23A	119.8
C23A-C24A-C25A	119.8(2)
C23A-C24A-C27A	118.8(2)
C25A-C24A-C27A	121.3(2)
C26A-C25A-C24A	119.3(2)
C26A-C25A-H25A	120.4
C24A-C25A-H25A	120.4
C25A-C26A-C21A	121.7(2)
C25A-C26A-H26A	119.2
C21A-C26A-H26A	119.2
N27A-C27A-C24A	177.5(3)
C5A-C30A-C31A	123.4(2)
C5A-C30A-C41A	120.5(2)
C31A-C30A-C41A	116.1(2)

C36A-C31A-C32A	118.0(2)
C36A-C31A-C30A	121.7(2)
C32A-C31A-C30A	120.3(2)
C33A-C32A-C31A	120.5(3)
C33A-C32A-H32A	119.8
C31A-C32A-H32A	119.8
C34A-C33A-C32A	120.3(3)
C34A-C33A-H33A	119.8
C32A-C33A-H33A	119.8
C35A-C34A-C33A	119.9(3)
C35A-C34A-H34A	120.1
C33A-C34A-H34A	120.1
C34A-C35A-C36A	120.1(3)
C34A-C35A-H35A	119.9
C36A-C35A-H35A	119.9
C35A-C36A-C31A	121.2(3)
C35A-C36A-H36A	119.4
C31A-C36A-H36A	119.4
C46A-C41A-C42A	118.8(3)
C46A-C41A-C30A	120.3(3)
C42A-C41A-C30A	120.9(3)
C41A-C42A-C43A	119.9(4)
C41A-C42A-H42A	120.0
C43A-C42A-H42A	120.0
C44A-C43A-C42A	120.2(4)
C44A-C43A-H43A	119.9
C42A-C43A-H43A	119.9
C43A-C44A-C45A	120.9(4)
C43A-C44A-H44A	119.6
C45A-C44A-H44A	119.6
C44A-C45A-C46A	119.2(4)
C44A-C45A-H45A	120.4
C46A-C45A-H45A	120.4
C41A-C46A-C45A	121.0(3)
C41A-C46A-H46A	119.5
C45A-C46A-H46A	119.5
C7B-C1B-C2B	118.5(2)
C7B-C1B-C6B	118.4(2)
C2B-C1B-C6B	60.59(15)
C7B-C1B-H1B	116.0
C2B-C1B-H1B	116.0
C6B-C1B-H1B	116.0
C9B-C2B-C1B	118.5(2)
C9B-C2B-C3B	121.5(2)
C1B-C2B-C3B	113.89(19)
C9B-C2B-C6B	121.3(2)
C1B-C2B-C6B	60.53(15)
C3B-C2B-C6B	105.74(18)
C21B-C3B-C2B	116.85(19)
C21B-C3B-C4B	113.40(18)
C2B-C3B-C4B	101.89(18)
C21B-C3B-H3B	108.1
C2B-C3B-H3B	108.1
C4B-C3B-H3B	108.1
C8B-C4B-C5B	108.41(19)
C8B-C4B-C3B	107.78(19)
C5B-C4B-C3B	101.28(18)
C8B-C4B-H4B	112.9
C5B-C4B-H4B	112.9
C3B-C4B-H4B	112.9
C30B-C5B-C6B	130.2(2)
C30B-C5B-C4B	125.5(2)
C6B-C5B-C4B	104.30(19)
C5B-C6B-C1B	112.8(2)
C5B-C6B-C2B	107.11(19)
C1B-C6B-C2B	58.88(15)
C5B-C6B-H6B	120.7
C1B-C6B-H6B	120.7
C2B-C6B-H6B	120.7
C8B-C7B-C1B	116.7(2)
C8B-C7B-H7B	121.7
C1B-C7B-H7B	121.7
C7B-C8B-C4B	115.6(2)
C7B-C8B-H8B	122.2
C4B-C8B-H8B	122.2
O9B-C9B-C10B	120.5(2)
O9B-C9B-C2B	121.0(2)
C10B-C9B-C2B	118.4(2)
C11B-C10B-C15B	118.8(3)
C11B-C10B-C9B	122.4(2)
C15B-C10B-C9B	118.8(2)
C10B-C11B-C12B	120.5(3)
C10B-C11B-H11B	119.7
C12B-C11B-H11B	119.7
C13B-C12B-C11B	119.1(3)
C13B-C12B-H12B	120.5
C11B-C12B-H12B	120.5
C14B-C13B-C12B	120.6(3)
C14B-C13B-H13B	119.7
C12B-C13B-H13B	119.7
C15B-C14B-C13B	120.5(3)
C15B-C14B-H14B	119.8
C13B-C14B-H14B	119.8
C14B-C15B-C10B	120.5(3)
C14B-C15B-H15B	119.7
C10B-C15B-H15B	119.7
C22B-C21B-C26B	118.4(2)
C22B-C21B-C3B	122.5(2)
C26B-C21B-C3B	119.1(2)
C23B-C22B-C21B	121.0(2)
C23B-C22B-H22B	119.5
C21B-C22B-H22B	119.5
C24B-C23B-C22B	119.7(2)
C24B-C23B-H23B	120.1
C22B-C23B-H23B	120.1
C23B-C24B-C25B	119.9(2)
C23B-C24B-C27B	120.1(2)
C25B-C24B-C27B	119.9(2)
C26B-C25B-C24B	119.7(2)
C26B-C25B-H25B	120.1
C24B-C25B-H25B	120.1
C25B-C26B-C21B	121.3(2)
C25B-C26B-H26B	119.4
C21B-C26B-H26B	119.4
N27B-C27B-C24B	177.5(3)
C5B-C30B-C41B	124.4(2)
C5B-C30B-C31B	119.3(2)
C41B-C30B-C31B	116.3(2)
C32B-C31B-C36B	117.6(3)
C32B-C31B-C30B	120.5(2)
C36B-C31B-C30B	121.9(3)
C33B-C32B-C31B	122.2(3)
C33B-C32B-H32B	118.9
C31B-C32B-H32B	118.9
C34B-C33B-C32B	119.5(3)
C34B-C33B-H33B	120.3
C32B-C33B-H33B	120.3
C33B-C34B-C35B	120.4(3)
C33B-C34B-H34B	119.8
C35B-C34B-H34B	119.8

C34B-C35B-C36B	120.4(3)
C34B-C35B-H35B	119.8
C36B-C35B-H35B	119.8
C31B-C36B-C35B	119.9(3)
C31B-C36B-H36B	120.0
C35B-C36B-H36B	120.0
C46B-C41B-C42B	117.7(2)
C46B-C41B-C30B	122.5(2)
C42B-C41B-C30B	119.8(2)
C43B-C42B-C41B	121.1(3)
C43B-C42B-H42B	119.4
C41B-C42B-H42B	119.4
C44B-C43B-C42B	120.3(3)
C44B-C43B-H43B	119.8
C42B-C43B-H43B	119.8
C43B-C44B-C45B	119.7(3)
C43B-C44B-H44B	120.1
C45B-C44B-H44B	120.1
C44B-C45B-C46B	119.9(3)
C44B-C45B-H45B	120.0
C46B-C45B-H45B	120.0
C45B-C46B-C41B	121.2(3)
C45B-C46B-H46B	119.4
C41B-C46B-H46B	119.4

(3,3-Diphenyl-indan-1-yl)-*p*-tolyl-methanone (11e)

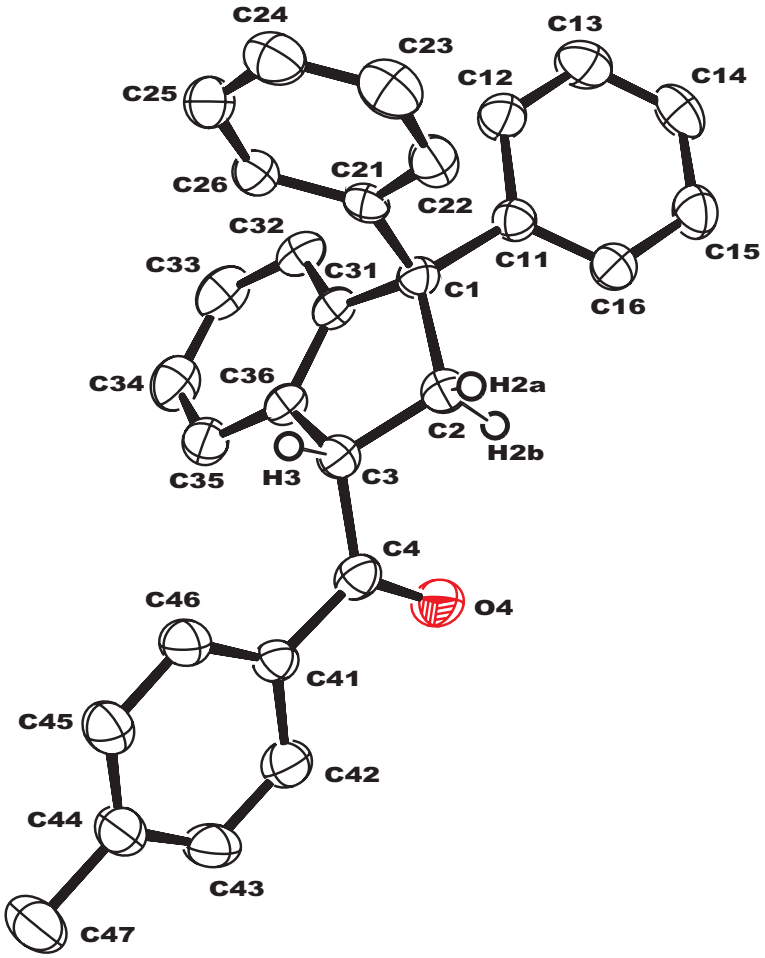


Table 1: Crystal data and structure refinement for **11e**.

Empirical formula	$C_{29}H_{24}O$	
Formula weight	388.48	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	2	
Unit cell dimensions	a = 8.5190(2) Å	α = 73.0570(11) deg.
	b = 12.5850(3) Å	β = 86.7680(12) deg.
	c = 10.2410(1) Å	γ = 98.8770(9) deg.
Volume	1031.73(4) $Å^3$	
Density (calculated)	1.25 g/cm^3	
Absorption coefficient	0.07 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.49 x 0.17 x 0.06 mm^3	
Crystal colour	colorless	
Theta range for data collection	1.7 to 24.7 deg.	
Index ranges	$-10\le h\le 9$, $-14\le k\le 14$, $-12\le l\le 12$	
Reflections collected	14378	
Independent reflections	14378 (R(int) = 0.0000)	
Observed reflections	9690 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	14378 / 0 / 285	
Goodness-of-fit on F^2	1.00	
Final R indices ($I>2\sigma(I)$)	R1 = 0.048, wR2 = 0.112	
Largest diff. peak and hole	0.17 and -0.18 $eÅ^{-3}$	

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **11e**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
C1	0.2965(1)	0.7563(1)	1.0264(1)	0.0292(3)
C2	0.1737(2)	0.6590(1)	1.0077(1)	0.0335(3)
H2A	0.1079(15)	0.6177(10)	1.0931(13)	0.036(4)
H2B	0.2324(13)	0.6118(10)	0.9704(11)	0.032(3)
C3	0.0735(2)	0.7132(1)	0.8966(1)	0.0307(3)
H3	-0.0182(15)	0.7394(9)	0.9354(12)	0.036(3)
C4	0.0173(2)	0.6381(1)	0.8089(1)	0.0336(3)
O4	0.0989(1)	0.5711(1)	0.7903(1)	0.0490(3)
C11	0.4510(1)	0.7212(1)	1.0799(1)	0.0301(3)
C12	0.5619(2)	0.7992(1)	1.1142(1)	0.0411(3)
C13	0.7030(2)	0.7722(1)	1.1622(1)	0.0482(4)
C14	0.7363(2)	0.6660(1)	1.1786(1)	0.0433(4)
C15	0.6269(2)	0.5870(1)	1.1472(1)	0.0428(3)
C16	0.4860(2)	0.6144(1)	1.0979(1)	0.0368(3)
C21	0.2172(1)	0.8093(1)	1.1258(1)	0.0281(3)
C22	0.1856(2)	0.7487(1)	1.2644(1)	0.0383(3)
C23	0.1145(2)	0.7919(1)	1.3573(1)	0.0472(4)
C24	0.0733(2)	0.8972(1)	1.3143(2)	0.0463(4)
C25	0.1032(2)	0.9581(1)	1.1783(1)	0.0418(3)
C26	0.1745(1)	0.9150(1)	1.0845(1)	0.0334(3)
C31	0.3212(1)	0.8376(1)	0.8807(1)	0.0299(3)
C32	0.4446(2)	0.9268(1)	0.8184(1)	0.0360(3)
C33	0.4356(2)	0.9949(1)	0.6872(1)	0.0449(4)
C34	0.3048(2)	0.9753(1)	0.6191(1)	0.0459(4)
C35	0.1817(2)	0.8854(1)	0.6797(1)	0.0384(3)
C36	0.1906(1)	0.8169(1)	0.8102(1)	0.0300(3)
C41	-0.1299(1)	0.6507(1)	0.7402(1)	0.0306(3)
C42	-0.1598(2)	0.5968(1)	0.6407(1)	0.0394(3)
C43	-0.2925(2)	0.6070(1)	0.5715(1)	0.0446(4)
C44	-0.4031(2)	0.6693(1)	0.6007(1)	0.0415(3)
C45	-0.3750(2)	0.7214(1)	0.7002(2)	0.0470(4)
C46	-0.2409(2)	0.7132(1)	0.7692(1)	0.0423(3)
C47	-0.5505(2)	0.6786(1)	0.5270(2)	0.0605(4)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **11e**.

Atom	x	y	z	U_{eq}
H2A	0.1079(15)	0.6177(10)	1.0931(13)	0.036(4)
H2B	0.2324(13)	0.6118(10)	0.9704(11)	0.032(3)
H3	-0.0182(15)	0.7394(9)	0.9354(12)	0.036(3)
H12	0.5400	0.8727	1.1042	0.049
H13	0.7774	0.8272	1.1842	0.058
H14	0.8338	0.6472	1.2111	0.052
H15	0.6485	0.5130	1.1594	0.051
H16	0.4120	0.5591	1.0762	0.044
H22	0.2135	0.6760	1.2959	0.046
H23	0.0940	0.7488	1.4515	0.057
H24	0.0247	0.9271	1.3782	0.056
H25	0.0749	1.0308	1.1477	0.050
H26	0.1943	0.9587	0.9905	0.040
H32	0.5346	0.9411	0.8655	0.043
H33	0.5204	1.0559	0.6436	0.054

H34	0.2989	1.0237	0.5296	0.055
H35	0.0922	0.8713	0.6320	0.046
H42	-0.0870	0.5523	0.6204	0.047
H43	-0.3090	0.5709	0.5027	0.054
H45	-0.4499	0.7640	0.7218	0.056
H46	-0.2241	0.7505	0.8369	0.051
H47A	-0.5260	0.6784	0.4324	0.091
H47B	-0.5866	0.7490	0.5261	0.091
H47C	-0.6351	0.6143	0.5744	0.091

Table 4: Anisotropic displacement parameters ($Å^2$) for **11e**. 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	0.0269(7)	0.0264(6)	0.0353(7)	-0.0108(6)	-0.0050(6)	0.0038(5)
C2	0.0338(8)	0.0292(7)	0.0364(8)	-0.0094(7)	-0.0063(6)	0.0026(6)
C3	0.0286(7)	0.0308(7)	0.0343(7)	-0.0115(6)	-0.0055(6)	0.0063(6)
C4	0.0310(7)	0.0289(7)	0.0403(8)	-0.0117(6)	-0.0012(6)	0.0023(6)
O4	0.0399(6)	0.0493(6)	0.0739(7)	-0.0360(6)	-0.0187(5)	0.0180(5)
C11	0.0282(7)	0.0316(7)	0.0310(7)	-0.0105(6)	-0.0037(5)	0.0050(6)
C12	0.0335(8)	0.0368(8)	0.0557(9)	-0.0175(7)	-0.0119(7)	0.0058(6)
C13	0.0342(8)	0.0539(9)	0.0577(10)	-0.0208(8)	-0.0130(7)	0.0013(7)
C14	0.0291(8)	0.0620(10)	0.0389(8)	-0.0109(7)	-0.0077(6)	0.0153(7)
C15	0.0424(9)	0.0437(8)	0.0456(9)	-0.0127(7)	-0.0079(7)	0.0179(7)
C16	0.0342(8)	0.0365(7)	0.0408(8)	-0.0125(6)	-0.0070(6)	0.0074(6)
C21	0.0204(6)	0.0325(7)	0.0320(7)	-0.0115(6)	-0.0070(5)	0.0017(5)
C22	0.0362(8)	0.0391(7)	0.0384(8)	-0.0087(6)	-0.0074(6)	0.0075(6)
C23	0.0434(9)	0.0646(10)	0.0332(8)	-0.0153(7)	0.0002(7)	0.0093(8)
C24	0.0389(8)	0.0672(10)	0.0448(9)	-0.0305(8)	-0.0082(7)	0.0180(8)
C25	0.0373(8)	0.0460(8)	0.0512(9)	-0.0230(7)	-0.0110(7)	0.0160(7)
C26	0.0318(7)	0.0355(7)	0.0347(7)	-0.0122(6)	-0.0069(6)	0.0071(6)
C31	0.0315(7)	0.0269(6)	0.0334(7)	-0.0130(6)	0.0002(6)	0.0058(6)
C32	0.0337(8)	0.0319(7)	0.0428(8)	-0.0156(6)	0.0021(6)	0.0011(6)
C33	0.0504(9)	0.0336(7)	0.0432(9)	-0.0084(7)	0.0131(7)	-0.0023(7)
C34	0.0615(10)	0.0376(8)	0.0332(8)	-0.0043(7)	0.0027(7)	0.0083(7)
C35	0.0455(9)	0.0366(7)	0.0344(8)	-0.0114(6)	-0.0055(6)	0.0099(7)
C36	0.0333(7)	0.0276(6)	0.0321(7)	-0.0131(6)	-0.0027(6)	0.0069(6)
C41	0.0302(7)	0.0275(6)	0.0324(7)	-0.0086(6)	-0.0040(6)	0.0005(5)
C42	0.0400(8)	0.0377(8)	0.0429(8)	-0.0162(7)	-0.0046(7)	0.0061(6)
C43	0.0507(9)	0.0471(8)	0.0389(8)	-0.0192(7)	-0.0133(7)	0.0022(7)
C44	0.0383(8)	0.0405(8)	0.0410(8)	-0.0064(7)	-0.0108(7)	0.0024(7)
C45	0.0417(9)	0.0540(9)	0.0559(9)	-0.0254(8)	-0.0171(7)	0.0195(7)
C46	0.0415(9)	0.0470(8)	0.0491(9)	-0.0259(7)	-0.0144(7)	0.0144(7)
C47	0.0530(10)	0.0652(10)	0.0625(11)	-0.0144(9)	-0.0283(8)	0.0097(8)

Table 5: Bond lengths (Å) and angles (deg) for **11e**.

C1-C31	1.5252(16)	C13-C14	1.3746(19)
C1-C11	1.5321(16)	C14-C15	1.3762(18)
C1-C2	1.5466(16)	C15-C16	1.3820(17)
C1-C21	1.5483(16)	C21-C26	1.3857(16)
C2-C3	1.5255(17)	C21-C22	1.3899(17)
C3-C36	1.5194(17)	C22-C23	1.3805(18)
C3-C4	1.5268(16)	C23-C24	1.3755(19)
C4-O4	1.2213(14)	C24-C25	1.3673(19)
C4-C41	1.4786(17)	C25-C26	1.3867(17)
C11-C16	1.3838(16)	C31-C32	1.3839(16)
C11-C12	1.3895(16)	C31-C36	1.3919(17)
C12-C13	1.3774(18)	C32-C33	1.3814(17)

C33-C34	1.3756(19)
C34-C35	1.3837(18)
C35-C36	1.3762(17)
C41-C46	1.3914(17)
C41-C42	1.3933(16)
C42-C43	1.3699(18)
C43-C44	1.3869(19)
C44-C45	1.3762(18)
C44-C47	1.5037(19)
C45-C46	1.3789(18)
C31-C1-C11	113.57(10)
C31-C1-C2	100.32(10)
C11-C1-C2	114.47(10)
C31-C1-C21	110.10(9)
C11-C1-C21	109.09(9)
C2-C1-C21	108.98(10)
C3-C2-C1	106.47(10)
C36-C3-C2	102.00(10)
C36-C3-C4	110.13(10)
C2-C3-C4	113.34(10)
O4-C4-C41	119.97(11)
O4-C4-C3	119.42(11)
C41-C4-C3	120.52(11)
C16-C11-C12	117.58(12)
C16-C11-C1	123.30(11)
C12-C11-C1	119.11(10)
C13-C12-C11	121.47(12)
C14-C13-C12	120.16(13)
C13-C14-C15	119.28(13)
C14-C15-C16	120.49(12)
C15-C16-C11	121.01(12)
C26-C21-C22	117.29(12)
C26-C21-C1	123.60(11)
C22-C21-C1	119.11(11)
C23-C22-C21	121.43(12)
C24-C23-C22	120.38(13)
C25-C24-C23	119.08(13)
C24-C25-C26	120.79(13)
C21-C26-C25	121.04(12)
C32-C31-C36	119.79(12)
C32-C31-C1	129.59(11)
C36-C31-C1	110.50(10)
C33-C32-C31	119.36(12)
C34-C33-C32	120.53(13)
C33-C34-C35	120.55(13)
C36-C35-C34	119.12(13)
C35-C36-C31	120.63(12)
C35-C36-C3	128.89(11)
C31-C36-C3	110.47(11)
C46-C41-C42	117.82(12)
C46-C41-C4	123.82(11)
C42-C41-C4	118.37(11)
C43-C42-C41	121.13(12)
C42-C43-C44	120.96(13)
C45-C44-C43	118.09(13)
C45-C44-C47	120.87(13)
C43-C44-C47	121.03(13)
C44-C45-C46	121.57(13)
C45-C46-C41	120.42(13)

(3,3-Diphenyl-indan-1-yl)-(4-methoxy-phenyl)-methanone (11f)

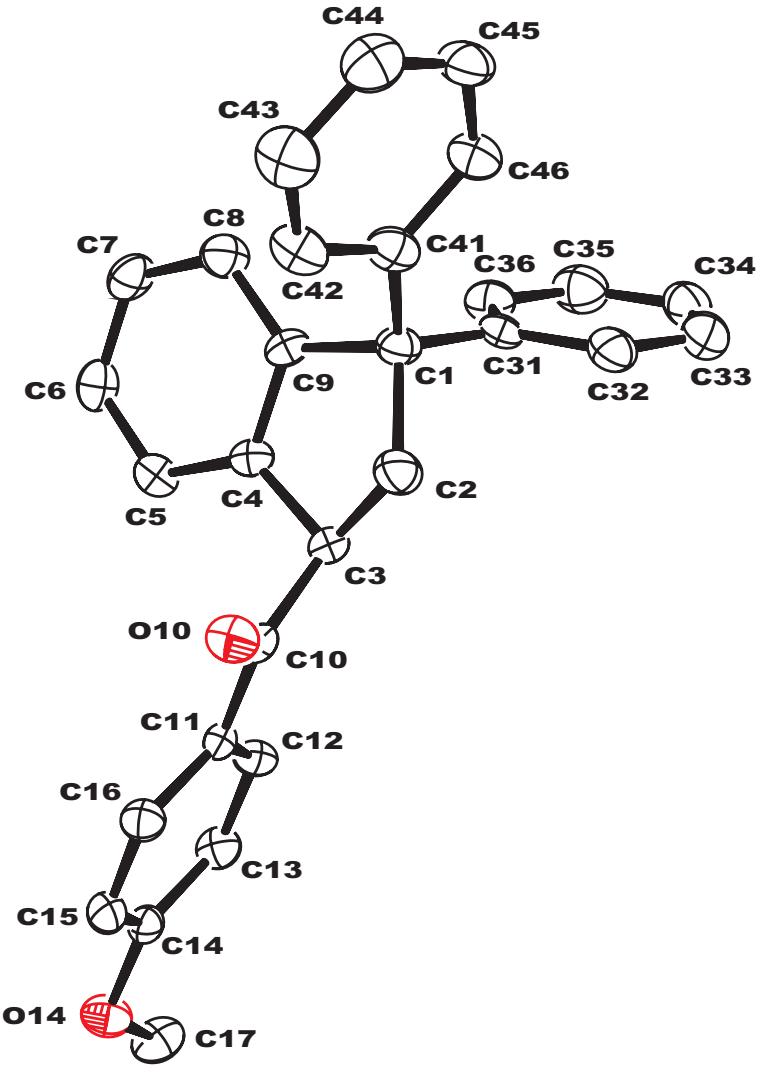


Table 1: Crystal data and structure refinement for **11f**.

Empirical formula	$C_{29}H_{24}O_2$	
Formula weight	404.48	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	Pccn	
Z	8	
Unit cell dimensions	a = 15.277(3) Å	α = 90.0 deg.
	b = 37.640(8) Å	β = 90.0 deg.
	c = 7.251(2) Å	γ = 90.0 deg.
Volume	4169.4(15) $Å^3$	
Density (calculated)	1.29 g/cm^3	
Absorption coefficient	0.08 mm^{-1}	
Crystal shape	plates	
Crystal size	0.18 x 0.12 x 0.05 mm^3	
Crystal colour	colourless	
Theta range for data collection	1.4 to 20.8 deg.	
Index ranges	$-15 \le h \le 15$, $-37 \le k \le 24$, $-6 \le l \le 7$	
Reflections collected	10547	
Independent reflections	2173 (R(int) = 0.0737)	
Observed reflections	1621 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.99	
Refinement method	Full-matrix least-squares on F^2	

Data/restraints/parameters	2173 / 0 / 281
Goodness-of-fit on F^2	1.08
Final R indices ($I>2\sigma(I)$)	R1 = 0.061, wR2 = 0.133
Largest diff. peak and hole	0.21 and -0.20 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **11f**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
O10	0.5809(2)	0.4534(1)	0.1516(4)	0.0303(8)
O14	0.3401(2)	0.5751(1)	0.4487(4)	0.0305(8)
C1	0.4946(3)	0.3515(1)	0.1048(6)	0.0261(11)
C2	0.5365(3)	0.3830(1)	0.2135(7)	0.0326(12)
C3	0.4668(3)	0.4127(1)	0.2201(6)	0.0247(11)
C4	0.4129(3)	0.4053(1)	0.0496(6)	0.0216(11)
C5	0.3547(3)	0.4277(1)	-0.0429(6)	0.0240(11)
C6	0.3170(3)	0.4161(1)	-0.2036(6)	0.0289(12)
C7	0.3352(3)	0.3824(1)	-0.2730(7)	0.0319(12)
C8	0.3917(3)	0.3601(1)	-0.1823(6)	0.0317(12)
C9	0.4306(3)	0.3716(1)	-0.0187(6)	0.0234(11)
C10	0.5070(3)	0.4498(1)	0.2135(6)	0.0214(11)
C11	0.4576(3)	0.4814(1)	0.2771(6)	0.0191(10)
C12	0.3779(3)	0.4798(1)	0.3692(6)	0.0273(12)
C13	0.3362(3)	0.5105(1)	0.4278(6)	0.0269(12)
C14	0.3740(3)	0.5430(1)	0.3945(6)	0.0226(11)
C15	0.4529(3)	0.5450(1)	0.3022(6)	0.0262(11)
C16	0.4934(3)	0.5144(1)	0.2433(6)	0.0251(11)
C17	0.2674(3)	0.5743(1)	0.5735(6)	0.0339(12)
C31	0.4472(3)	0.3266(1)	0.2375(6)	0.0278(12)
C32	0.4932(3)	0.3115(1)	0.3836(7)	0.0354(13)
C33	0.4538(4)	0.2882(1)	0.5068(7)	0.0448(14)
C34	0.3665(4)	0.2797(1)	0.4879(7)	0.0444(15)
C35	0.3189(3)	0.2951(1)	0.3449(7)	0.0422(14)
C36	0.3587(3)	0.3180(1)	0.2220(7)	0.0324(12)
C41	0.5629(3)	0.3318(1)	-0.0151(7)	0.0300(12)
C42	0.6114(3)	0.3508(1)	-0.1422(7)	0.0360(13)
C43	0.6722(3)	0.3340(1)	-0.2543(7)	0.0431(14)
C44	0.6856(3)	0.2981(1)	-0.2421(7)	0.0410(14)
C45	0.6374(3)	0.2786(1)	-0.1195(7)	0.0379(14)
C46	0.5758(3)	0.2952(1)	-0.0059(7)	0.0340(13)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **11f**.

Atom	x	y	z	U_{eq}
H2A	0.5525	0.3754	0.3398	0.039
H2B	0.5900	0.3915	0.1501	0.039
H3	0.4298	0.4101	0.3331	0.030
H5	0.3414	0.4506	0.0047	0.029
H6	0.2780	0.4312	-0.2685	0.035
H7	0.3082	0.3748	-0.3843	0.038
H8	0.4041	0.3371	-0.2301	0.038
H12	0.3517	0.4573	0.3925	0.033
H13	0.2817	0.5090	0.4905	0.032
H15	0.4791	0.5675	0.2794	0.031
H16	0.5471	0.5161	0.1779	0.030
H17A	0.2159	0.5647	0.5102	0.051

H17B	0.2547	0.5984	0.6164	0.051
H17C	0.2818	0.5592	0.6794	0.051
H32	0.5532	0.3173	0.3996	0.042
H33	0.4871	0.2781	0.6042	0.054
H34	0.3392	0.2637	0.5711	0.053
H35	0.2584	0.2898	0.3317	0.051
H36	0.3251	0.3282	0.1251	0.039
H42	0.6029	0.3757	-0.1531	0.043
H43	0.7051	0.3475	-0.3405	0.052
H44	0.7279	0.2868	-0.3181	0.049
H45	0.6459	0.2537	-0.1114	0.046
H46	0.5424	0.2814	0.0782	0.041

Table 4: Anisotropic displacement parameters ($Å^2$) for **11f**. 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}
O10	0.0263(19)	0.0298(19)	0.035(2)	-0.0033(15)	0.0051(16)	-0.0013(16)
O14	0.0273(18)	0.0274(19)	0.037(2)	-0.0067(16)	0.0034(16)	0.0056(15)
C1	0.027(3)	0.024(2)	0.028(3)	-0.005(2)	-0.003(2)	0.004(2)
C2	0.035(3)	0.027(3)	0.036(3)	-0.002(2)	-0.009(3)	0.001(2)
C3	0.031(3)	0.023(3)	0.020(3)	-0.003(2)	-0.002(2)	-0.001(2)
C4	0.018(2)	0.024(3)	0.023(3)	-0.004(2)	0.004(2)	-0.002(2)
C5	0.016(2)	0.024(2)	0.033(3)	0.000(2)	0.002(2)	0.000(2)
C6	0.020(3)	0.037(3)	0.029(3)	0.006(2)	-0.003(2)	0.000(2)
C7	0.030(3)	0.039(3)	0.027(3)	-0.002(3)	-0.009(2)	-0.005(3)
C8	0.032(3)	0.029(3)	0.034(3)	-0.004(3)	-0.002(3)	0.000(2)
C9	0.022(2)	0.028(3)	0.021(3)	-0.005(2)	-0.002(2)	-0.002(2)
C10	0.023(3)	0.026(3)	0.016(3)	-0.001(2)	-0.002(2)	-0.001(2)
C11	0.022(2)	0.020(3)	0.015(2)	0.001(2)	-0.001(2)	0.000(2)
C12	0.033(3)	0.022(3)	0.027(3)	-0.004(2)	-0.002(2)	-0.006(2)
C13	0.024(3)	0.031(3)	0.026(3)	-0.002(2)	0.004(2)	-0.002(2)
C14	0.027(3)	0.022(3)	0.019(3)	0.000(2)	-0.003(2)	0.004(2)
C15	0.031(3)	0.024(3)	0.024(3)	0.002(2)	-0.002(2)	-0.005(2)
C16	0.024(2)	0.025(3)	0.026(3)	-0.002(2)	0.002(2)	0.001(2)
C17	0.027(3)	0.043(3)	0.031(3)	-0.010(2)	0.003(2)	0.011(2)
C31	0.037(3)	0.018(2)	0.028(3)	-0.005(2)	0.002(2)	0.011(2)
C32	0.040(3)	0.028(3)	0.038(3)	-0.005(3)	-0.006(3)	0.010(3)
C33	0.066(4)	0.034(3)	0.034(3)	-0.002(3)	0.000(3)	0.016(3)
C34	0.071(4)	0.028(3)	0.034(3)	0.002(3)	0.013(3)	0.001(3)
C35	0.045(3)	0.037(3)	0.045(4)	-0.004(3)	0.007(3)	-0.007(3)
C36	0.033(3)	0.031(3)	0.033(3)	-0.006(2)	0.004(2)	0.000(2)
C41	0.025(3)	0.027(3)	0.039(3)	-0.005(2)	-0.005(2)	-0.003(2)
C42	0.033(3)	0.028(3)	0.047(3)	-0.003(3)	0.002(3)	0.001(3)
C43	0.035(3)	0.043(4)	0.051(4)	0.001(3)	0.007(3)	-0.008(3)
C44	0.033(3)	0.049(4)	0.041(3)	-0.005(3)	0.005(3)	0.004(3)
C45	0.044(3)	0.029(3)	0.041(3)	-0.009(3)	-0.002(3)	0.010(3)
C46	0.035(3)	0.027(3)	0.039(3)	-0.003(2)	0.001(3)	-0.003(2)

Table 5: Bond lengths (Å) and angles (deg) for **11f**.

O10-C10	1.222(5)	C2-H2A	0.9900
O14-C14	1.373(5)	C2-H2B	0.9900
O14-C17	1.433(5)	C3-C4	1.511(6)
C1-C9	1.526(6)	C3-C10	1.526(6)
C1-C31	1.527(6)	C3-H3	1.0000
C1-C41	1.549(6)	C4-C9	1.388(6)
C1-C2	1.561(6)	C4-C5	1.397(6)
C2-C3	1.546(6)	C5-C6	1.371(6)

C5-H5	0.9500
C6-C7	1.391(6)
C6-H6	0.9500
C7-C8	1.373(6)
C7-H7	0.9500
C8-C9	1.396(6)
C8-H8	0.9500
C10-C11	1.481(6)
C11-C16	1.382(5)
C11-C12	1.390(6)
C12-C13	1.386(6)
C12-H12	0.9500
C13-C14	1.376(6)
C13-H13	0.9500
C14-C15	1.381(6)
C15-C16	1.374(6)
C15-H15	0.9500
C16-H16	0.9500
C17-H17A	0.9800
C17-H17B	0.9800
C17-H17C	0.9800
C31-C32	1.391(6)
C31-C36	1.394(6)
C32-C33	1.389(7)
C32-H32	0.9500
C33-C34	1.379(7)
C33-H33	0.9500
C34-C35	1.392(7)
C34-H34	0.9500
C35-C36	1.382(6)
C35-H35	0.9500
C36-H36	0.9500
C41-C42	1.382(6)
C41-C46	1.392(6)
C42-C43	1.387(6)
C42-H42	0.9500
C43-C44	1.370(7)
C43-H43	0.9500
C44-C45	1.366(7)
C44-H44	0.9500
C45-C46	1.398(6)
C45-H45	0.9500
C46-H46	0.9500

C14-O14-C17	117.0(3)
C9-C1-C31	111.8(3)
C9-C1-C41	109.9(4)
C31-C1-C41	112.2(3)
C9-C1-C2	100.5(3)
C31-C1-C2	110.1(4)
C41-C1-C2	111.7(4)
C3-C2-C1	106.4(3)
C3-C2-H2A	110.5
C1-C2-H2A	110.5
C3-C2-H2B	110.5
C1-C2-H2B	110.5
H2A-C2-H2B	108.6
C4-C3-C10	111.3(3)
C4-C3-C2	102.5(3)
C10-C3-C2	112.5(3)
C4-C3-H3	110.1
C10-C3-H3	110.1
C2-C3-H3	110.1
C9-C4-C5	120.2(4)
C9-C4-C3	110.8(4)
C5-C4-C3	128.9(4)
C6-C5-C4	118.9(4)
C6-C5-H5	120.5
C4-C5-H5	120.5
C5-C6-C7	120.9(4)
C5-C6-H6	119.6
C7-C6-H6	119.6
C8-C7-C6	120.7(4)
C8-C7-H7	119.7
C6-C7-H7	119.7
C7-C8-C9	119.0(4)
C7-C8-H8	120.5
C9-C8-H8	120.5
C4-C9-C8	120.3(4)
C4-C9-C1	111.6(4)
C8-C9-C1	128.1(4)
O10-C10-C11	119.7(4)
O10-C10-C3	119.1(4)
C11-C10-C3	121.2(4)
C16-C11-C12	118.0(4)
C16-C11-C10	117.8(4)
C12-C11-C10	124.2(4)
C13-C12-C11	121.0(4)
C13-C12-H12	119.5
C11-C12-H12	119.5
C14-C13-C12	119.6(4)
C14-C13-H13	120.2
C12-C13-H13	120.2
O14-C14-C13	125.2(4)
O14-C14-C15	114.8(4)
C13-C14-C15	120.0(4)
C16-C15-C14	119.9(4)
C16-C15-H15	120.1
C14-C15-H15	120.1
C15-C16-C11	121.4(4)
C15-C16-H16	119.3
C11-C16-H16	119.3
O14-C17-H17A	109.5
O14-C17-H17B	109.5
H17A-C17-H17B	109.5
O14-C17-H17C	109.5
H17A-C17-H17C	109.5
H17B-C17-H17C	109.5
C32-C31-C36	117.2(4)
C32-C31-C1	119.4(4)
C36-C31-C1	123.3(4)
C33-C32-C31	121.9(5)
C33-C32-H32	119.1
C31-C32-H32	119.1
C34-C33-C32	120.1(5)
C34-C33-H33	120.0
C32-C33-H33	120.0
C33-C34-C35	118.9(5)
C33-C34-H34	120.5
C35-C34-H34	120.5
C36-C35-C34	120.7(5)
C36-C35-H35	119.7
C34-C35-H35	119.7
C35-C36-C31	121.2(5)
C35-C36-H36	119.4
C31-C36-H36	119.4
C42-C41-C46	117.9(4)
C42-C41-C1	119.2(4)
C46-C41-C1	122.9(4)
C41-C42-C43	120.9(4)

C41-C42-H42	119.5
C43-C42-H42	119.5
C44-C43-C42	120.8(5)
C44-C43-H43	119.6
C42-C43-H43	119.6
C45-C44-C43	119.3(5)
C45-C44-H44	120.3
C43-C44-H44	120.3
C44-C45-C46	120.5(4)
C44-C45-H45	119.8
C46-C45-H45	119.8
C41-C46-C45	120.5(5)
C41-C46-H46	119.7
C45-C46-H46	119.7

II. Computational Studies on the intermediates and products

General remarks. All calculations were carried out on an AMD Athlon64 X2 architecture using Gaussian 03: x86–Linux–G03 Revision C.01:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; AL̃Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.01, *Gaussian, Inc., Wallingford CT*, 2004.

Geometry optimizations were carried out using the restricted Becke Perdew 86 Functionals [RBP86/6–31+G(d,p)]:

J. P. Perdew, *Phys. Rev. B* 1986, **33**, 8822.

Single point energy calculation were carried out using the *Møller–Plesset* correlation energy correction truncated at second-order [RMP2/6-311++G (2d,2p)//RBP86/6–31+G(d,p)]:

C. Møller, M. S. Plesset *Phys. Rev*., 1934, **46**, 618.

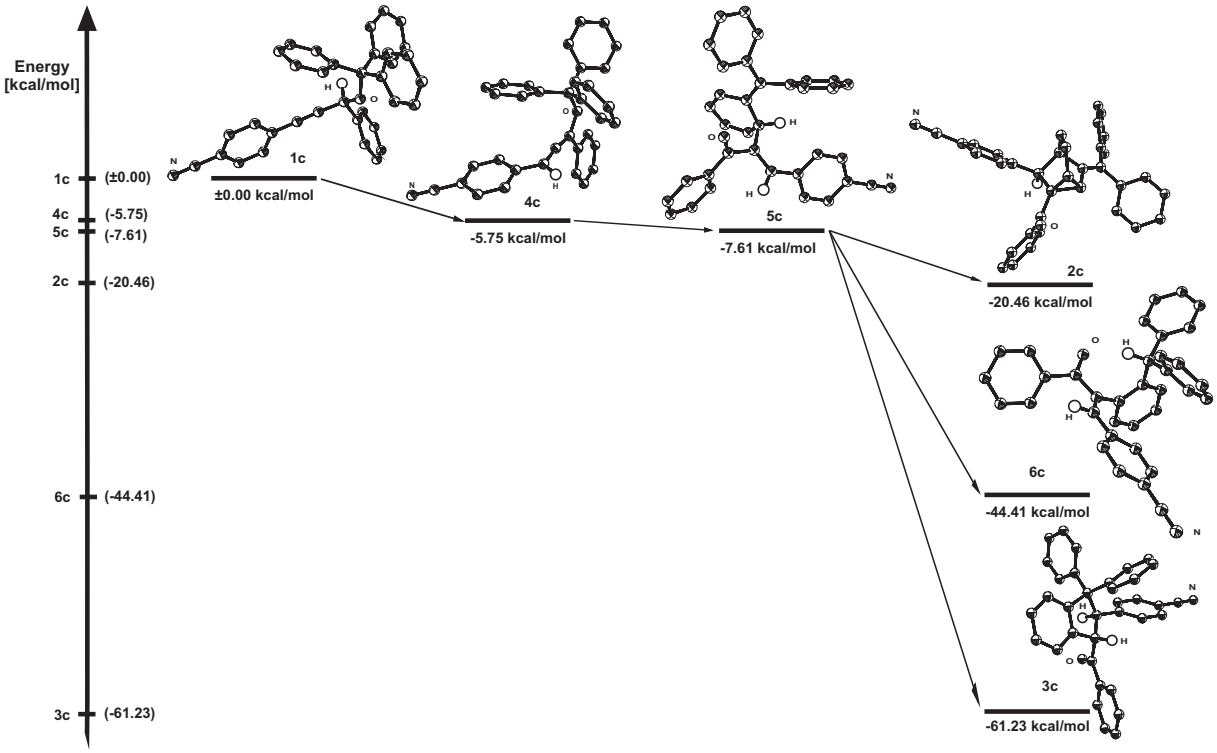
M. Head-Gordon, J. A. Pople, M. J. Frisch, *Chem. Phys. Lett.*, 1988, **153**, 503.

M. J. Frisch, M. Head-Gordon, J. A. Pople, *Chem. Phys. Lett.*, 1990, **166**, 275.

M. J. Frisch, M. Head-Gordon, J. A. Pople, *Chem. Phys. Lett.*, 1990, **166**, 281.

M. Head-Gordon, T. Head-Gordon, *Chem. Phys. Lett.*, 1994, **220**, 122.

S. Saebo, J. Almlof, *Chem. Phys. Lett.*, 1989, **154**, 83.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2c (-20.46)
6c (-44.41)
3c (-61.23)
1c
±0.00 kcal/mol
4c
-5.75 kcal/mol
5c
-7.61 kcal/mol
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6c
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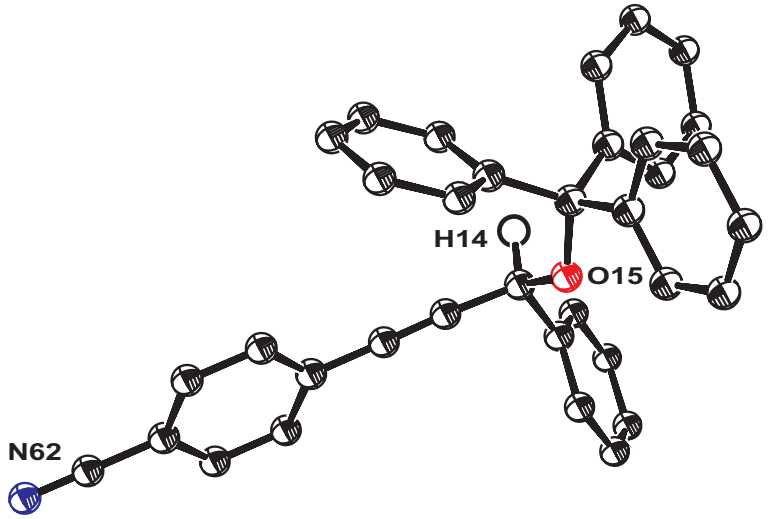
3c
-61.23 kcal/mol

Propargyl trityl ether 1c



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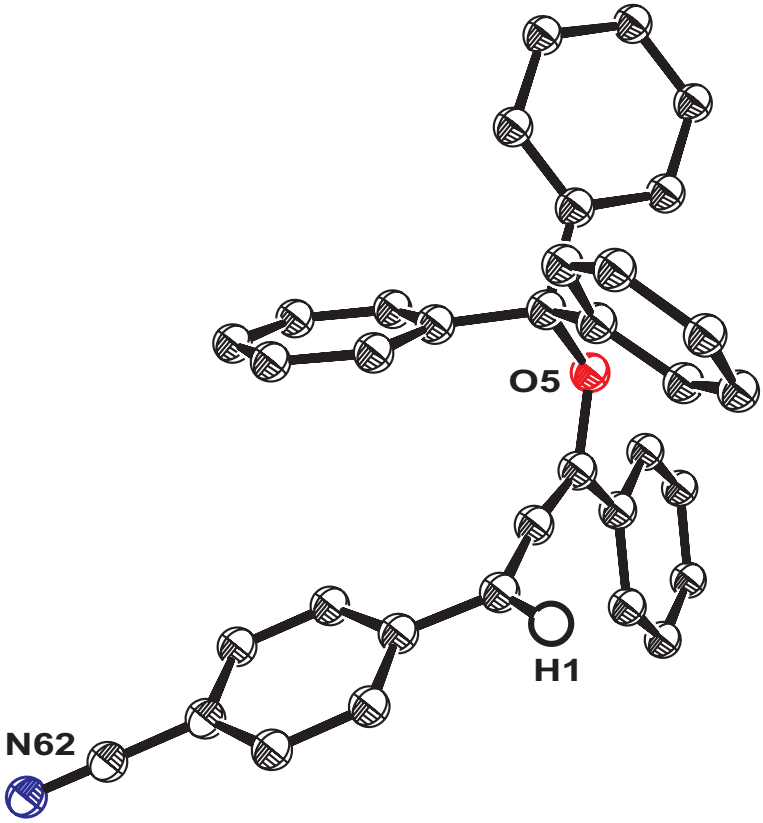
C	2.32365400	0.63036800	–0.15618200
C	3.71288700	0.31797800	–0.06876600
C	6.46849300	–0.30565600	0.10256400
C	4.14824200	–1.03399100	–0.06805800
C	4.68333900	1.35136500	0.01897600
C	6.04352300	1.04559800	0.10164300
C	5.50730900	–1.34282900	0.01789800
H	3.40153200	–1.83002900	–0.13835100
H	4.35369600	2.39419300	0.02037300
H	6.78689100	1.84512000	0.16747400
H	5.83830100	–2.38534000	0.01862800
C	–0.29459600	1.26415200	–0.31551100
H	–0.65458700	1.13887100	–1.35648900
O	–1.11300800	0.46705000	0.58210800
C	–1.79798700	–0.70318600	0.03444600
C	–0.47003700	2.73200400	0.07779300
C	–0.79329200	5.43772000	0.80397500
C	–0.89983600	3.67612000	–0.87250600
C	–0.19601200	3.15133500	1.39540900
C	–0.36360900	4.49616900	1.75746300
C	–1.05842600	5.02592100	–0.51220400
H	–1.11622800	3.35424100	–1.89766700
H	0.14744600	2.41881200	2.13316000
H	–0.15349200	4.81278600	2.78461100
H	–1.39274500	5.75273300	–1.26001100
H	–0.91905900	6.48795800	1.08730500
C	–2.56397300	–1.29860000	1.24356100
C	–4.01828100	–2.40661300	3.40823400
C	–3.33024400	–2.47138600	1.07330500
C	–2.53812100	–0.68669600	2.51108600
C	–3.26152800	–1.23847600	3.58453300
C	–4.04811900	–3.02283500	2.14430200

H	–3.36596100	–2.96213700	0.09541000
H	–1.94753400	0.22005100	2.65525300
H	–3.22816400	–0.74776900	4.56333300
H	–4.63409500	–3.93506600	1.98953900
H	–4.58082300	–2.83424600	4.24479000
C	–0.75367700	–1.69967100	–0.51966800
C	1.27399100	–3.45281600	–1.45929200
C	–0.15041300	–2.64040600	0.34267400
C	–0.30193500	–1.63928700	–1.85631900
C	0.69919400	–2.50721900	–2.32349700
C	0.84959300	–3.50976100	–0.12017100
H	–0.47124600	–2.69550600	1.38695600
H	–0.74126600	–0.91549500	–2.54991500
H	1.02655000	–2.44288500	–3.36659100
H	1.29125800	–4.23952600	0.56717800
H	2.04338000	–4.14058100	–1.82650600
C	–2.86617600	–0.25719500	–0.99689300
C	–4.97887400	0.54773700	–2.71355900
C	–3.48606300	1.00122300	–0.84204300
C	–3.33800000	–1.11381900	–2.01501200
C	–4.38355800	–0.71492400	–2.86534000
C	–4.52539100	1.40352800	–1.69547400
H	–3.15000100	1.66387600	–0.03960000
H	–2.88956200	–2.10272300	–2.15138600
H	–4.73018400	–1.39670900	–3.64939700
H	–4.98651900	2.38727300	–1.55683700
H	–5.79126300	0.85942000	–3.37832900
C	7.86502100	–0.62234400	0.18839400
N	9.01186000	–0.88286600	0.25869100

Energy RMP2 = –1475.0194704 Hartree

Tentative Intermediate 4c



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C	0.70832700	0.93990300	0.88623500
C	–0.36145200	1.52565700	0.35272400
O	–1.52766800	0.89331400	–0.05356600
C	–1.65692300	–0.57013000	–0.07791000
C	–3.06633700	–0.78394800	–0.68905600
C	–5.68779200	–1.23471600	–1.66130300
C	–4.11693600	0.09734600	–0.35810500
C	–3.34835400	–1.89825500	–1.50372300
C	–4.64979000	–2.12308400	–1.98412000
C	–5.41401200	–0.12211100	–0.84720100
H	–3.91438600	0.96045200	0.28182800
H	–2.54764200	–2.59237300	–1.77731500
H	–4.84663000	–2.99360400	–2.61889800
H	–6.21443500	0.57854300	–0.58628600
H	–6.70062400	–1.40691200	–2.04009200
C	–0.55774500	–1.13993300	–0.99829100
C	1.35818800	–2.13312000	–2.83699700
C	–0.51840600	–0.66818600	–2.33060900
C	0.39773500	–2.09175300	–0.59590200
C	1.34301600	–2.59103300	–1.51097900
C	0.43024900	–1.15583900	–3.24066800
H	–1.24778700	0.08172900	–2.65316600
H	0.41678000	–2.44503900	0.43821300

H	2.07476200	−3.33388100	−1.17687000
H	0.43817000	−0.77947500	−4.26917200
H	2.09200400	−2.52598900	−3.54860000
C	−1.71710400	−1.14735500	1.35473400
C	−2.03128700	−2.23388100	3.95884900
C	−1.80153100	−0.30642700	2.48247800
C	−1.83300500	−2.54156400	1.55092100
C	−1.97881000	−3.08041600	2.83854800
C	−1.95117900	−0.84507400	3.77217900
H	−1.75829400	0.77776900	2.35629900
H	−1.83076600	−3.21593500	0.68881300
H	−2.06290200	−4.16528200	2.96264000
H	−2.01139100	−0.16960700	4.63233100
H	−2.14824200	−2.65252000	4.96378900
C	−0.44212100	2.99862100	0.12355400
C	−0.59421700	5.79137000	−0.32010500
C	−1.49300400	3.54786800	−0.64589900
C	0.52916800	3.86947900	0.66917300
C	0.45314400	5.25053000	0.44883300
C	−1.56367600	4.93366000	−0.86406000
H	−2.24894200	2.88379000	−1.07193500
H	1.34597000	3.45466200	1.26884300
H	1.21434000	5.90851700	0.88120900
H	−2.38367200	5.34194600	−1.46452500
H	−0.65259300	6.87124300	−0.49125300
C	3.07893600	0.12378300	0.93848000
C	5.59252900	−0.62023300	−0.13531900
C	4.11864300	−0.33939700	1.78037200
C	3.32153000	0.20719100	−0.45446600
C	4.55819400	−0.15607200	−0.98792000
C	5.36142100	−0.71045300	1.25815500
H	3.94405600	−0.40638900	2.86014000
H	2.52180500	0.56000300	−1.11352900
H	4.73909900	−0.08709800	−2.06443100
H	6.15813700	−1.06819700	1.91666500
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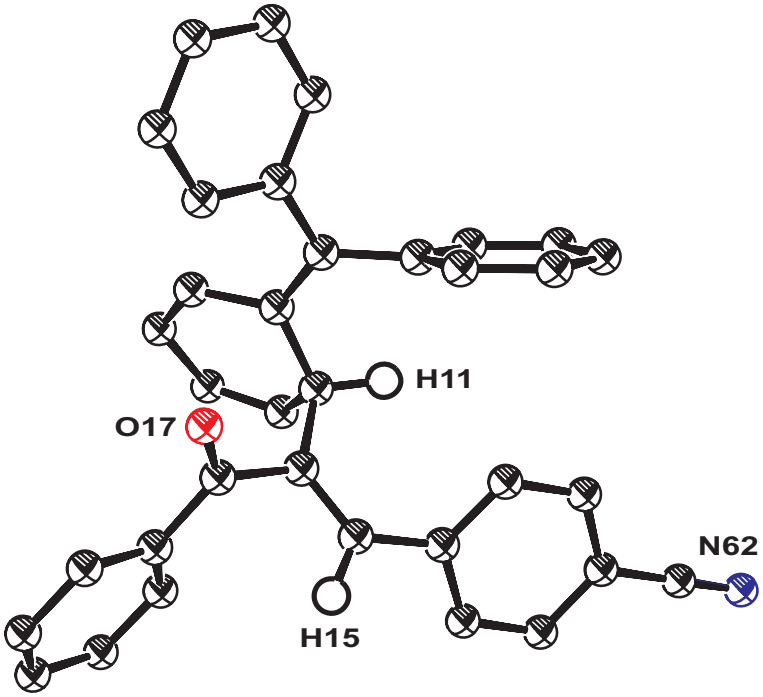
N	7.90669300	−1.30914400	−1.13347400

Energy RMP2 = −1475.0286324 Hartree

Tentative intermediate 5c



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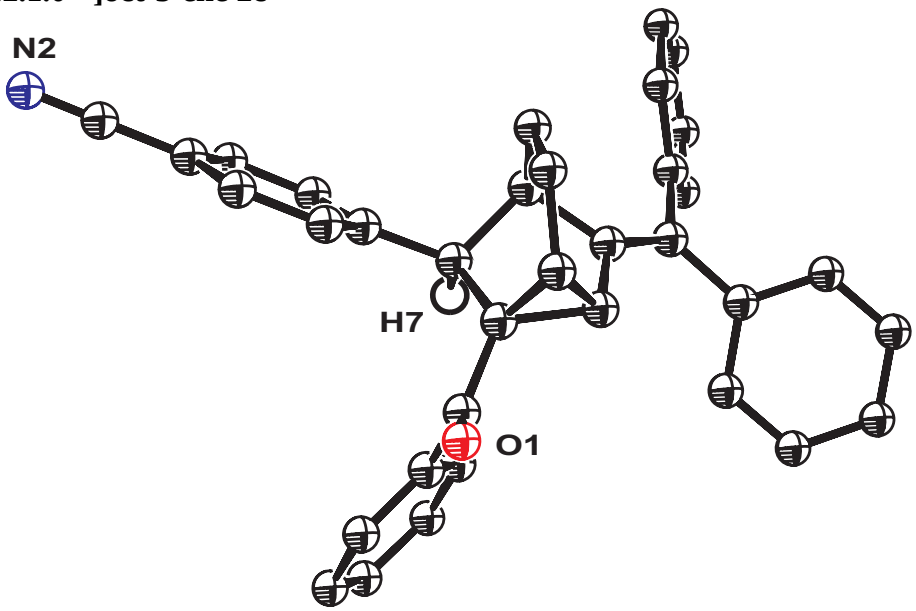
C	0.04455000	0.22466600	1.07690700
C	0.37806800	1.05841800	2.30769300
C	–1.40427500	–0.28674200	1.06455800
C	–1.99947800	1.48339900	2.67904100
H	–0.34178900	2.33205400	3.86095600
H	1.43799900	1.17755800	2.55774800
H	–2.76371900	2.03230800	3.23899900
H	–3.44150400	0.30880100	1.63626200
H	0.73970100	–0.62444000	1.02844300
C	–1.75513500	–1.45763900	0.41351200
C	0.38044500	1.15322100	–0.12293200
C	1.61261500	1.26744300	–0.69440800
H	1.74321300	2.09635300	–1.40642700
C	–0.70212100	2.03864600	–0.70930200
O	–1.65811100	1.50081300	–1.28850800
C	2.83658100	0.46521100	–0.48699000
C	5.26330900	–0.97098500	–0.14415000
C	4.08367700	1.13878500	–0.42684300
C	2.83853600	–0.94918900	–0.41170600
C	4.03039600	–1.65967000	–0.23877400
C	5.28087800	0.44113200	–0.24733200
H	4.10610000	2.23076200	–0.51267800
H	1.90338300	–1.50416200	–0.52945800
H	4.01404600	–2.75193100	–0.19074600
H	6.23307300	0.97635500	–0.19015100
C	–0.57626000	3.53194500	–0.64864400

C	–0.44550900	6.34743000	–0.57748700
C	–1.42953200	4.30875600	–1.46698800
C	0.34021400	4.18221100	0.20791800
C	0.39961900	5.58411700	0.24628800
C	–1.36038600	5.70628600	–1.43538700
H	–2.13699600	3.78851900	–2.12025400
H	0.98805300	3.58479900	0.85624400
H	1.10475400	6.08159900	0.92037300
H	–2.01810600	6.30110000	–2.07780800
H	–0.39355200	7.44111600	–0.55114000
C	–0.74244300	–2.47910300	0.00312200
C	1.07736000	–4.52015300	–0.75700200
C	–0.63811700	–2.89193400	–1.34651600
C	0.07528100	–3.11895300	0.96652300
C	0.97348800	–4.13163400	0.59055200
C	0.27062400	–3.89324300	–1.72394300
H	–1.27483500	–2.41530500	–2.09903900
H	–0.01849500	–2.83103100	2.01972800
H	1.58410500	–4.62526800	1.35438400
H	0.34405100	–4.19008200	–2.77561000
H	1.77376700	–5.31275600	–1.05028200
C	–3.16555100	–1.79928000	0.06884400
C	–5.82737600	–2.48468400	–0.63190900
C	–3.67697600	–3.09308900	0.33528600
C	–4.00664900	–0.86377000	–0.58326600
C	–5.32368900	–1.20616600	–0.92804100
C	–4.99702600	–3.42782300	–0.00006000
H	–3.03266800	–3.83471300	0.81959900
H	–3.59934800	0.11794000	–0.84556500
H	–5.95486900	–0.47292500	–1.44190700
H	–5.37768200	–4.42901800	0.22900800
H	–6.85520500	–2.74905100	–0.90221900
C	6.48656700	–1.69841100	0.03765600
N	7.49050300	–2.29590000	0.18956300

Energy RMP2 = –1475.0316008 Hartree

Tricyclo[3.2.1.0^{2,7}]oct-3-ene 2c

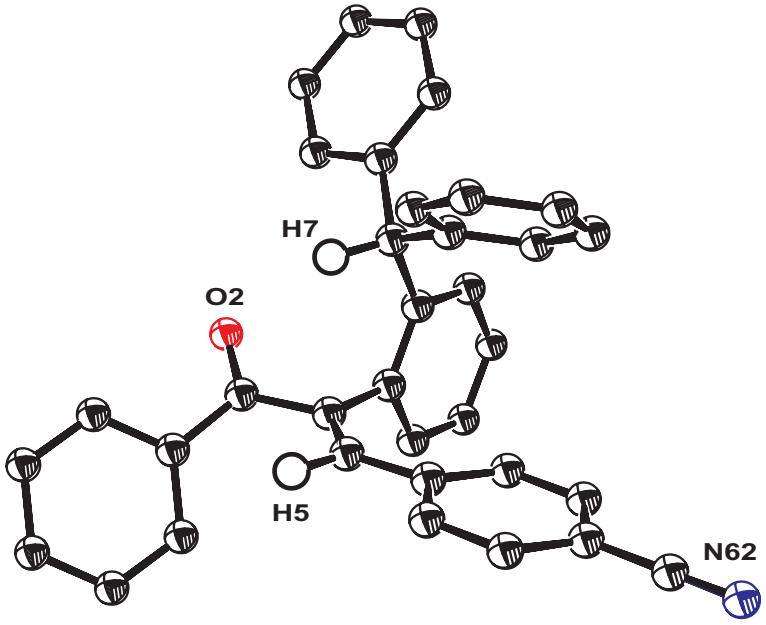


ATOM	X	Y	Z
O	–1.90279100	2.68699600	–2.10209700
N	–7.44452300	–3.05609900	0.34725100
C	–0.35909200	0.29527400	–2.48906600
H	–0.52320900	1.01612000	–3.29529300
C	–0.79663100	0.80820300	–1.11092300
C	–1.06265700	–0.29986100	–0.07934700
H	–0.80664900	0.07751900	0.92663900
C	0.07523400	–1.35686300	–0.44442100
H	0.23574300	–2.08138300	0.36606900
C	1.26566900	–0.41401100	–0.66577300
C	0.71624500	0.71509200	–1.45581400
H	1.30315100	1.60741100	–1.68151700
C	–0.49068200	–1.15245800	–2.78823800
H	–0.75653700	–1.47337000	–3.80039200
C	–0.26844800	–2.01100500	–1.76803000
H	–0.35144400	–3.09819100	–1.85972600
C	–1.48321000	2.15503600	–1.06395400
C	–1.64400800	2.85900800	0.25420400
C	–2.70995200	3.77602100	0.39499800
H	–3.39209700	3.91525500	–0.44924100
C	–2.88260400	4.48456000	1.59109900
H	–3.72179800	5.17986200	1.69674000
C	–1.97630900	4.30718700	2.65310600
H	–2.10771400	4.86623900	3.58550200
C	–0.89822600	3.41601300	2.51410800
H	–0.18092000	3.28901400	3.33163700
C	–0.73828200	2.68775600	1.32504300
H	0.11295500	2.00748500	1.21834200
C	–2.46786300	–0.86534800	–0.01632000
C	–3.40016500	–0.71454900	–1.06496900
H	–3.12473600	–0.14789700	–1.95896400

C	–4.68205600	–1.27232800	–0.97694800
H	–5.39769000	–1.14532300	–1.79438800
C	–5.05872900	–2.00348200	0.17331000
C	–4.13506700	–2.15630700	1.23554000
H	–4.42692100	–2.71278900	2.13083700
C	–2.86235100	–1.58680400	1.13335200
H	–2.15723000	–1.70120300	1.96505400
C	–6.36980500	–2.58032700	0.26834000
C	2.53931900	–0.56207600	–0.18734800
C	2.97660700	–1.79953500	0.52788400
C	3.71135600	–1.69796700	1.73452800
H	3.95226900	–0.70556000	2.13046500
C	4.12171000	–2.84569600	2.42803400
H	4.67858100	–2.74248200	3.36553000
C	3.82488300	–4.12388800	1.92112200
H	4.15278200	–5.02001900	2.45813600
C	3.11810000	–4.24176100	0.71264900
H	2.90131300	–5.23191100	0.29742000
C	2.70044900	–3.09205200	0.02185000
H	2.18114500	–3.18878100	–0.93730800
C	3.58150500	0.49977000	–0.36028900
C	3.35078400	1.84695400	0.00283600
H	2.39008400	2.12651800	0.44784300
C	4.34410500	2.82463400	–0.17194200
H	4.14258100	3.86023700	0.12222700
C	5.59365400	2.47349600	–0.70940000
H	6.36893700	3.23454100	–0.84585100
C	5.84436900	1.13499100	–1.06055600
H	6.81674000	0.84934200	–1.47583200
C	4.85345600	0.15877400	–0.87981100
H	5.05678700	–0.88262500	–1.15103700

Energy RMP2 = –1475.0520786 Hartree

Triphenylmethyl enone 6c

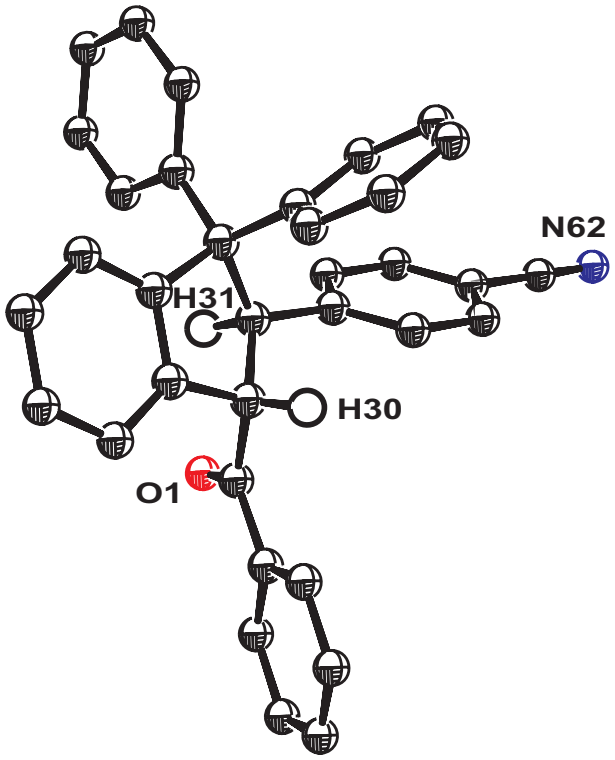


ATOM	X	Y	Z
C	–0.24331500	2.61180000	0.13759900
O	–1.48291500	2.69053800	0.15543000
C	0.43437900	1.32457700	0.54061000
C	1.61875100	0.99293200	–0.06451500
H	1.99765200	1.72471600	–0.79013900
C	–1.81181400	–0.56137900	–0.23804800
H	–1.56528400	0.38220500	–0.75575400
C	0.56902400	3.80775000	–0.28574700
C	1.82514800	4.11955700	0.28256200
H	2.26287200	3.45564600	1.03457600
C	2.49787800	5.29588300	–0.08534900
H	3.46174300	5.53762100	0.37454000
C	1.93391600	6.16129900	–1.03797500
H	2.46390600	7.07353000	–1.33146000
C	0.68222400	5.85927900	–1.60676200
H	0.23852600	6.53449300	–2.34583600
C	–0.00262200	4.69944800	–1.22193600
H	–0.98872200	4.46313300	–1.63356300
C	–0.29477300	0.49618700	1.55770800
C	–1.36361700	–0.37732200	1.21979900
C	–2.00163200	–1.08568700	2.26022800
H	–2.84383500	–1.74003300	2.01083300
C	–1.60403600	–0.94952500	3.59888700
H	–2.12187600	–1.51408800	4.38140700
C	–0.55824200	–0.07332100	3.92985200
H	–0.24834200	0.05793000	4.97171700
C	0.08200300	0.64778400	2.91142400
H	0.89375400	1.34066400	3.16041400
C	–3.34144200	–0.70669300	–0.35083500
C	–3.97395400	–1.92349600	–0.67146300

H	–3.36967400	–2.81283900	–0.87738000
C	–5.37712100	–2.00591100	–0.74390900
H	–5.84994500	–2.96151700	–0.99588700
C	–6.16643000	–0.87091600	–0.50136300
H	–7.25825800	–0.93407900	–0.56083000
C	–5.54230500	0.35048900	–0.18756600
H	–6.14725800	1.24505300	–0.00302100
C	–4.14376300	0.43209600	–0.11289700
H	–3.65665500	1.38238400	0.13284100
C	–1.05033100	–1.67125900	–0.97368100
C	–0.75944200	–1.50507100	–2.34489400
H	–1.05674000	–0.57534800	–2.84474800
C	–0.10611400	–2.51051900	–3.07482800
H	0.11181900	–2.35697700	–4.13732200
C	0.26830600	–3.70966000	–2.44351300
H	0.78038800	–4.49539000	–3.00873000
C	–0.01626000	–3.88893400	–1.07993500
H	0.27237700	–4.81848100	–0.57722600
C	–0.66669700	–2.87694500	–0.35171800
H	–0.87510000	–3.02687800	0.71323300
C	2.48553500	–0.18510100	0.05362300
C	2.30503100	–1.25026900	0.97507400
H	1.45256000	–1.24314700	1.65584300
C	3.20988500	–2.31194800	1.03114700
H	3.05990200	–3.12399200	1.74822100
C	4.32607100	–2.34936800	0.16027500
C	4.52055900	–1.29948400	–0.76862300
H	5.38011300	–1.32426000	–1.44422800
C	3.61287400	–0.24005700	–0.81037000
H	3.77102700	0.57152600	–1.52928000
C	5.25285300	–3.44279400	0.21954300
N	6.01360000	–4.34095700	0.26770200

Energy RMP2 = –1475.0902385 Hartree

Indane 3c



ATOM	X	Y	Z
O	2.15237000	0.05823200	–2.26728300
C	2.38762100	–0.09936500	–1.06403800
C	1.24443300	–0.47243300	–0.09797300
C	–0.13530300	0.02614600	–0.60983100
C	–1.20270100	–0.97295400	0.05659700
C	1.02054500	–1.97914100	0.01759700
C	1.96303300	–3.01834100	0.05754000
C	1.50819000	–4.34585100	0.16822000
C	0.13103300	–4.62519300	0.23679900
C	–0.81070000	–3.58041500	0.19670100
C	–0.35875300	–2.25767100	0.08558900
C	3.78596400	0.04618500	–0.53442500
C	4.79955800	0.43086000	–1.44384500
C	6.12219700	0.58202200	–1.01280200
C	6.45559000	0.34586900	0.33482400
C	5.45927200	–0.04172300	1.24672200
C	4.13078300	–0.18798200	0.81694400
C	–1.54927600	–0.49871400	1.48875400
C	–1.01019100	–1.11782600	2.63604500
C	–1.30691600	–0.64354700	3.92747800
C	–2.15475700	0.46085800	4.09985100
C	–2.70291800	1.08782500	2.96708600
C	–2.39970800	0.61608100	1.68106200
C	–2.46334300	–1.19765800	–0.81440700
C	–3.73156600	–1.41894600	–0.23345000
C	–4.85701600	–1.71455500	–1.02284800
C	–4.74237800	–1.80339500	–2.41815700

C	–3.48334400	–1.61262600	–3.01161900
C	–2.36140300	–1.32296300	–2.21943400
H	1.45945200	–0.06432300	0.90741000
H	–0.12462200	–0.20962300	–1.68676200
H	3.03577100	–2.80872800	–0.00899300
H	2.23295900	–5.16644500	0.18916100
H	–0.21155800	–5.66252800	0.31231400
H	–1.88386900	–3.79507400	0.24064700
H	4.51615000	0.60629300	–2.48611100
H	6.89756800	0.88417800	–1.72437800
H	7.49051100	0.46379300	0.67292000
H	5.71572800	–0.22909600	2.29446800
H	3.36959800	–0.49636300	1.54018700
H	–0.35853400	–1.98999600	2.52717600
H	–0.87609700	–1.14914300	4.79853000
H	–2.39089100	0.82788000	5.10419800
H	–3.36794200	1.95038700	3.08214200
H	–2.84190400	1.11312900	0.81219600
H	–3.84777000	–1.35960800	0.85226400
H	–5.82579200	–1.87545600	–0.53766000
H	–5.61869200	–2.02683400	–3.03542800
H	–3.36765400	–1.69585300	–4.09762700
H	–1.39134200	–1.21730300	–2.71557400
C	–0.38740900	1.51820500	–0.50131900
C	–1.12302600	2.16402400	–1.52117900
C	0.08849200	2.30533200	0.57062400
C	–1.38680300	3.53718700	–1.47673600
H	–1.49426700	1.57487500	–2.36594700
C	–0.15485000	3.68250800	0.62780800
H	0.65225800	1.84088700	1.38523600
C	–0.90005100	4.31128300	–0.39687100
H	–1.95725900	4.01986100	–2.27549400
H	0.22324700	4.27742800	1.46417600
C	–1.15544000	5.72290000	–0.34305100
N	–1.36673700	6.88084300	–0.29661700

Energy RMP2 = –1475.1170548 Hartree