SUPPLEMENTARY MATERIALS

4,5-Di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene

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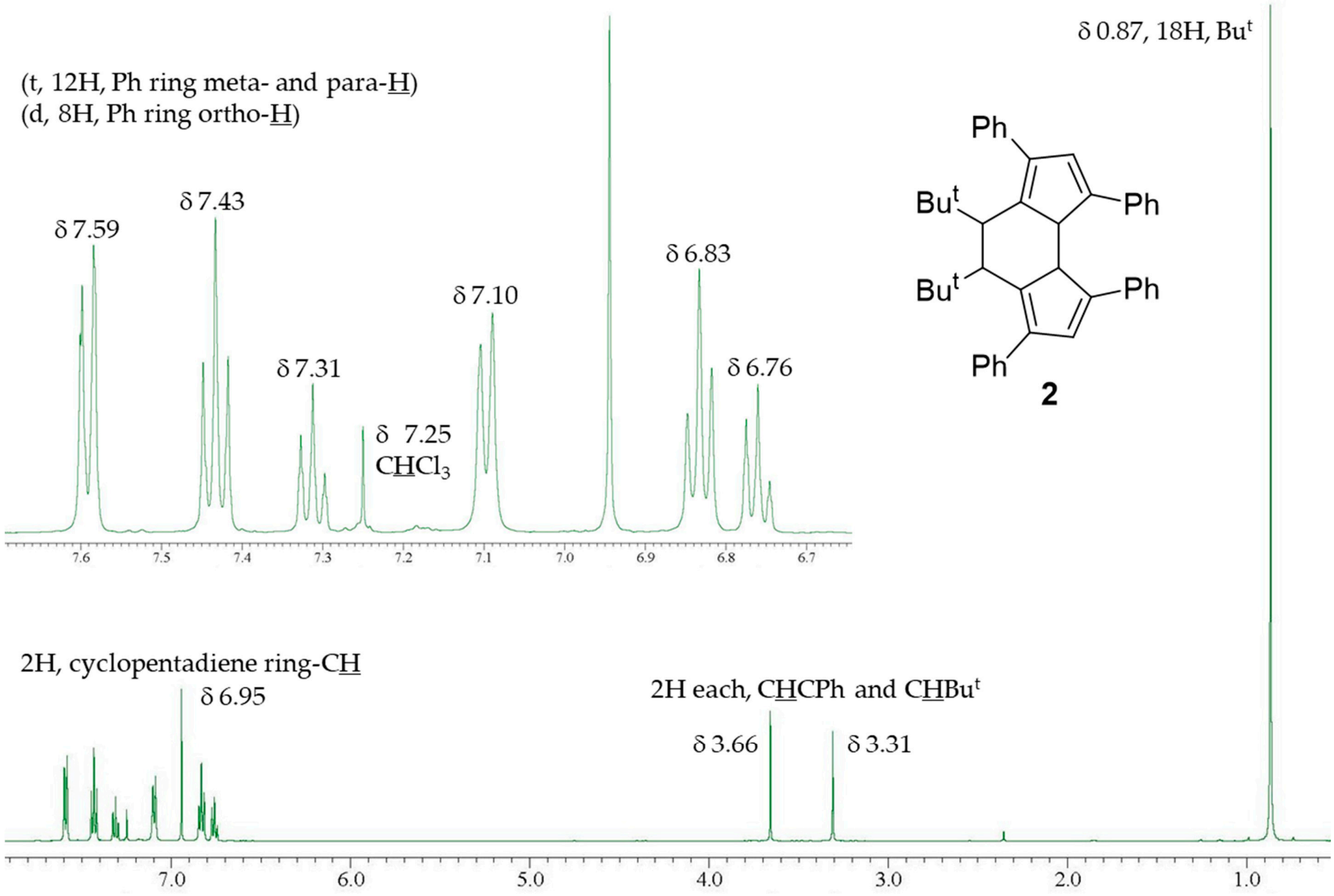


Figure S1. ^{1}H NMR spectrum of crude product **2** (500 MHz, $CDCl_3$).

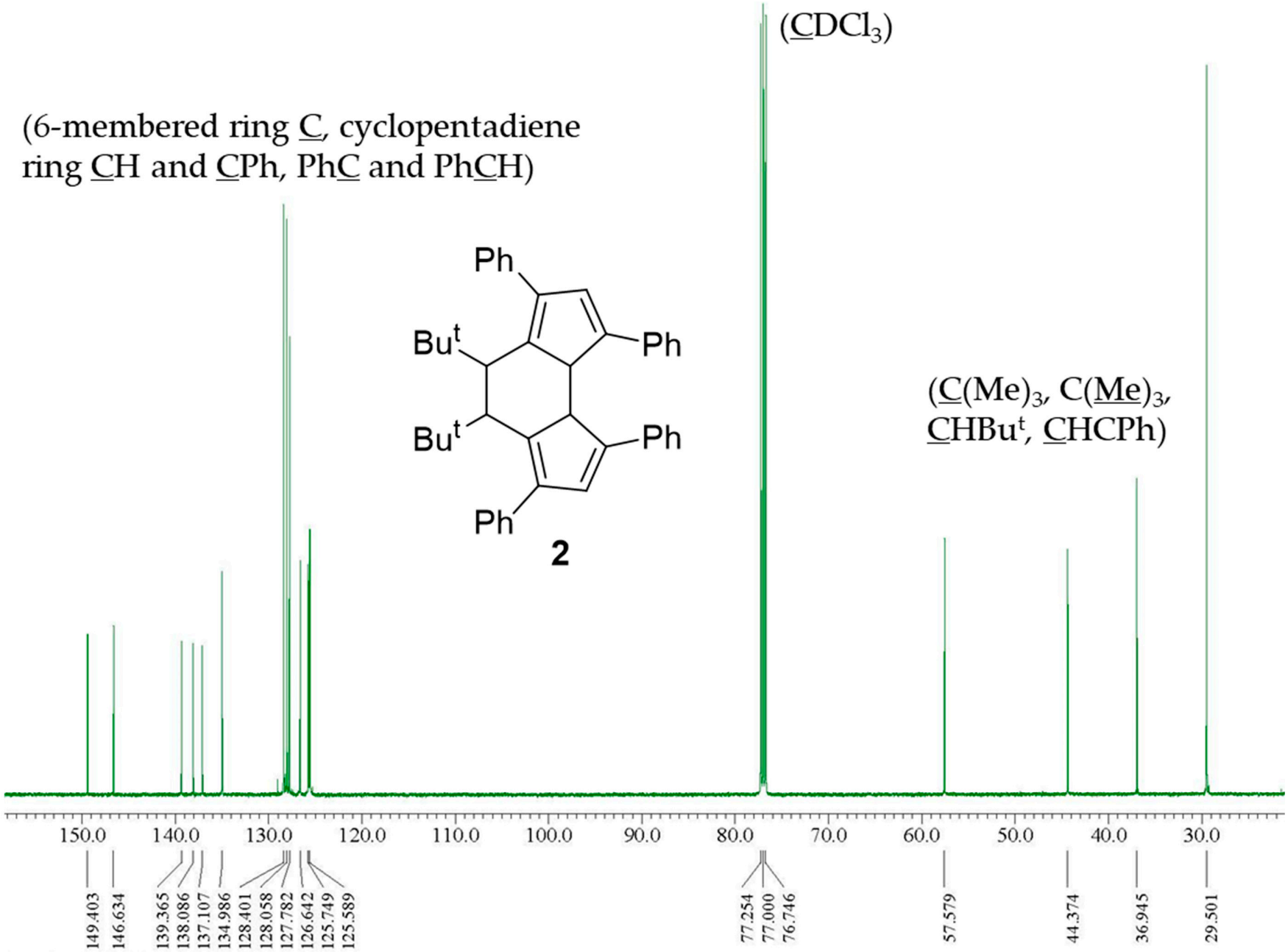
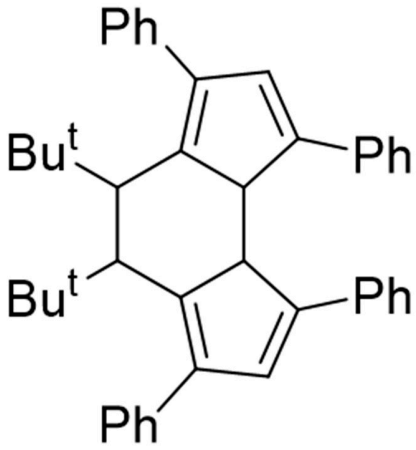


Figure S2. ^{13}C NMR Spectrum of crude product **2** (126 MHz, $CDCl_3$).



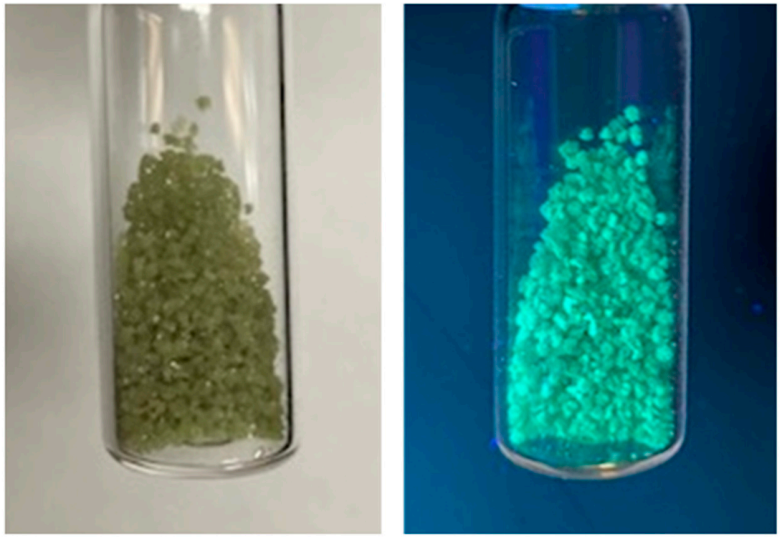


Figure S3. ^{1}H NMR spectrum of crystalline **2** ($CDCl_3$, compare to Figure S1). Crystals were obtained from hot iPrOH by slow cooling and evaporation. Photo inset shows green ambient light fluorescence of **2** (photo A), and green fluorescence under long-wave UV (photo B).

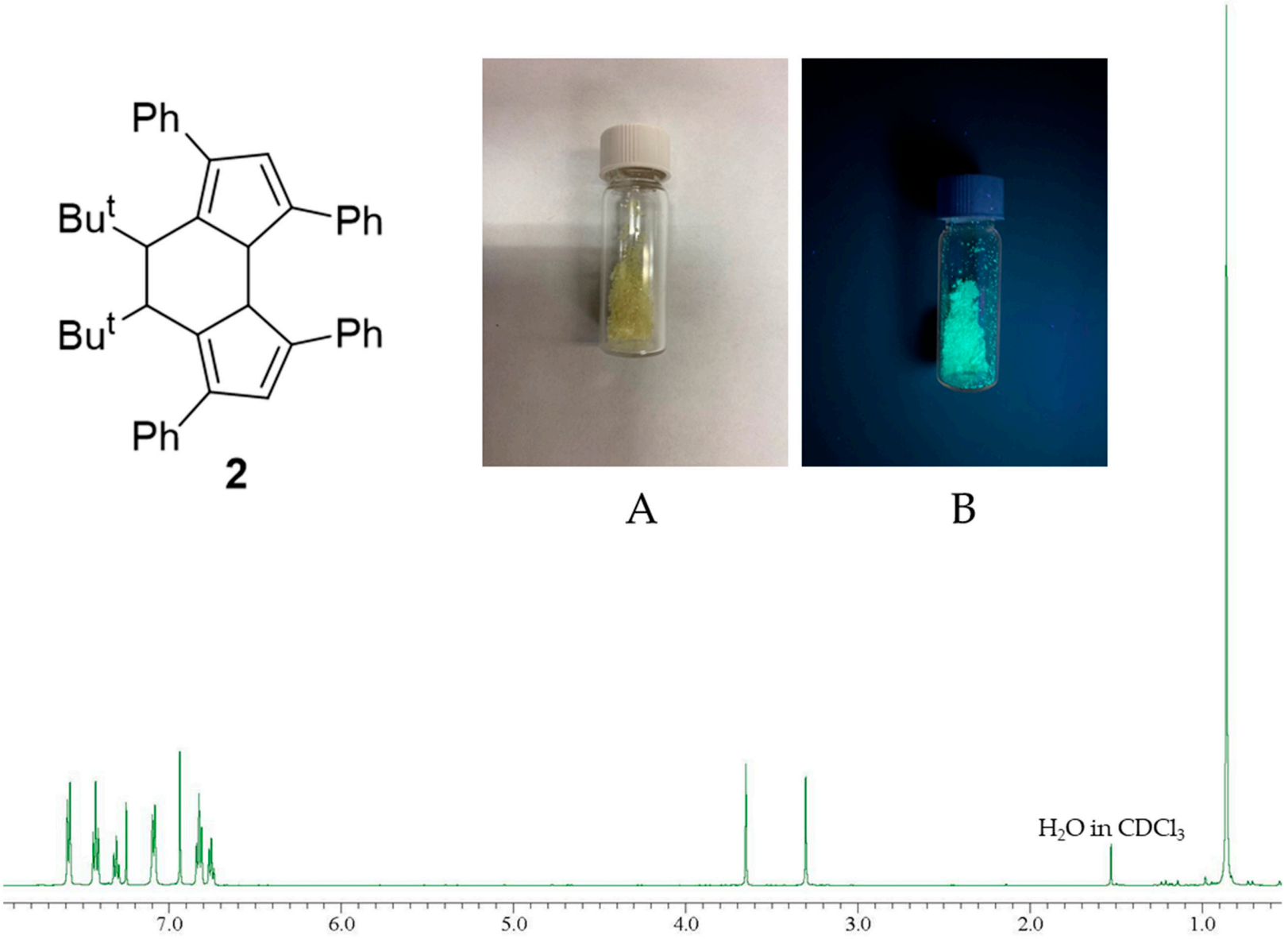


Figure S4. ^{1}H NMR spectrum of crystalline **2** ($CDCl_3$, compare to Figures S1 and S3). Crystals were obtained from hot 2-butanol by slow cooling and evaporation. Photo inset shows ambient light fluorescence of **2** (photo A), and green fluorescence under long-wave UV (photo B). Note that **2** (crystalline material from 2-butanol) in photo A appears with a slightly different color compared to that of **2** (crystalline material from iPrOH, photo A, Figure S3).

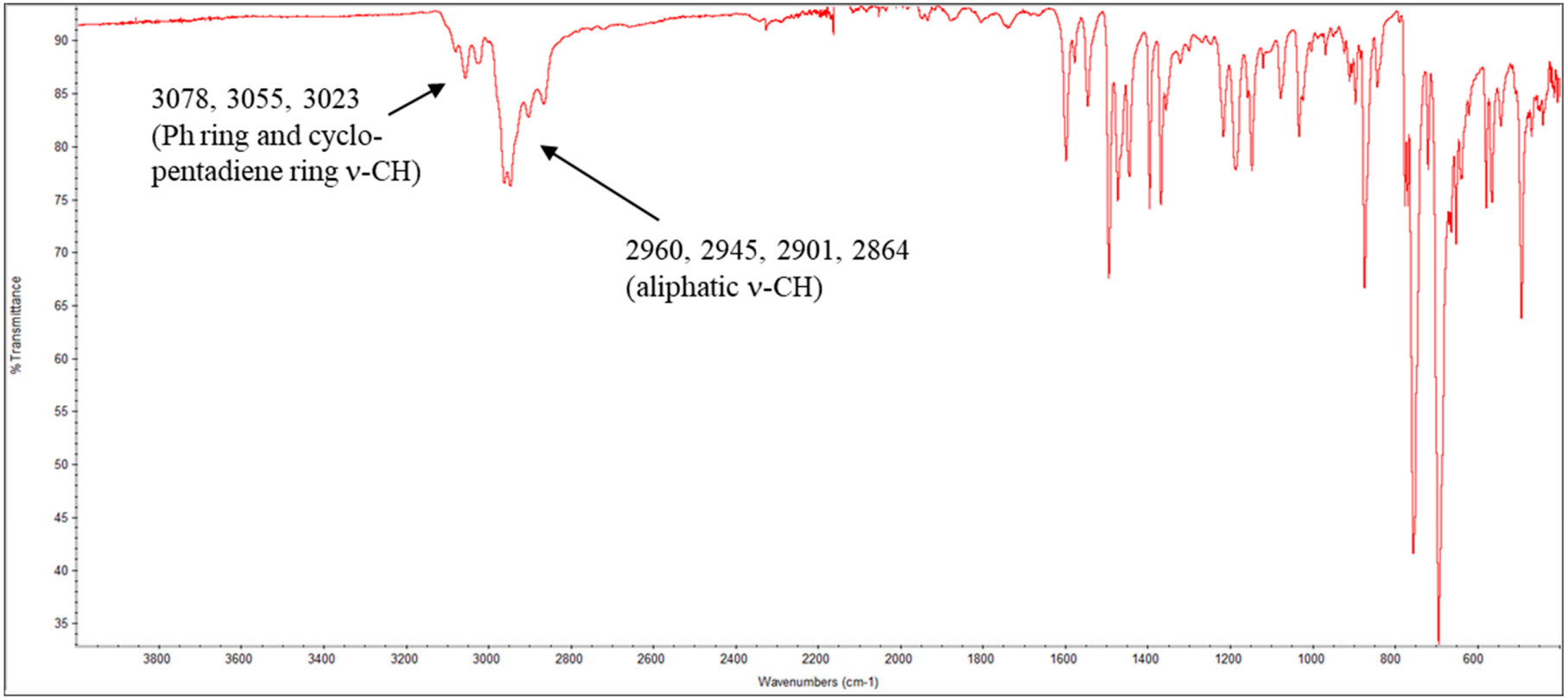


Figure S5. FTIR spectrum of crystalline **2** (ATR). The crystalline sample of **2** was obtained from hot iPrOH by slow cooling and evaporation.

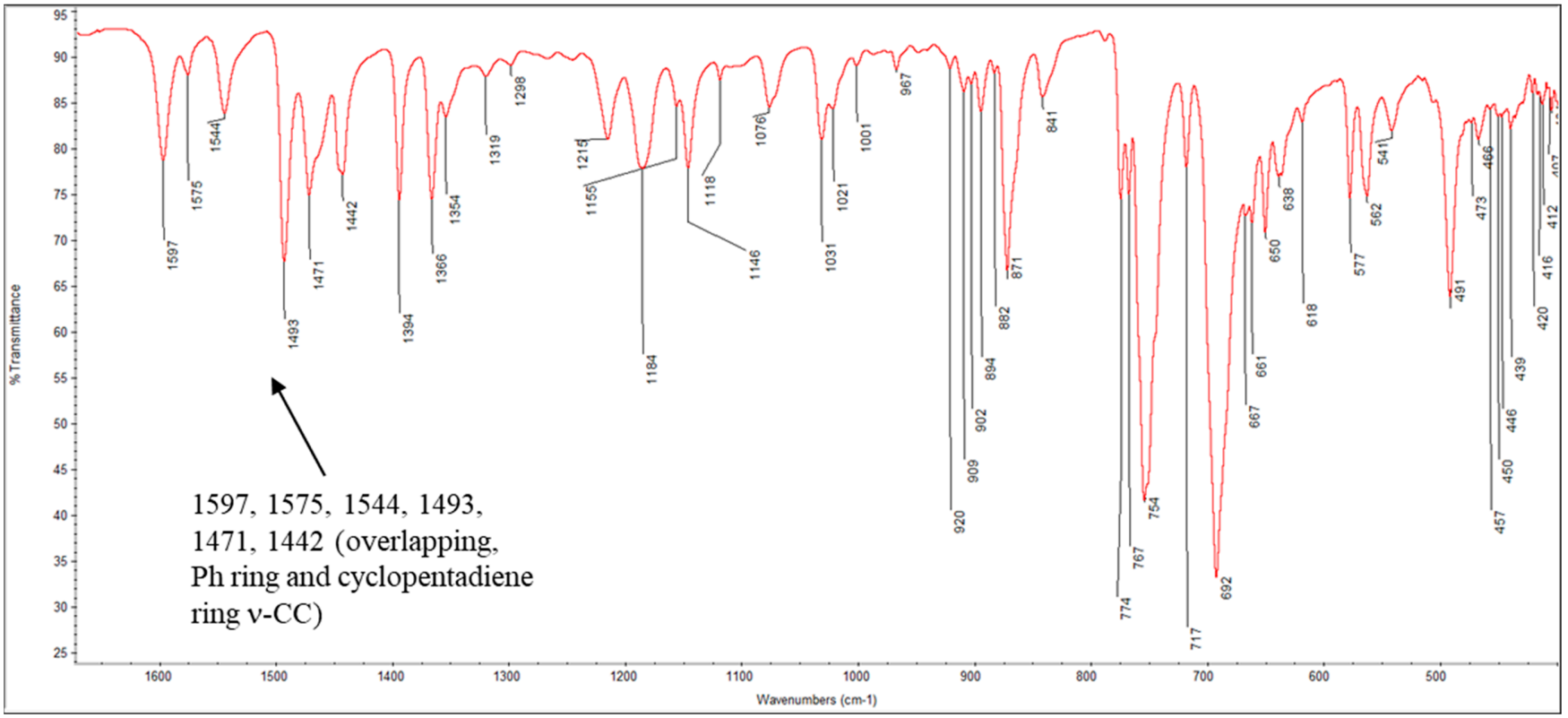


Figure S5A. Expansion of the FTIR spectrum of crystalline **2** (ATR). The crystalline sample of **2** was obtained from hot iPrOH by slow cooling and evaporation.

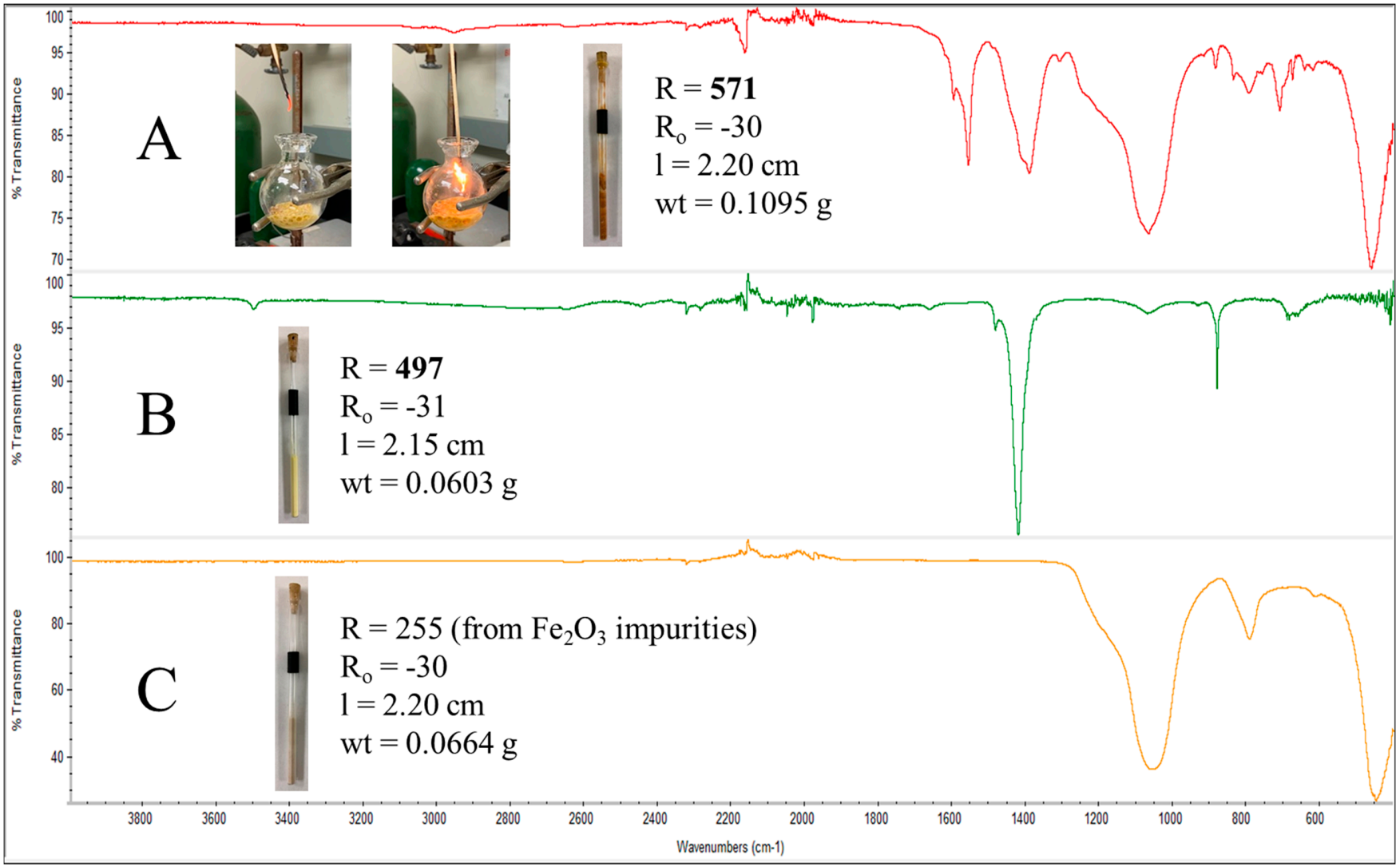


Figure S6. Comparison of FTIR spectra of dry filtered by-product contaminated with celite (spectrum A), authentic sample of KO_2 (spectrum B), and celite (spectrum C). Effervescence was observed upon hydrolysis of the by-product, and re-kindled a wood splint, indicating the generation of O_2 (spectrum A photos). Magnetic susceptibility tubes packed with the by-product contaminated with celite (spectrum A photo), authentic KO_2 (97%, spectrum B photo), and celite (spectrum C photo), indicating paramagnetism of the by-product, consistent with KO_2 formation in the reaction mixture.

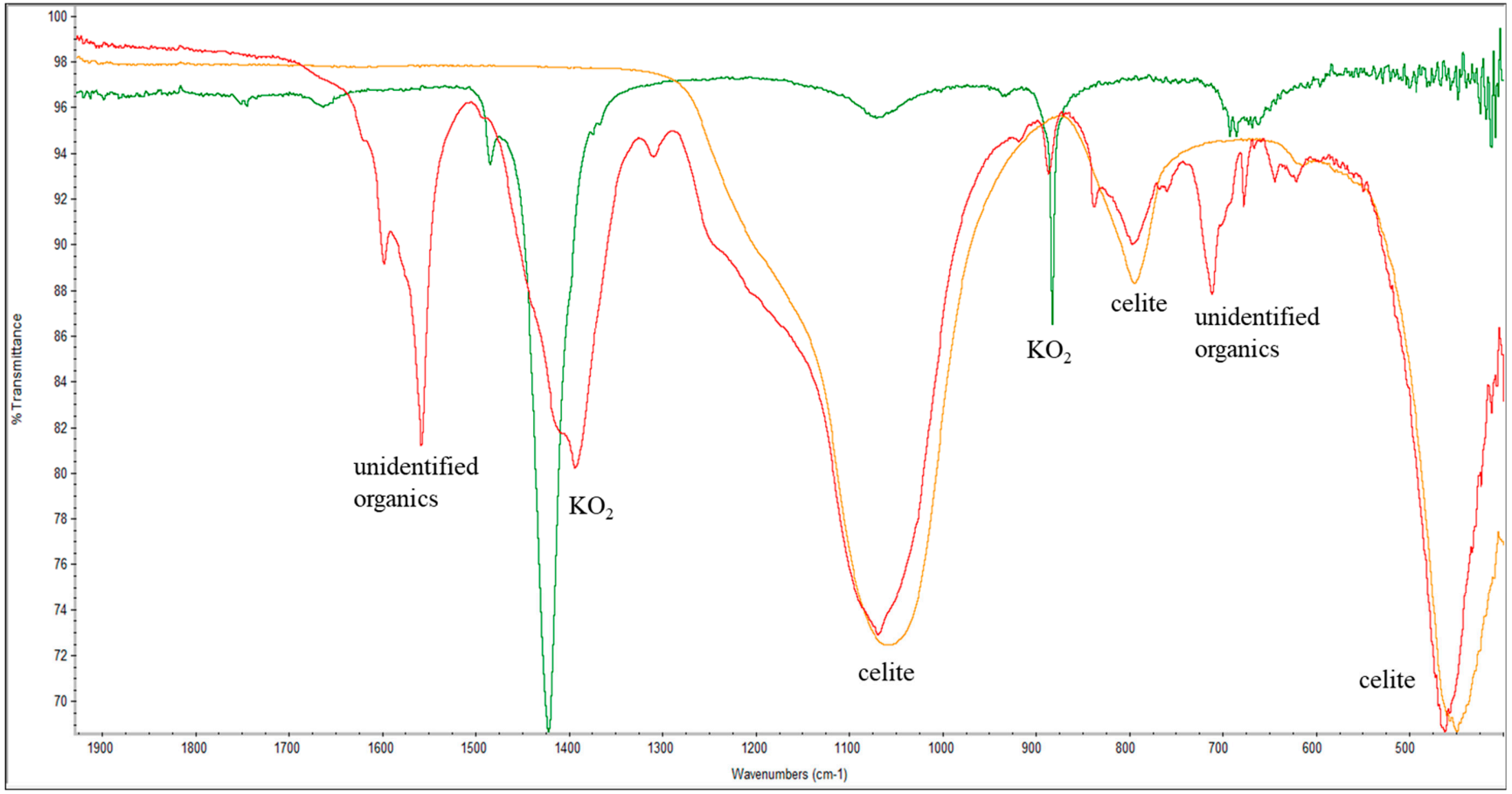


Figure S7. Overlay of the FTIR (ATR) spectra (400 – 1900 cm^{-1}) of the dry filtered by-product contaminated with celite (red spectrum), authentic KO_2 (green spectrum) and celite (orange spectrum), showing presence of KO_2 in the by-product.

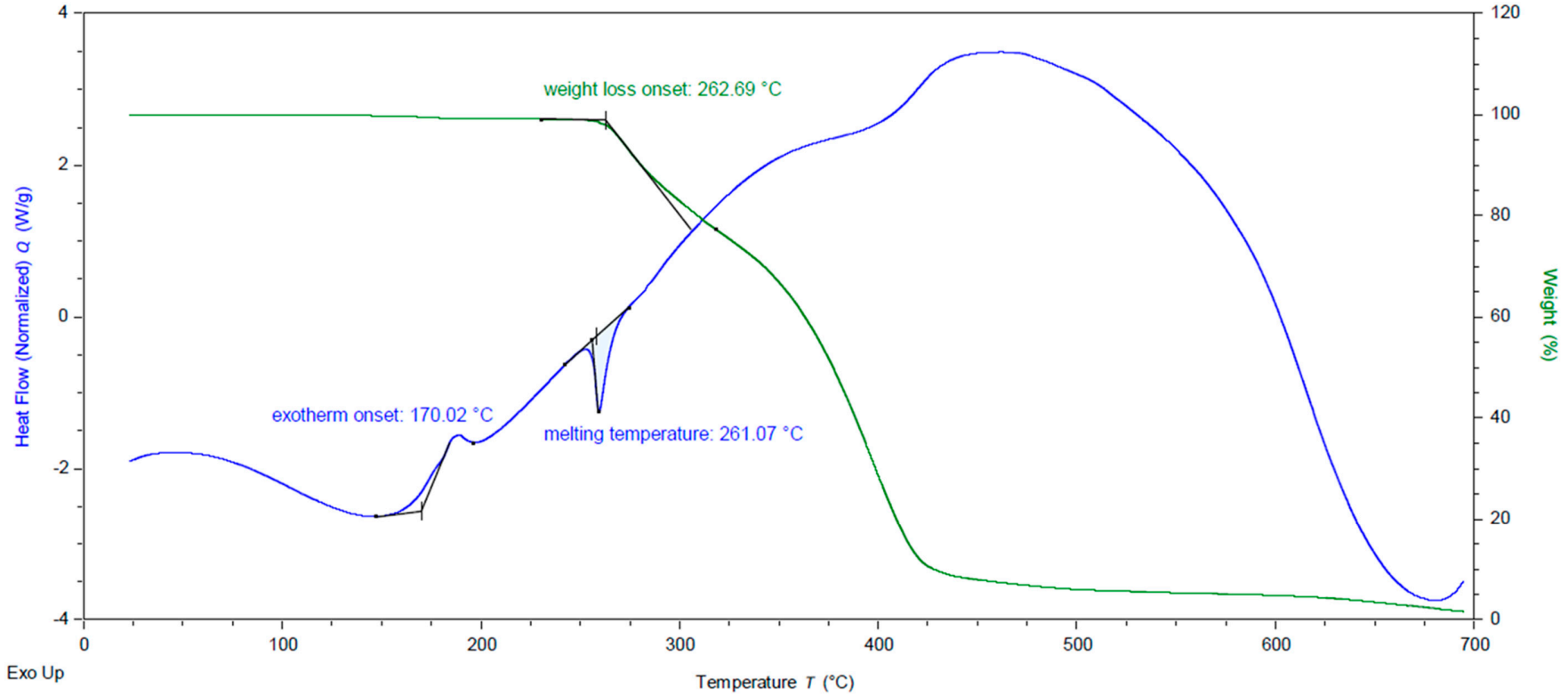


Figure S8. SDT thermogram of **2** (crystalline sample from iPrOH under N_2, ambient to 700º C, 10º C/min).

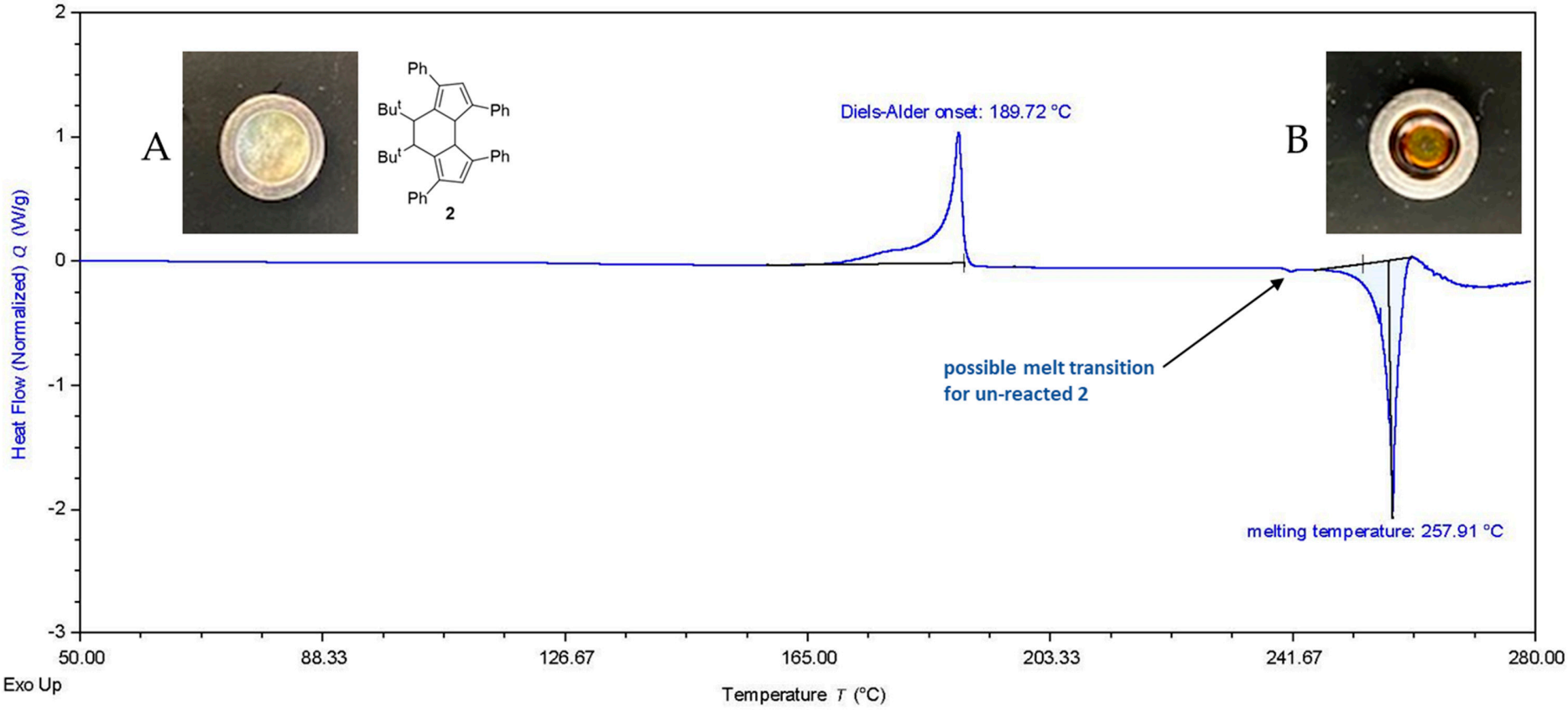


Figure S9. DSC thermogram of **2** (crystalline sample from iPrOH under N_2, open Al pan, ambient to 280º C, 5º C/min). Insets show appearance of a powdered sample of **2** in Al pan at the beginning of the analysis (photo A), and dark brown appearance of residue after melting and some decomposition (photo B).

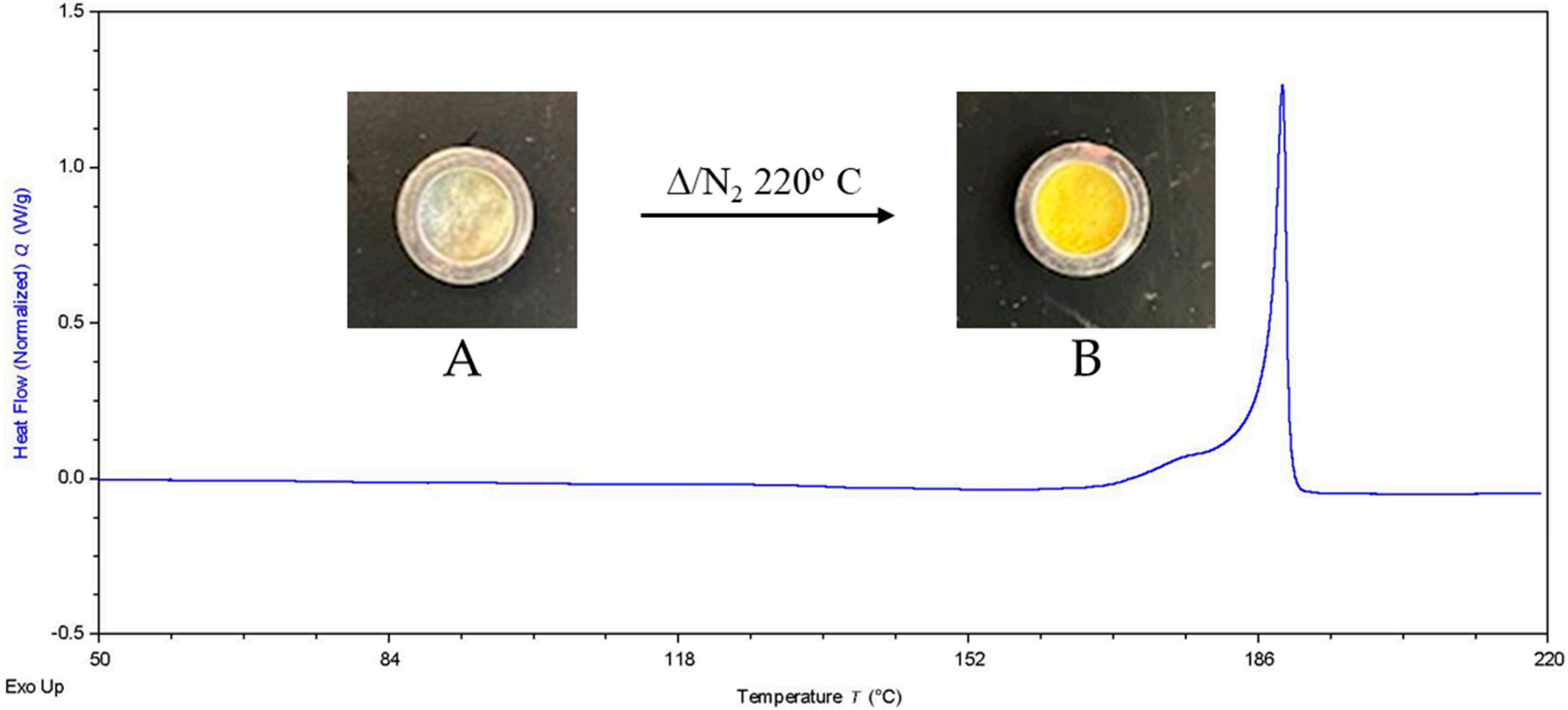


Figure S10. DSC thermogram of **2** (crystalline sample from iPrOH under N_2, open Al pan, ambient to 220° C, 5° C/min). Insets show appearance of a powdered sample of **2** in Al pan at the beginning of the analysis (photo A), and yellow appearance of residue from conversion of **2** to a possible Diels-Alder adduct (photo B).

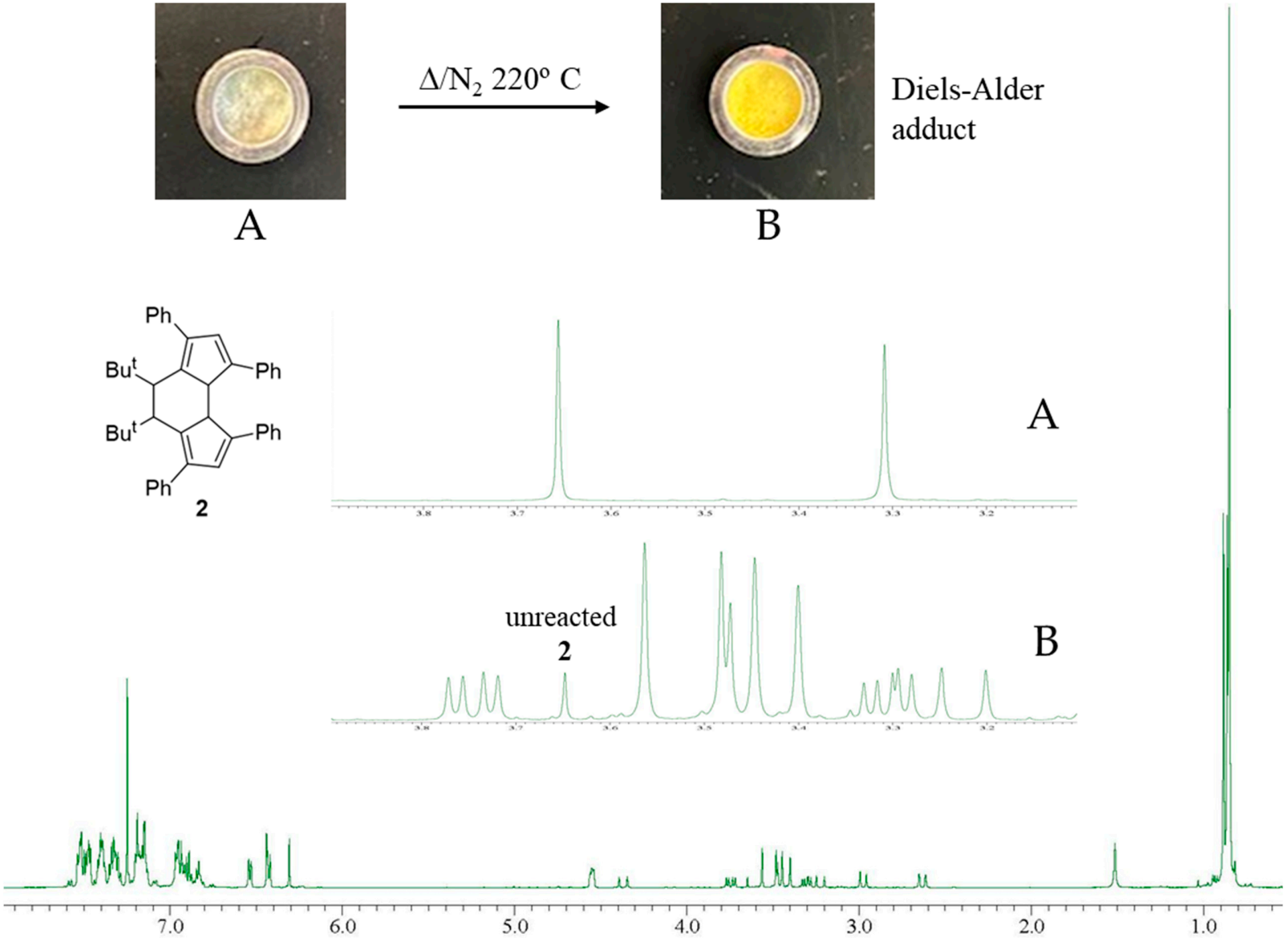


Figure S11. ^{1}H NMR spectrum of yellow residue in DSC pan after pyrolysis of **2** (in $CDCl_3$, crystalline sample from iPrOH, under N_2, open Al pan, ambient to 220° C, 5° C/min), indicating formation of a possible Diels-Alder adduct. Comparison of an expansion of the ^{1}H NMR spectrum of pure **2** (A) with that of the yellow converted product (B) shows some un-converted **2** after pyrolysis to 220° C.

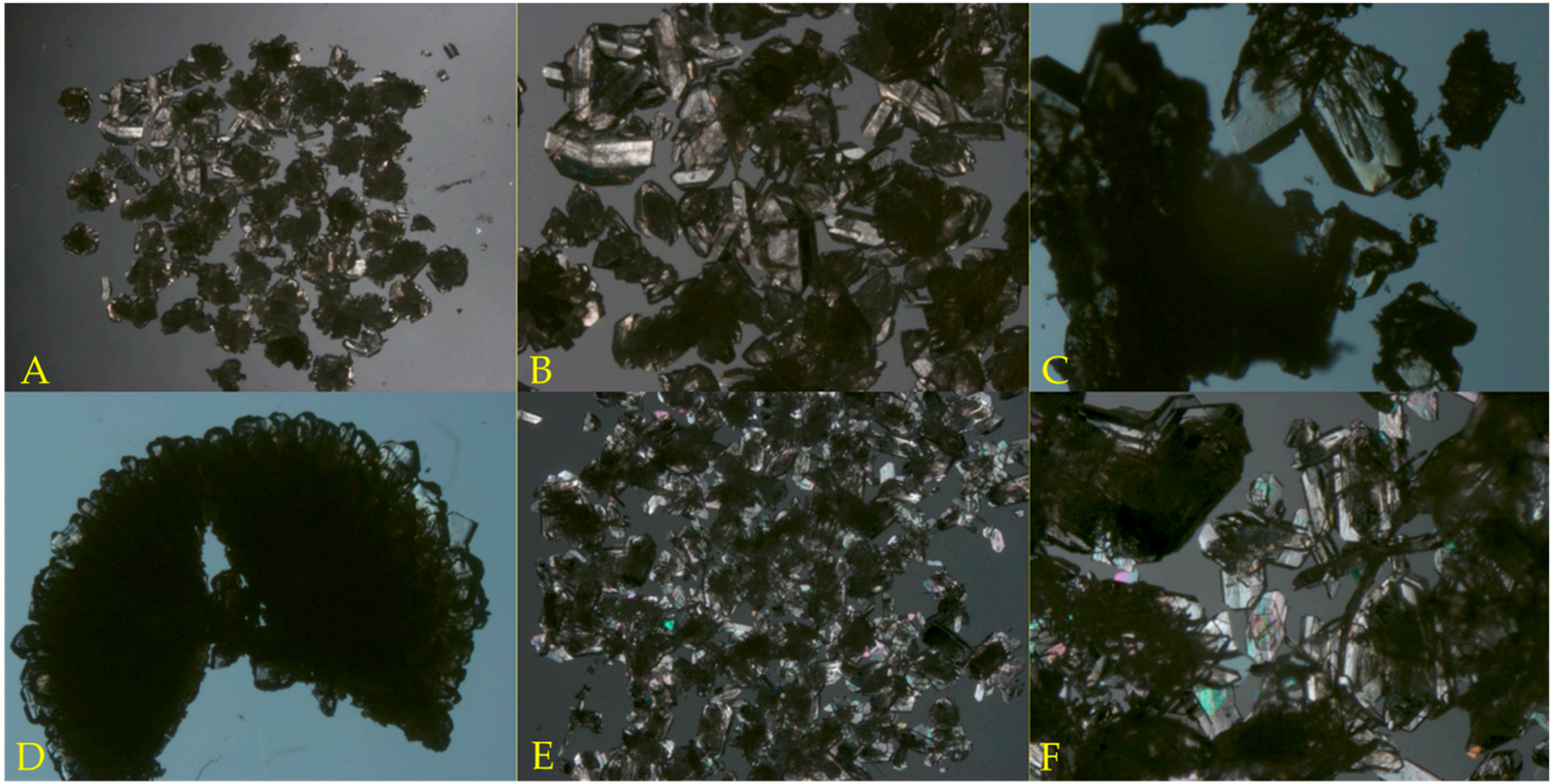


Figure S12. Microscopic images of crystalline samples of **2** taken under polarized transmitted light. Crystals from iPrOH (A), iPrOH magnified view (B), 50/50 THF/MeOH magnified view (C), 50/50 THF/MeOH MeCN layer (D), 2-butanol (E), 2-butanol magnified view (F). Images were taken using a Zeiss Stereo Discovery V12 stereomicroscope.

Single Crystal X-ray Diffraction Study – Experimental Summary (Crystals from iPrOH)

The single crystal X-ray diffraction studies were carried out on a Rigaku Synergy-i dual source (Cu, Mo) single crystal diffractometer using the Cu K_α radiation source (λ = 1.54184 Å) and a Bantam HyPIX-3000 direct photon counting detector. Crystals of the subject compound were grown from iPrOH solution. A 0.184 x 0.164 x 0.055 mm^3 colorless translucent prism crystal was mounted on a Cryoloop with Paratone-N oil.

Data were collected in a nitrogen gas stream at 100.01(12) K using ϖ scans. Crystal-to-detector distance was 40 mm using exposure times of 1 and 4 seconds with a scan width of 0.50°. Data collection was 99.8 % complete to 68.251° in θ. A total of 63674 reflections were collected. 11957 reflections were found to be symmetry independent, with an R_{int} of 0.0211. Indexing and unit cell refinement indicated a **primitive monoclinic** lattice. The space group was found to be **$P2_1/c$.** The data were integrated using the CrysAlisPro software program (Rigaku Oxford Diffraction, 2019, 1.171.40.53) and scaled using an empirical absorption correction implemented in the SCALE 3 ABSPACK software program as well as a numerical absorption correction based on Gaussian integration over a multifaceted crystal model. Solution by direct methods (SHELXT-2014/5) produced a complete phasing model consistent with the proposed structure.

All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL- 2016/6). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL.

Notes: Excellent data and stable refinement. The asymmetric unit consists of two molecules of 4,5-di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene **2**. The molecule crystallizes out as the racemate.

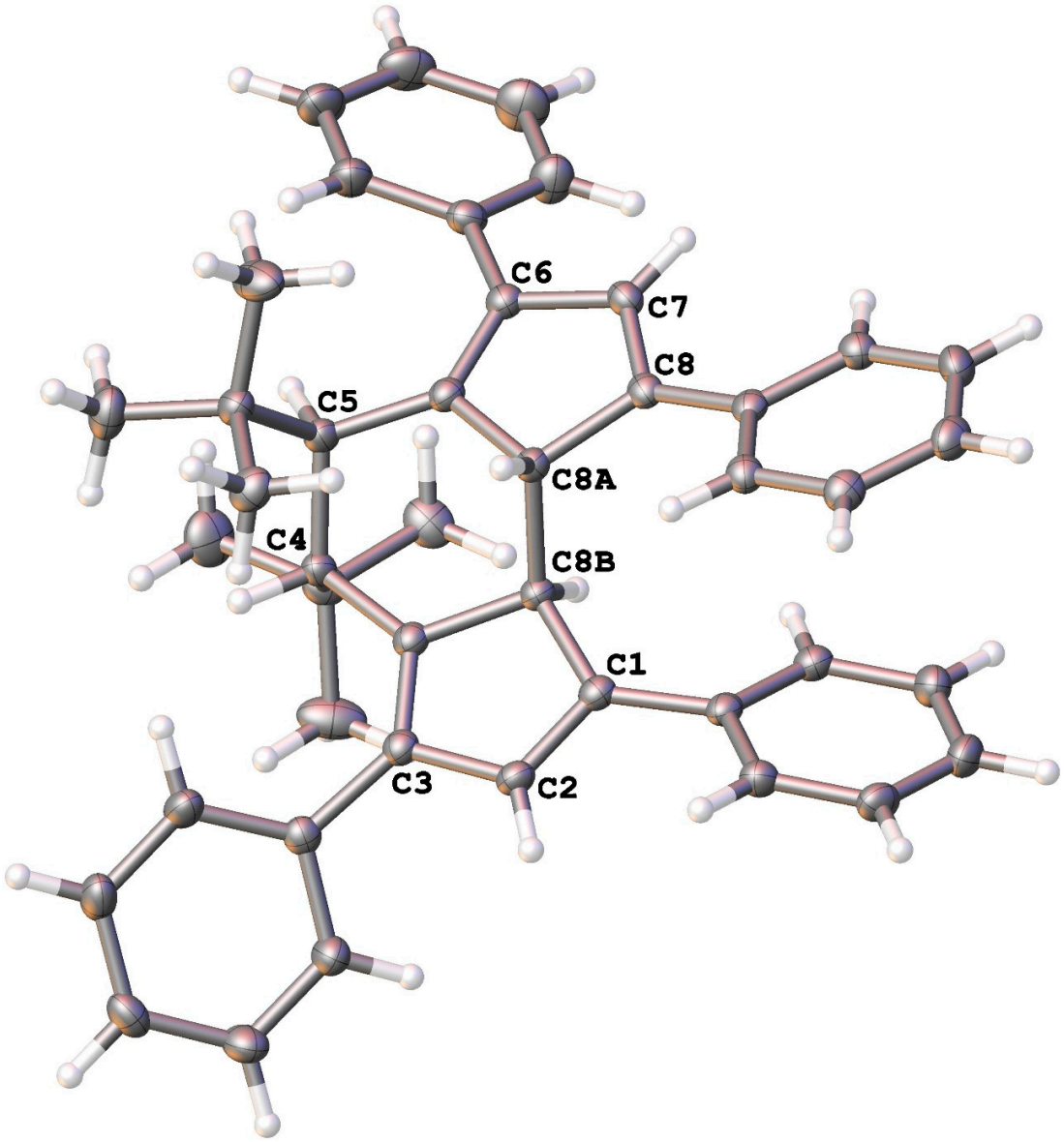


Figure S13. Thermal ellipsoid view of the molecular structure of 4,5-di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene **2** (crystal obtained from iPrOH solution). Thermal ellipsoids are shown at the 50% probability level.

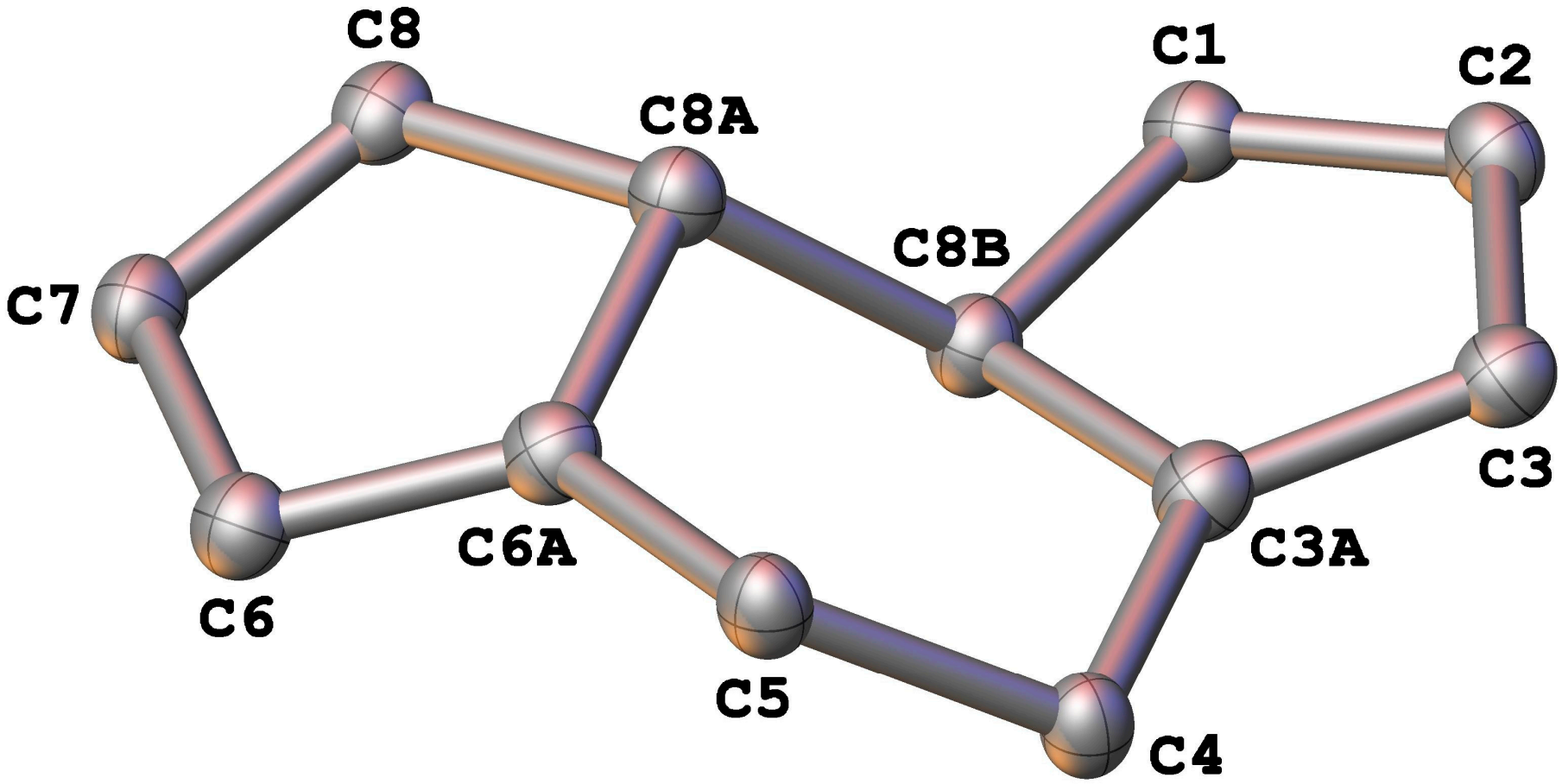


Figure S14. Thermal ellipsoid view of the core structure of **2**, showing two cyclopentadiene rings fused to a central 6–membered ring. Ph groups, Bu^t groups and H atoms were omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

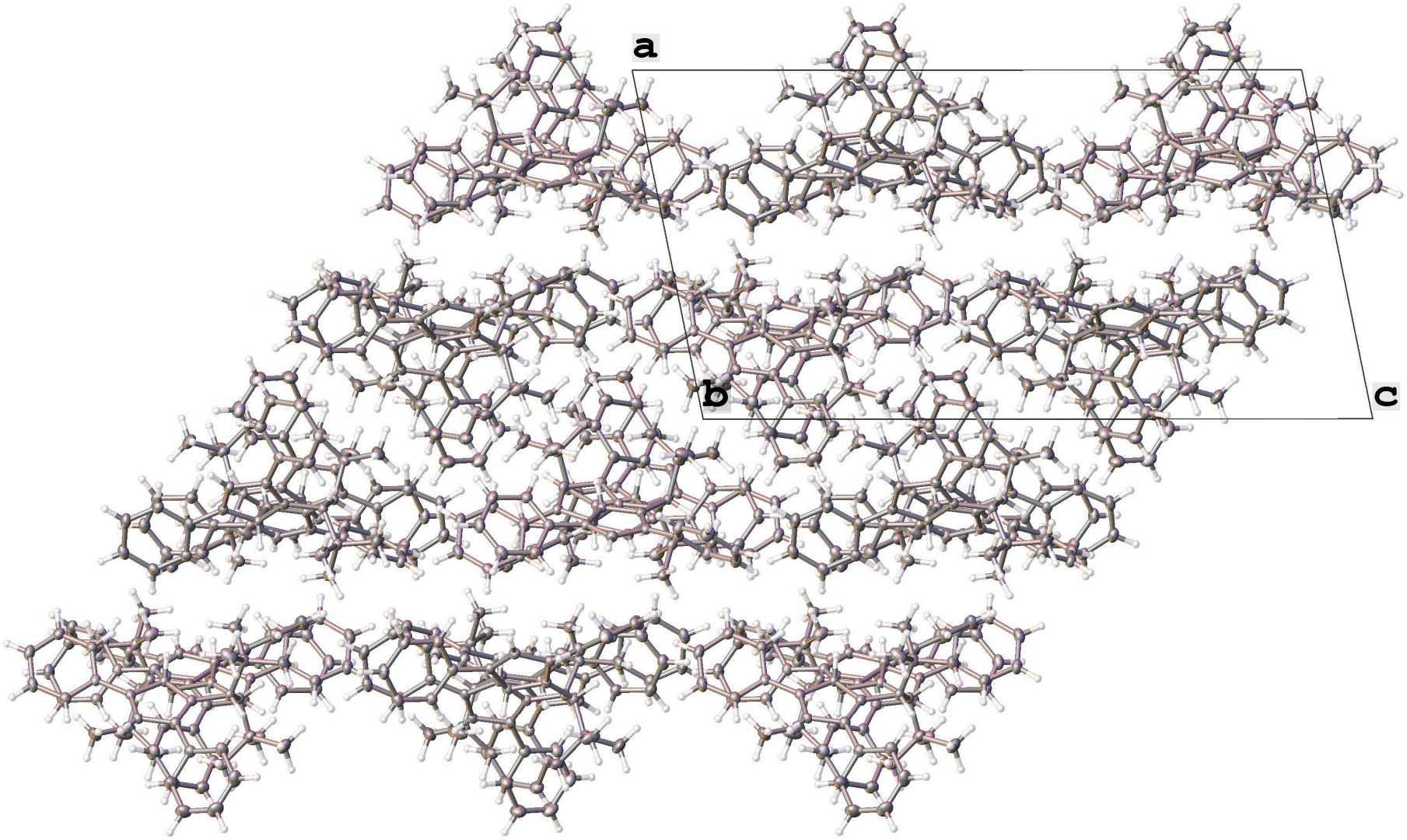


Figure S15. Thermal ellipsoid view of the molecular packing of **2**, view along the b-axis direction (crystal obtained from iPrOH solution). Thermal ellipsoids are shown at the 50% probability level.

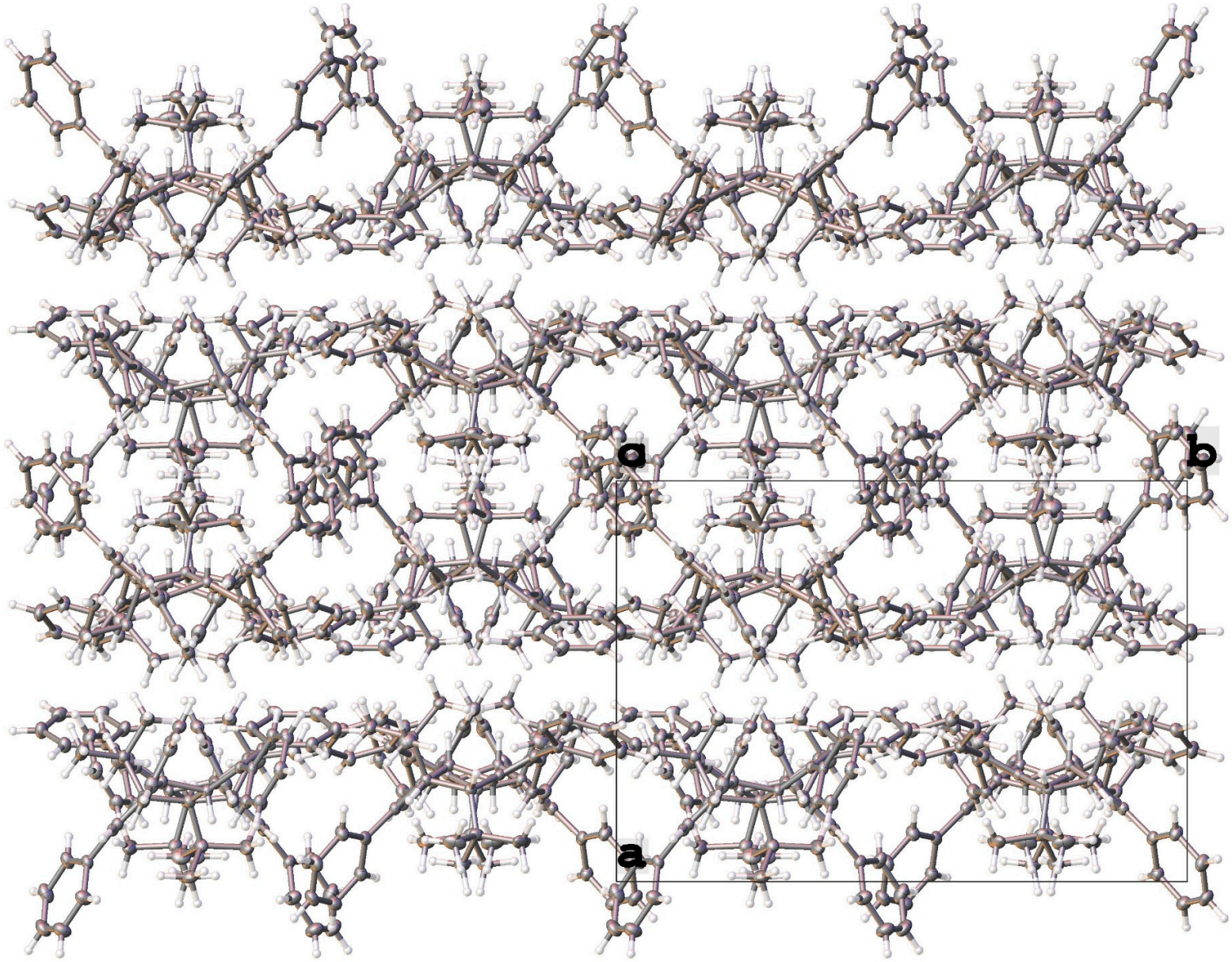


Figure S16. Thermal ellipsoid view of the molecular packing of **2**, view along the c-axis direction. Thermal ellipsoids are shown at the 50% probability level.

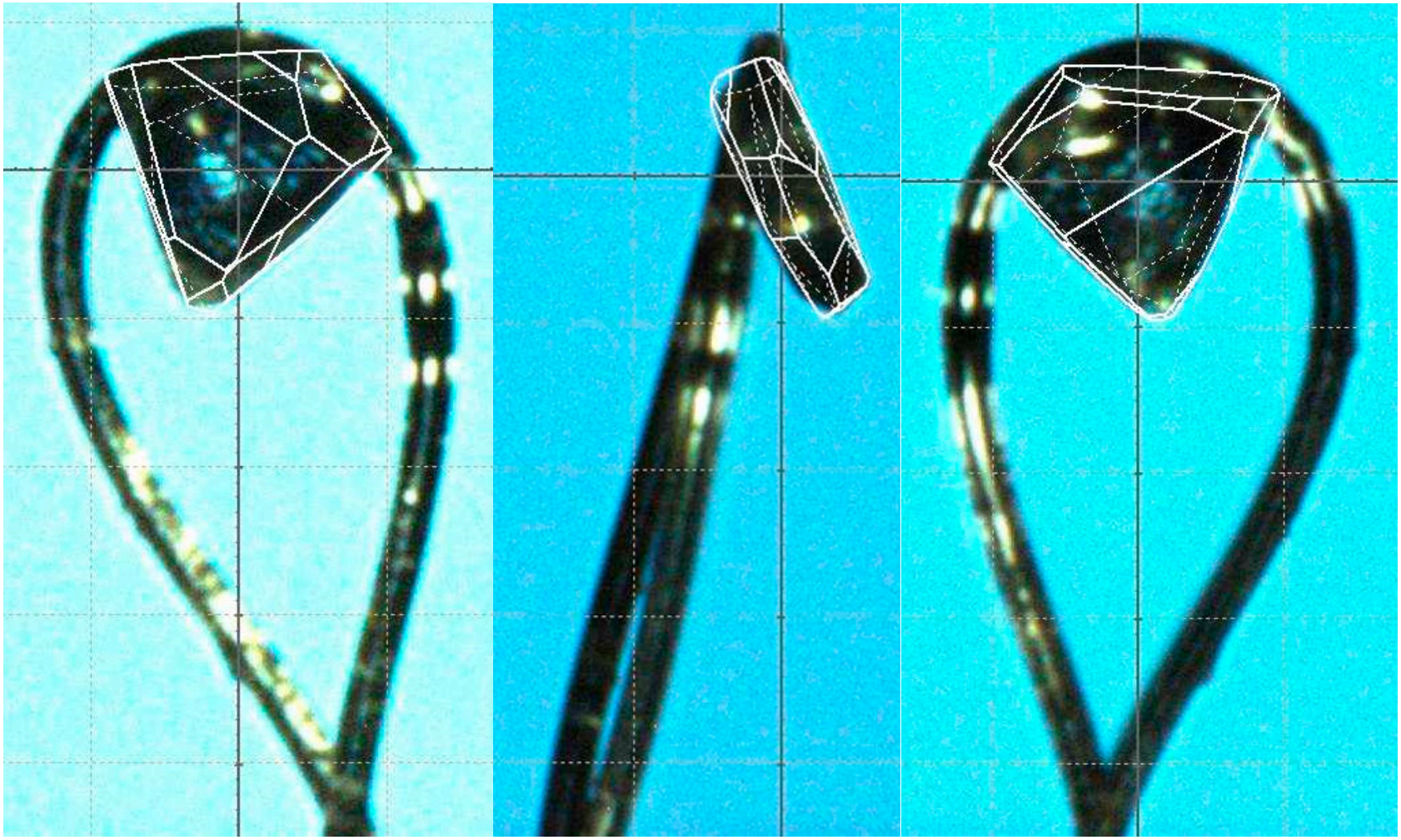


Figure S17. Images of the mounted crystal of **2** (THInd1ABS). A 0.184 x 0.164 x 0.055 mm^3 translucent colorless prism crystal was selected from crystals that were grown from a hot iPrOH solution by slow cooling and evaporation.

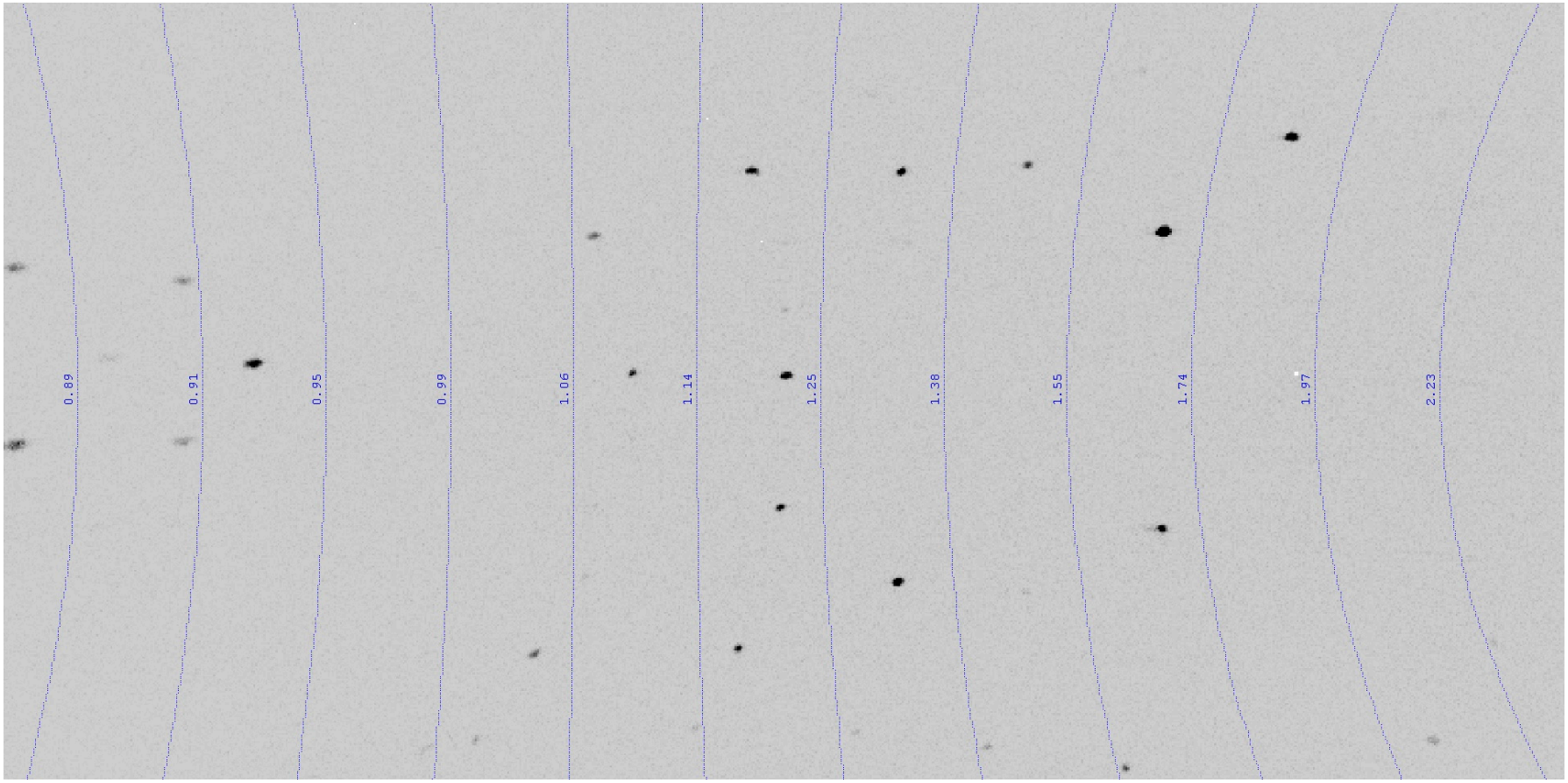


Figure S18. Example frame taken from the series of runs (run 4, frame 66), demonstrating excellent diffraction for the selected crystal of **2** (THInd1ABS).

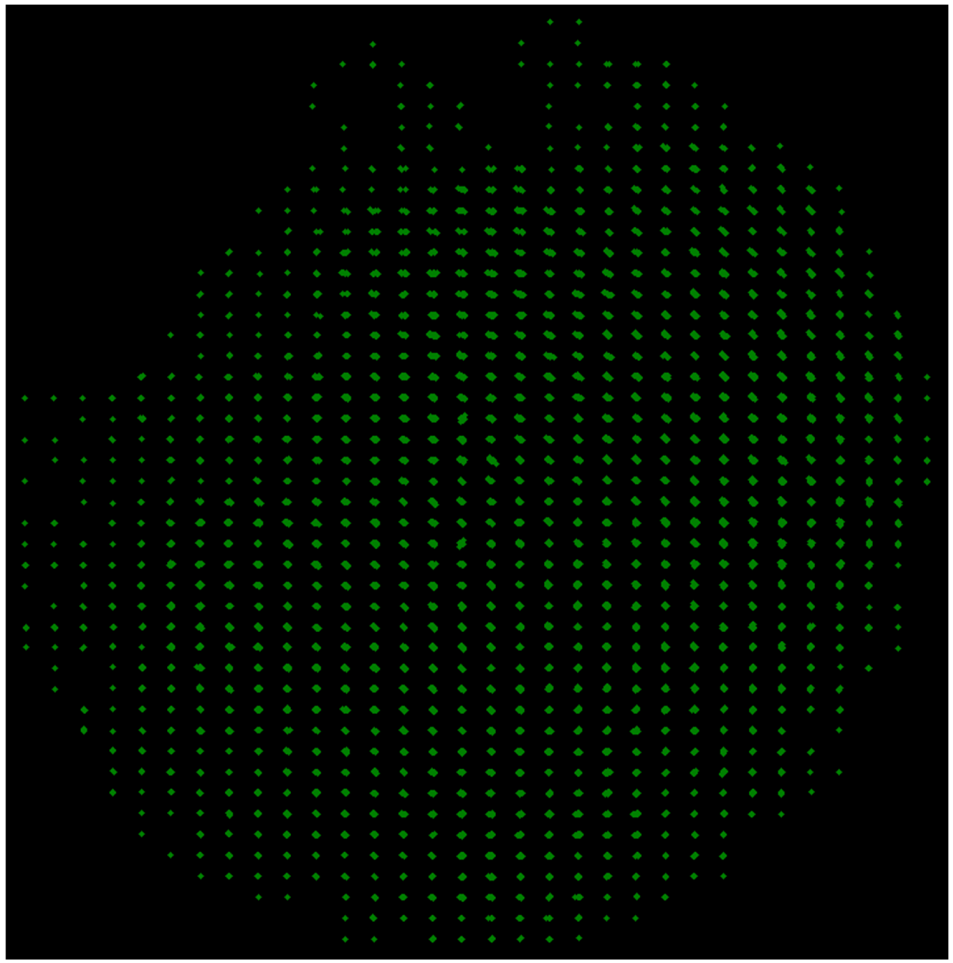


Figure S19. Reciprocal space plot for **2** (THInd1ABS). View down the c* reciprocal lattice vector.

Table S1. Crystal data and structure refinement for 4,5-di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene **2** (THInd1ABS, crystal obtained from iPrOH solution).

Identification code	thind1abs (CCDC No. 2263159)	
Empirical formula	C44 H44	
Formula weight	572.79	
Temperature	100.01(12) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.66820(10) Å	α= 90°.
	b = 19.08900(10) Å	β= 101.4620(10)°.
	c = 25.66600(10) Å	γ = 90°.
Volume	6563.02(7) $Å^3$	
Z	8	
Density (calculated)	1.159 Mg/m^3	
Absorption coefficient	0.486 mm^{-1}	
F(000)	2464	
Crystal size	0.184 x 0.164 x 0.055 mm^3	
Theta range for data collection	2.906 to 68.251°.	
Index ranges	-16<=h<=16, -22<=k<=22, -30<=l<=25	
Reflections collected	63674	
Independent reflections	11957 [R(int) = 0.0211]	
Completeness to theta = 67.684°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.628	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11957 / 0 / 806	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0904	
R indices (all data)	R1 = 0.0404, wR2 = 0.0926	
Extinction coefficient	0.00024(2)	
Largest diff. peak and hole	0.244 and -0.179 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2** (THInd1ABS). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7148(1)	1587(1)	3949(1)	19(1)
C(2)	6704(1)	1203(1)	3528(1)	20(1)
C(3)	6936(1)	1464(1)	3032(1)	19(1)
C(3A)	7543(1)	2029(1)	3145(1)	19(1)
C(4)	7996(1)	2482(1)	2775(1)	19(1)
C(5)	7892(1)	3277(1)	2906(1)	19(1)
C(6)	8708(1)	3823(1)	3808(1)	20(1)
C(6A)	8049(1)	3391(1)	3494(1)	18(1)
C(7)	8572(1)	3743(1)	4356(1)	19(1)
C(8)	7878(1)	3253(1)	4393(1)	18(1)
C(8A)	7501(1)	2954(1)	3841(1)	18(1)
C(8B)	7736(1)	2167(1)	3743(1)	18(1)
C(9)	7171(1)	1374(1)	4504(1)	19(1)
C(10)	8008(1)	1483(1)	4907(1)	22(1)
C(11)	8033(1)	1238(1)	5419(1)	27(1)
C(12)	7226(1)	877(1)	5538(1)	28(1)
C(13)	6388(1)	767(1)	5144(1)	26(1)
C(14)	6358(1)	1016(1)	4633(1)	23(1)
C(15)	6576(1)	1069(1)	2530(1)	20(1)
C(16)	6591(1)	335(1)	2554(1)	25(1)
C(17)	6225(1)	-72(1)	2110(1)	29(1)
C(18)	5835(1)	243(1)	1628(1)	28(1)
C(19)	5824(1)	965(1)	1594(1)	30(1)

C(20)	6192(1)	1374(1)	2038(1)	26(1)
C(21)	9515(1)	4270(1)	3677(1)	22(1)
C(22)	9475(1)	4615(1)	3194(1)	29(1)
C(23)	10289(1)	4988(1)	3090(1)	35(1)
C(24)	11158(1)	5039(1)	3470(1)	36(1)
C(25)	11209(1)	4712(1)	3952(1)	37(1)
C(26)	10404(1)	4333(1)	4054(1)	31(1)
C(27)	7459(1)	3108(1)	4866(1)	18(1)
C(28)	7985(1)	3285(1)	5376(1)	22(1)
C(29)	7591(1)	3144(1)	5822(1)	27(1)
C(30)	6671(1)	2818(1)	5772(1)	27(1)
C(31)	6132(1)	2655(1)	5272(1)	24(1)
C(32)	6517(1)	2808(1)	4824(1)	21(1)
C(33)	9098(1)	2272(1)	2741(1)	24(1)
C(34)	9144(1)	1480(1)	2657(1)	39(1)
C(35)	9367(1)	2631(1)	2254(1)	38(1)
C(36)	9880(1)	2470(1)	3230(1)	31(1)
C(37)	6903(1)	3624(1)	2589(1)	23(1)
C(38)	5956(1)	3218(1)	2623(1)	27(1)
C(39)	6986(1)	3696(1)	2005(1)	33(1)
C(40)	6764(1)	4359(1)	2805(1)	35(1)
C(1')	2580(1)	3218(1)	2446(1)	20(1)
C(2')	1939(1)	3746(1)	2289(1)	21(1)
C(3')	1821(1)	3876(1)	1717(1)	20(1)
C(3A')	2423(1)	3424(1)	1518(1)	18(1)
C(4')	2544(1)	3327(1)	952(1)	19(1)
C(5')	2293(1)	2555(1)	765(1)	19(1)
C(6')	3143(1)	1429(1)	1189(1)	19(1)
C(6A')	2661(1)	2047(1)	1209(1)	18(1)
C(7')	3357(1)	1126(1)	1721(1)	21(1)

C(8')	3019(1)	1536(1)	2074(1)	19(1)
C(8A')	2527(1)	2173(1)	1777(1)	18(1)
C(8B')	2908(1)	2926(1)	1957(1)	18(1)
C(9')	2999(1)	3027(1)	3000(1)	20(1)
C(10')	3904(1)	2669(1)	3138(1)	21(1)
C(11')	4297(1)	2494(1)	3662(1)	24(1)
C(12')	3797(1)	2680(1)	4060(1)	29(1)
C(13')	2903(1)	3043(1)	3933(1)	28(1)
C(14')	2505(1)	3215(1)	3410(1)	24(1)
C(15')	1084(1)	4395(1)	1447(1)	21(1)
C(16')	196(1)	4479(1)	1635(1)	24(1)
C(17')	-539(1)	4939(1)	1397(1)	28(1)
C(18')	-409(1)	5333(1)	962(1)	31(1)
C(19')	465(1)	5265(1)	772(1)	31(1)
C(20')	1207(1)	4806(1)	1014(1)	27(1)
C(21')	3363(1)	1025(1)	731(1)	20(1)
C(22')	3849(1)	1295(1)	347(1)	23(1)
C(23')	4059(1)	877(1)	-60(1)	25(1)
C(24')	3773(1)	182(1)	-97(1)	25(1)
C(25')	3287(1)	-94(1)	280(1)	30(1)
C(26')	3088(1)	320(1)	690(1)	28(1)
C(27')	3024(1)	1322(1)	2626(1)	19(1)
C(28')	3821(1)	928(1)	2907(1)	23(1)
C(29')	3819(1)	697(1)	3418(1)	26(1)
C(30')	3036(1)	865(1)	3666(1)	28(1)
C(31')	2247(1)	1260(1)	3394(1)	26(1)
C(32')	2236(1)	1480(1)	2878(1)	22(1)
C(33')	3586(1)	3584(1)	846(1)	22(1)
C(34')	3858(1)	4301(1)	1103(1)	30(1)
C(35')	3501(1)	3669(1)	244(1)	31(1)

C(36')	4455(1)	3091(1)	1063(1)	24(1)
C(37')	1169(1)	2448(1)	488(1)	25(1)
C(38')	421(1)	2705(1)	815(1)	27(1)
C(39')	973(1)	2836(1)	-46(1)	41(1)
C(40')	987(1)	1666(1)	375(1)	41(1)

Table S3. Bond lengths [Å] and angles [°] for **2** (THInd1ABS).

C(1)-C(2)	1.3457(16)
C(1)-C(8B)	1.5227(15)
C(1)-C(9)	1.4742(15)
C(2)-H(2)	0.9500
C(2)-C(3)	1.4614(16)
C(3)-C(3A)	1.3565(16)
C(3)-C(15)	1.4886(16)
C(3A)-C(4)	1.5065(15)
C(3A)-C(8B)	1.5275(15)
C(4)-H(4)	1.0000
C(4)-C(5)	1.5662(16)
C(4)-C(33)	1.5777(16)
C(5)-H(5)	1.0000
C(5)-C(6A)	1.4997(15)
C(5)-C(37)	1.5790(16)
C(6)-C(6A)	1.3597(16)
C(6)-C(7)	1.4641(16)
C(6)-C(21)	1.4849(16)
C(6A)-C(8A)	1.5206(15)

C(7)-H(7)	0.9500
C(7)-C(8)	1.3484(16)
C(8)-C(8A)	1.5184(15)
C(8)-C(27)	1.4696(15)
C(8A)-H(8A)	1.0000
C(8A)-C(8B)	1.5677(15)
C(8B)-H(8B)	1.0000
C(9)-C(10)	1.3974(17)
C(9)-C(14)	1.4007(17)
C(10)-H(10)	0.9500
C(10)-C(11)	1.3875(17)
C(11)-H(11)	0.9500
C(11)-C(12)	1.3861(19)
C(12)-H(12)	0.9500
C(12)-C(13)	1.3859(19)
C(13)-H(13)	0.9500
C(13)-C(14)	1.3873(17)
C(14)-H(14)	0.9500
C(15)-C(16)	1.4024(17)
C(15)-C(20)	1.3927(17)
C(16)-H(16)	0.9500
C(16)-C(17)	1.3870(18)
C(17)-H(17)	0.9500
C(17)-C(18)	1.3845(19)
C(18)-H(18)	0.9500
C(18)-C(19)	1.3810(19)
C(19)-H(19)	0.9500
C(19)-C(20)	1.3898(18)
C(20)-H(20)	0.9500
C(21)-C(22)	1.3949(17)

C(21)-C(26)	1.3995(18)
C(22)-H(22)	0.9500
C(22)-C(23)	1.3913(19)
C(23)-H(23)	0.9500
C(23)-C(24)	1.381(2)
C(24)-H(24)	0.9500
C(24)-C(25)	1.376(2)
C(25)-H(25)	0.9500
C(25)-C(26)	1.3860(19)
C(26)-H(26)	0.9500
C(27)-C(28)	1.4025(16)
C(27)-C(32)	1.3938(17)
C(28)-H(28)	0.9500
C(28)-C(29)	1.3846(17)
C(29)-H(29)	0.9500
C(29)-C(30)	1.3866(19)
C(30)-H(30)	0.9500
C(30)-C(31)	1.3823(18)
C(31)-H(31)	0.9500
C(31)-C(32)	1.3883(17)
C(32)-H(32)	0.9500
C(33)-C(34)	1.5290(18)
C(33)-C(35)	1.5338(18)
C(33)-C(36)	1.5249(18)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800

C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.5266(17)
C(37)-C(39)	1.5319(17)
C(37)-C(40)	1.5337(18)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(1')-C(2')	1.3444(17)
C(1')-C(8B')	1.5210(15)
C(1')-C(9')	1.4691(16)
C(2')-H(2')	0.9500
C(2')-C(3')	1.4654(16)
C(3')-C(3A')	1.3602(16)
C(3')-C(15')	1.4826(16)
C(3A')-C(4')	1.5040(15)
C(3A')-C(8B')	1.5224(16)
C(4')-H(4')	1.0000
C(4')-C(5')	1.5670(15)
C(4')-C(33')	1.5805(16)
C(5')-H(5')	1.0000
C(5')-C(6A')	1.5048(16)
C(5')-C(37')	1.5730(16)

C(6')-C(6A')	1.3573(16)
C(6')-C(7')	1.4577(16)
C(6')-C(21')	1.4859(16)
C(6A')-C(8A')	1.5242(15)
C(7')-H(7')	0.9500
C(7')-C(8')	1.3456(16)
C(8')-C(8A')	1.5201(16)
C(8')-C(27')	1.4720(16)
C(8A')-H(8A')	1.0000
C(8A')-C(8B')	1.5655(15)
C(8B')-H(8B')	1.0000
C(9')-C(10')	1.3952(17)
C(9')-C(14')	1.4039(16)
C(10')-H(10')	0.9500
C(10')-C(11')	1.3860(17)
C(11')-H(11')	0.9500
C(11')-C(12')	1.3846(18)
C(12')-H(12')	0.9500
C(12')-C(13')	1.3870(19)
C(13')-H(13')	0.9500
C(13')-C(14')	1.3845(18)
C(14')-H(14')	0.9500
C(15')-C(16')	1.4024(17)
C(15')-C(20')	1.3970(17)
C(16')-H(16')	0.9500
C(16')-C(17')	1.3828(18)
C(17')-H(17')	0.9500
C(17')-C(18')	1.3854(19)
C(18')-H(18')	0.9500
C(18')-C(19')	1.3831(19)

C(19')-H(19')	0.9500
C(19')-C(20')	1.3902(18)
C(20')-H(20')	0.9500
C(21')-C(22')	1.3927(16)
C(21')-C(26')	1.3968(17)
C(22')-H(22')	0.9500
C(22')-C(23')	1.3884(17)
C(23')-H(23')	0.9500
C(23')-C(24')	1.3821(18)
C(24')-H(24')	0.9500
C(24')-C(25')	1.3815(18)
C(25')-H(25')	0.9500
C(25')-C(26')	1.3852(18)
C(26')-H(26')	0.9500
C(27')-C(28')	1.4004(17)
C(27')-C(32')	1.3966(16)
C(28')-H(28')	0.9500
C(28')-C(29')	1.3853(17)
C(29')-H(29')	0.9500
C(29')-C(30')	1.3864(19)
C(30')-H(30')	0.9500
C(30')-C(31')	1.3857(19)
C(31')-H(31')	0.9500
C(31')-C(32')	1.3872(17)
C(32')-H(32')	0.9500
C(33')-C(34')	1.5324(17)
C(33')-C(35')	1.5346(16)
C(33')-C(36')	1.5314(17)
C(34')-H(34D)	0.9800
C(34')-H(34E)	0.9800

C(34')-H(34F)	0.9800
C(35')-H(35D)	0.9800
C(35')-H(35E)	0.9800
C(35')-H(35F)	0.9800
C(36')-H(36D)	0.9800
C(36')-H(36E)	0.9800
C(36')-H(36F)	0.9800
C(37')-C(38')	1.5274(17)
C(37')-C(39')	1.5331(19)
C(37')-C(40')	1.5317(19)
C(38')-H(38D)	0.9800
C(38')-H(38E)	0.9800
C(38')-H(38F)	0.9800
C(39')-H(39D)	0.9800
C(39')-H(39E)	0.9800
C(39')-H(39F)	0.9800
C(40')-H(40D)	0.9800
C(40')-H(40E)	0.9800
C(40')-H(40F)	0.9800

C(2)-C(1)-C(8B)	107.62(10)
C(2)-C(1)-C(9)	122.94(10)
C(9)-C(1)-C(8B)	128.58(10)
C(1)-C(2)-H(2)	124.1
C(1)-C(2)-C(3)	111.89(10)
C(3)-C(2)-H(2)	124.1
C(2)-C(3)-C(15)	119.44(10)
C(3A)-C(3)-C(2)	108.24(10)
C(3A)-C(3)-C(15)	132.10(10)
C(3)-C(3A)-C(4)	129.19(10)

C(3)-C(3A)-C(8B)	109.22(10)
C(4)-C(3A)-C(8B)	121.59(10)
C(3A)-C(4)-H(4)	106.3
C(3A)-C(4)-C(5)	110.81(9)
C(3A)-C(4)-C(33)	113.86(10)
C(5)-C(4)-H(4)	106.3
C(5)-C(4)-C(33)	112.70(9)
C(33)-C(4)-H(4)	106.3
C(4)-C(5)-H(5)	106.2
C(4)-C(5)-C(37)	113.64(9)
C(6A)-C(5)-C(4)	110.86(9)
C(6A)-C(5)-H(5)	106.2
C(6A)-C(5)-C(37)	113.22(9)
C(37)-C(5)-H(5)	106.2
C(6A)-C(6)-C(7)	108.02(10)
C(6A)-C(6)-C(21)	130.51(11)
C(7)-C(6)-C(21)	121.27(10)
C(5)-C(6A)-C(8A)	121.39(10)
C(6)-C(6A)-C(5)	129.01(10)
C(6)-C(6A)-C(8A)	109.41(10)
C(6)-C(7)-H(7)	124.3
C(8)-C(7)-C(6)	111.39(10)
C(8)-C(7)-H(7)	124.3
C(7)-C(8)-C(8A)	107.98(10)
C(7)-C(8)-C(27)	125.67(10)
C(27)-C(8)-C(8A)	125.81(10)
C(6A)-C(8A)-H(8A)	109.6
C(6A)-C(8A)-C(8B)	106.96(9)
C(8)-C(8A)-C(6A)	102.94(9)
C(8)-C(8A)-H(8A)	109.6

C(8)-C(8A)-C(8B)	117.84(9)
C(8B)-C(8A)-H(8A)	109.6
C(1)-C(8B)-C(3A)	103.04(9)
C(1)-C(8B)-C(8A)	120.10(9)
C(1)-C(8B)-H(8B)	108.0
C(3A)-C(8B)-C(8A)	109.04(9)
C(3A)-C(8B)-H(8B)	108.0
C(8A)-C(8B)-H(8B)	108.0
C(10)-C(9)-C(1)	122.21(11)
C(10)-C(9)-C(14)	117.86(11)
C(14)-C(9)-C(1)	119.83(10)
C(9)-C(10)-H(10)	119.5
C(11)-C(10)-C(9)	120.97(11)
C(11)-C(10)-H(10)	119.5
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-C(10)	120.40(12)
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-C(11)	119.46(11)
C(13)-C(12)-H(12)	120.3
C(12)-C(13)-H(13)	119.9
C(12)-C(13)-C(14)	120.26(12)
C(14)-C(13)-H(13)	119.9
C(9)-C(14)-H(14)	119.5
C(13)-C(14)-C(9)	121.05(11)
C(13)-C(14)-H(14)	119.5
C(16)-C(15)-C(3)	117.87(10)
C(20)-C(15)-C(3)	124.94(11)
C(20)-C(15)-C(16)	117.16(11)
C(15)-C(16)-H(16)	119.2

C(17)-C(16)-C(15)	121.58(11)
C(17)-C(16)-H(16)	119.2
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-C(16)	120.17(12)
C(18)-C(17)-H(17)	119.9
C(17)-C(18)-H(18)	120.4
C(19)-C(18)-C(17)	119.14(12)
C(19)-C(18)-H(18)	120.4
C(18)-C(19)-H(19)	119.6
C(18)-C(19)-C(20)	120.72(12)
C(20)-C(19)-H(19)	119.6
C(15)-C(20)-H(20)	119.4
C(19)-C(20)-C(15)	121.22(12)
C(19)-C(20)-H(20)	119.4
C(22)-C(21)-C(6)	124.88(11)
C(22)-C(21)-C(26)	116.73(11)
C(26)-C(21)-C(6)	118.34(11)
C(21)-C(22)-H(22)	119.3
C(23)-C(22)-C(21)	121.33(12)
C(23)-C(22)-H(22)	119.3
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-C(22)	120.66(13)
C(24)-C(23)-H(23)	119.7
C(23)-C(24)-H(24)	120.5
C(25)-C(24)-C(23)	119.00(13)
C(25)-C(24)-H(24)	120.5
C(24)-C(25)-H(25)	119.8
C(24)-C(25)-C(26)	120.48(13)
C(26)-C(25)-H(25)	119.8
C(21)-C(26)-H(26)	119.1

C(25)-C(26)-C(21)	121.78(13)
C(25)-C(26)-H(26)	119.1
C(28)-C(27)-C(8)	120.91(10)
C(32)-C(27)-C(8)	121.21(10)
C(32)-C(27)-C(28)	117.85(10)
C(27)-C(28)-H(28)	119.6
C(29)-C(28)-C(27)	120.83(11)
C(29)-C(28)-H(28)	119.6
C(28)-C(29)-H(29)	119.8
C(28)-C(29)-C(30)	120.38(11)
C(30)-C(29)-H(29)	119.8
C(29)-C(30)-H(30)	120.2
C(31)-C(30)-C(29)	119.52(11)
C(31)-C(30)-H(30)	120.2
C(30)-C(31)-H(31)	119.9
C(30)-C(31)-C(32)	120.20(12)
C(32)-C(31)-H(31)	119.9
C(27)-C(32)-H(32)	119.4
C(31)-C(32)-C(27)	121.14(11)
C(31)-C(32)-H(32)	119.4
C(34)-C(33)-C(4)	109.02(10)
C(34)-C(33)-C(35)	107.64(11)
C(35)-C(33)-C(4)	108.46(10)
C(36)-C(33)-C(4)	114.38(10)
C(36)-C(33)-C(34)	108.67(11)
C(36)-C(33)-C(35)	108.47(11)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34B)	109.5

H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(5)	113.98(10)
C(38)-C(37)-C(39)	109.33(10)
C(38)-C(37)-C(40)	106.03(11)
C(39)-C(37)-C(5)	108.55(10)
C(39)-C(37)-C(40)	108.10(11)
C(40)-C(37)-C(5)	110.69(10)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39B)	109.5

H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(2')-C(1')-C(8B')	107.91(10)
C(2')-C(1')-C(9')	125.67(11)
C(9')-C(1')-C(8B')	125.87(10)
C(1')-C(2')-H(2')	124.3
C(1')-C(2')-C(3')	111.34(10)
C(3')-C(2')-H(2')	124.3
C(2')-C(3')-C(15')	120.67(10)
C(3A')-C(3')-C(2')	108.34(10)
C(3A')-C(3')-C(15')	130.83(11)
C(3')-C(3A')-C(4')	129.14(11)
C(3')-C(3A')-C(8B')	108.95(10)
C(4')-C(3A')-C(8B')	121.51(10)
C(3A')-C(4')-H(4')	106.3
C(3A')-C(4')-C(5')	110.71(9)
C(3A')-C(4')-C(33')	113.75(9)
C(5')-C(4')-H(4')	106.3
C(5')-C(4')-C(33')	112.89(9)
C(33')-C(4')-H(4')	106.3
C(4')-C(5')-H(5')	106.0
C(4')-C(5')-C(37')	113.22(9)
C(6A')-C(5')-C(4')	110.68(9)
C(6A')-C(5')-H(5')	106.0

C(6A')-C(5')-C(37')	114.12(10)
C(37')-C(5')-H(5')	106.0
C(6A')-C(6')-C(7')	108.59(10)
C(6A')-C(6')-C(21')	131.02(11)
C(7')-C(6')-C(21')	120.07(10)
C(5')-C(6A')-C(8A')	122.50(10)
C(6')-C(6A')-C(5')	128.56(10)
C(6')-C(6A')-C(8A')	108.94(10)
C(6')-C(7')-H(7')	124.2
C(8')-C(7')-C(6')	111.54(10)
C(8')-C(7')-H(7')	124.2
C(7')-C(8')-C(8A')	107.79(10)
C(7')-C(8')-C(27')	123.34(11)
C(27')-C(8')-C(8A')	128.36(10)
C(6A')-C(8A')-H(8A')	107.9
C(6A')-C(8A')-C(8B')	109.37(9)
C(8')-C(8A')-C(6A')	103.13(9)
C(8')-C(8A')-H(8A')	107.9
C(8')-C(8A')-C(8B')	119.95(9)
C(8B')-C(8A')-H(8A')	107.9
C(1')-C(8B')-C(3A')	103.09(9)
C(1')-C(8B')-C(8A')	116.44(9)
C(1')-C(8B')-H(8B')	110.1
C(3A')-C(8B')-C(8A')	106.52(9)
C(3A')-C(8B')-H(8B')	110.1
C(8A')-C(8B')-H(8B')	110.1
C(10')-C(9')-C(1')	121.47(10)
C(10')-C(9')-C(14')	118.02(11)
C(14')-C(9')-C(1')	120.49(11)
C(9')-C(10')-H(10')	119.4

C(11')-C(10')-C(9')	121.14(11)
C(11')-C(10')-H(10')	119.4
C(10')-C(11')-H(11')	120.0
C(12')-C(11')-C(10')	120.09(12)
C(12')-C(11')-H(11')	120.0
C(11')-C(12')-H(12')	120.1
C(11')-C(12')-C(13')	119.71(12)
C(13')-C(12')-H(12')	120.1
C(12')-C(13')-H(13')	119.8
C(14')-C(13')-C(12')	120.32(12)
C(14')-C(13')-H(13')	119.8
C(9')-C(14')-H(14')	119.6
C(13')-C(14')-C(9')	120.72(12)
C(13')-C(14')-H(14')	119.6
C(16')-C(15')-C(3')	117.98(11)
C(20')-C(15')-C(3')	124.66(11)
C(20')-C(15')-C(16')	117.36(11)
C(15')-C(16')-H(16')	119.2
C(17')-C(16')-C(15')	121.50(12)
C(17')-C(16')-H(16')	119.2
C(16')-C(17')-H(17')	119.9
C(16')-C(17')-C(18')	120.19(12)
C(18')-C(17')-H(17')	119.9
C(17')-C(18')-H(18')	120.3
C(19')-C(18')-C(17')	119.39(12)
C(19')-C(18')-H(18')	120.3
C(18')-C(19')-H(19')	119.8
C(18')-C(19')-C(20')	120.47(12)
C(20')-C(19')-H(19')	119.8
C(15')-C(20')-H(20')	119.5

C(19')-C(20')-C(15')	121.07(12)
C(19')-C(20')-H(20')	119.5
C(22')-C(21')-C(6')	124.68(11)
C(22')-C(21')-C(26')	117.56(11)
C(26')-C(21')-C(6')	117.73(10)
C(21')-C(22')-H(22')	119.4
C(23')-C(22')-C(21')	121.24(11)
C(23')-C(22')-H(22')	119.4
C(22')-C(23')-H(23')	119.8
C(24')-C(23')-C(22')	120.35(11)
C(24')-C(23')-H(23')	119.8
C(23')-C(24')-H(24')	120.4
C(25')-C(24')-C(23')	119.19(11)
C(25')-C(24')-H(24')	120.4
C(24')-C(25')-H(25')	119.7
C(24')-C(25')-C(26')	120.54(12)
C(26')-C(25')-H(25')	119.7
C(21')-C(26')-H(26')	119.4
C(25')-C(26')-C(21')	121.12(12)
C(25')-C(26')-H(26')	119.4
C(28')-C(27')-C(8')	119.99(10)
C(32')-C(27')-C(8')	122.01(11)
C(32')-C(27')-C(28')	117.97(11)
C(27')-C(28')-H(28')	119.6
C(29')-C(28')-C(27')	120.83(11)
C(29')-C(28')-H(28')	119.6
C(28')-C(29')-H(29')	119.7
C(28')-C(29')-C(30')	120.53(12)
C(30')-C(29')-H(29')	119.7
C(29')-C(30')-H(30')	120.4

C(31')-C(30')-C(29')	119.28(11)
C(31')-C(30')-H(30')	120.4
C(30')-C(31')-H(31')	119.8
C(30')-C(31')-C(32')	120.39(12)
C(32')-C(31')-H(31')	119.8
C(27')-C(32')-H(32')	119.5
C(31')-C(32')-C(27')	120.99(11)
C(31')-C(32')-H(32')	119.5
C(34')-C(33')-C(4')	110.75(9)
C(34')-C(33')-C(35')	107.62(10)
C(35')-C(33')-C(4')	108.39(10)
C(36')-C(33')-C(4')	113.99(9)
C(36')-C(33')-C(34')	106.76(10)
C(36')-C(33')-C(35')	109.15(10)
C(33')-C(34')-H(34D)	109.5
C(33')-C(34')-H(34E)	109.5
C(33')-C(34')-H(34F)	109.5
H(34D)-C(34')-H(34E)	109.5
H(34D)-C(34')-H(34F)	109.5
H(34E)-C(34')-H(34F)	109.5
C(33')-C(35')-H(35D)	109.5
C(33')-C(35')-H(35E)	109.5
C(33')-C(35')-H(35F)	109.5
H(35D)-C(35')-H(35E)	109.5
H(35D)-C(35')-H(35F)	109.5
H(35E)-C(35')-H(35F)	109.5
C(33')-C(36')-H(36D)	109.5
C(33')-C(36')-H(36E)	109.5
C(33')-C(36')-H(36F)	109.5
H(36D)-C(36')-H(36E)	109.5

H(36D)-C(36')-H(36F)	109.5
H(36E)-C(36')-H(36F)	109.5
C(38')-C(37')-C(5')	114.24(10)
C(38')-C(37')-C(39')	108.64(11)
C(38')-C(37')-C(40')	108.35(11)
C(39')-C(37')-C(5')	108.86(10)
C(40')-C(37')-C(5')	108.56(10)
C(40')-C(37')-C(39')	108.02(12)
C(37')-C(38')-H(38D)	109.5
C(37')-C(38')-H(38E)	109.5
C(37')-C(38')-H(38F)	109.5
H(38D)-C(38')-H(38E)	109.5
H(38D)-C(38')-H(38F)	109.5
H(38E)-C(38')-H(38F)	109.5
C(37')-C(39')-H(39D)	109.5
C(37')-C(39')-H(39E)	109.5
C(37')-C(39')-H(39F)	109.5
H(39D)-C(39')-H(39E)	109.5
H(39D)-C(39')-H(39F)	109.5
H(39E)-C(39')-H(39F)	109.5
C(37')-C(40')-H(40D)	109.5
C(37')-C(40')-H(40E)	109.5
C(37')-C(40')-H(40F)	109.5
H(40D)-C(40')-H(40E)	109.5
H(40D)-C(40')-H(40F)	109.5
H(40E)-C(40')-H(40F)	109.5

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2** (THInd1ABS). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(1)	16(1)	21(1)	2(1)	4(1)	2(1)
C(2)	21(1)	16(1)	22(1)	2(1)	4(1)	-1(1)
C(3)	21(1)	18(1)	19(1)	2(1)	4(1)	2(1)
C(3A)	21(1)	17(1)	19(1)	1(1)	4(1)	2(1)
C(4)	22(1)	18(1)	17(1)	-1(1)	5(1)	-3(1)
C(5)	22(1)	17(1)	18(1)	1(1)	4(1)	-3(1)
C(6)	22(1)	17(1)	20(1)	1(1)	4(1)	1(1)
C(6A)	21(1)	16(1)	19(1)	2(1)	4(1)	1(1)
C(7)	21(1)	18(1)	18(1)	-2(1)	1(1)	1(1)
C(8)	19(1)	17(1)	18(1)	1(1)	2(1)	4(1)
C(8A)	19(1)	17(1)	17(1)	1(1)	4(1)	0(1)
C(8B)	21(1)	16(1)	18(1)	1(1)	4(1)	0(1)
C(9)	25(1)	14(1)	20(1)	1(1)	6(1)	2(1)
C(10)	25(1)	18(1)	23(1)	1(1)	4(1)	0(1)
C(11)	32(1)	25(1)	21(1)	2(1)	1(1)	0(1)
C(12)	41(1)	25(1)	20(1)	4(1)	7(1)	-1(1)
C(13)	33(1)	22(1)	26(1)	1(1)	12(1)	-5(1)
C(14)	26(1)	20(1)	22(1)	-1(1)	5(1)	-2(1)
C(15)	18(1)	22(1)	20(1)	0(1)	5(1)	-2(1)
C(16)	30(1)	22(1)	22(1)	1(1)	2(1)	1(1)
C(17)	35(1)	21(1)	30(1)	-4(1)	3(1)	1(1)
C(18)	28(1)	32(1)	23(1)	-7(1)	4(1)	-6(1)
C(19)	34(1)	33(1)	20(1)	3(1)	-1(1)	-8(1)

C(20)	31(1)	22(1)	24(1)	4(1)	1(1)	-6(1)
C(21)	25(1)	18(1)	23(1)	-3(1)	6(1)	-3(1)
C(22)	35(1)	24(1)	27(1)	0(1)	4(1)	-9(1)
C(23)	46(1)	28(1)	32(1)	1(1)	13(1)	-13(1)
C(24)	34(1)	31(1)	46(1)	-3(1)	16(1)	-13(1)
C(25)	26(1)	42(1)	42(1)	0(1)	3(1)	-9(1)
C(26)	27(1)	36(1)	29(1)	4(1)	4(1)	-6(1)
C(27)	23(1)	14(1)	19(1)	1(1)	5(1)	4(1)
C(28)	25(1)	20(1)	21(1)	0(1)	3(1)	1(1)
C(29)	37(1)	26(1)	18(1)	-2(1)	3(1)	1(1)
C(30)	36(1)	26(1)	22(1)	3(1)	12(1)	4(1)
C(31)	24(1)	24(1)	25(1)	2(1)	9(1)	3(1)
C(32)	23(1)	20(1)	20(1)	0(1)	4(1)	3(1)
C(33)	24(1)	24(1)	27(1)	-3(1)	11(1)	-2(1)
C(34)	29(1)	28(1)	63(1)	-14(1)	18(1)	-1(1)
C(35)	34(1)	49(1)	34(1)	0(1)	18(1)	-2(1)
C(36)	21(1)	38(1)	34(1)	-6(1)	7(1)	3(1)
C(37)	27(1)	20(1)	20(1)	2(1)	2(1)	-1(1)
C(38)	23(1)	28(1)	29(1)	5(1)	2(1)	2(1)
C(39)	33(1)	41(1)	23(1)	8(1)	1(1)	-2(1)
C(40)	38(1)	23(1)	40(1)	-1(1)	-6(1)	6(1)
C(1')	21(1)	19(1)	19(1)	-3(1)	5(1)	-3(1)
C(2')	24(1)	20(1)	20(1)	-3(1)	6(1)	0(1)
C(3')	22(1)	17(1)	21(1)	-1(1)	4(1)	-1(1)
C(3A')	20(1)	17(1)	19(1)	-1(1)	4(1)	-2(1)
C(4')	20(1)	18(1)	18(1)	0(1)	4(1)	2(1)
C(5')	19(1)	20(1)	17(1)	-2(1)	3(1)	1(1)
C(6')	20(1)	18(1)	21(1)	-1(1)	5(1)	-3(1)
C(6A')	17(1)	19(1)	18(1)	-2(1)	3(1)	-4(1)
C(7')	24(1)	16(1)	24(1)	1(1)	6(1)	0(1)

C(8')	19(1)	17(1)	22(1)	0(1)	4(1)	-2(1)
C(8A')	18(1)	17(1)	19(1)	-1(1)	4(1)	-1(1)
C(8B')	20(1)	17(1)	18(1)	-1(1)	4(1)	-1(1)
C(9')	24(1)	17(1)	19(1)	-3(1)	4(1)	-5(1)
C(10')	23(1)	20(1)	21(1)	-2(1)	5(1)	-4(1)
C(11')	25(1)	22(1)	24(1)	-1(1)	0(1)	-3(1)
C(12')	37(1)	29(1)	19(1)	1(1)	0(1)	-5(1)
C(13')	37(1)	29(1)	20(1)	-3(1)	10(1)	-4(1)
C(14')	26(1)	23(1)	23(1)	-2(1)	7(1)	-1(1)
C(15')	25(1)	17(1)	22(1)	-4(1)	4(1)	1(1)
C(16')	27(1)	21(1)	25(1)	0(1)	6(1)	1(1)
C(17')	25(1)	27(1)	32(1)	-1(1)	7(1)	4(1)
C(18')	32(1)	25(1)	33(1)	3(1)	3(1)	10(1)
C(19')	38(1)	26(1)	30(1)	6(1)	10(1)	7(1)
C(20')	30(1)	24(1)	29(1)	2(1)	10(1)	5(1)
C(21')	21(1)	19(1)	20(1)	-1(1)	3(1)	2(1)
C(22')	29(1)	17(1)	24(1)	1(1)	7(1)	0(1)
C(23')	29(1)	25(1)	22(1)	2(1)	9(1)	4(1)
C(24')	27(1)	25(1)	22(1)	-6(1)	5(1)	4(1)
C(25')	39(1)	19(1)	35(1)	-7(1)	13(1)	-4(1)
C(26')	36(1)	21(1)	29(1)	-2(1)	14(1)	-4(1)
C(27')	22(1)	14(1)	21(1)	-1(1)	4(1)	-3(1)
C(28')	25(1)	18(1)	24(1)	-2(1)	4(1)	1(1)
C(29')	33(1)	19(1)	25(1)	1(1)	0(1)	1(1)
C(30')	40(1)	23(1)	21(1)	3(1)	6(1)	-5(1)
C(31')	30(1)	25(1)	26(1)	1(1)	12(1)	-4(1)
C(32')	23(1)	20(1)	24(1)	1(1)	5(1)	-2(1)
C(33')	25(1)	21(1)	22(1)	-1(1)	8(1)	-2(1)
C(34')	31(1)	21(1)	41(1)	-5(1)	14(1)	-4(1)
C(35')	33(1)	37(1)	25(1)	3(1)	10(1)	-3(1)

C(36')	22(1)	24(1)	27(1)	-3(1)	8(1)	-3(1)
C(37')	20(1)	29(1)	23(1)	-7(1)	-1(1)	2(1)
C(38')	20(1)	33(1)	28(1)	-5(1)	1(1)	0(1)
C(39')	28(1)	67(1)	24(1)	1(1)	-3(1)	8(1)
C(40')	23(1)	38(1)	57(1)	-24(1)	-6(1)	0(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2** (THInd1ABS).

	x	y	z	U(eq)
H(2)	6291	809	3552	24
H(4)	7583	2407	2411	23
H(5)	8455	3521	2785	23
H(7)	8927	4003	4649	23
H(8A)	6766	3038	3733	21
H(8B)	8462	2085	3889	22
H(10)	8567	1728	4830	27
H(11)	8607	1318	5688	32
H(12)	7246	707	5888	34
H(13)	5832	521	5223	31
H(14)	5776	943	4367	27
H(16)	6858	112	2882	30
H(17)	6242	-568	2138	35
H(18)	5579	-33	1324	33
H(19)	5562	1186	1264	36
H(20)	6181	1870	2006	32

H(22)	8880	4594	2931	35
H(23)	10247	5210	2755	42
H(24)	11712	5296	3398	43
H(25)	11801	4747	4217	45
H(26)	10456	4109	4389	37
H(28)	8619	3505	5415	27
H(29)	7954	3272	6164	33
H(30)	6413	2708	6080	33
H(31)	5496	2438	5235	29
H(32)	6131	2706	4482	25
H(34A)	9010	1236	2971	59
H(34B)	9810	1352	2601	59
H(34C)	8642	1346	2345	59
H(35A)	8877	2502	1935	56
H(35B)	10033	2480	2214	56
H(35C)	9363	3140	2302	56
H(36A)	9856	2977	3289	46
H(36B)	10544	2340	3173	46
H(36C)	9741	2222	3542	46
H(38A)	6011	2738	2497	41
H(38B)	5378	3448	2402	41
H(38C)	5869	3208	2993	41
H(39A)	7577	3976	1981	49
H(39B)	6388	3927	1806	49
H(39C)	7049	3230	1855	49
H(40A)	6740	4328	3183	53
H(40B)	6138	4561	2609	53
H(40C)	7324	4658	2759	53
H(2')	1605	4002	2518	25
H(4')	2026	3629	729	23

H(5')	2693	2458	486	22
H(7')	3694	693	1808	25
H(8A')	1797	2153	1779	22
H(8B')	3651	2948	2004	22
H(10')	4256	2543	2868	26
H(11')	4911	2246	3748	29
H(12')	4065	2559	4419	35
H(13')	2561	3175	4206	34
H(14')	1891	3463	3327	28
H(16')	97	4213	1933	29
H(17')	-1134	4986	1532	34
H(18')	-916	5646	796	37
H(19')	558	5534	475	37
H(20')	1808	4771	883	32
H(22')	4041	1774	363	28
H(23')	4401	1070	-314	30
H(24')	3909	-103	-377	30
H(25')	3087	-572	258	36
H(26')	2759	120	948	33
H(28')	4369	818	2745	27
H(29')	4359	422	3601	32
H(30')	3040	710	4018	34
H(31')	1711	1381	3562	31
H(32')	1684	1743	2694	27
H(34D)	3346	4644	953	45
H(34E)	4506	4451	1033	45
H(34F)	3897	4267	1488	45
H(35D)	3338	3216	70	47
H(35E)	4137	3838	172	47
H(35F)	2973	4007	108	47

H(36D)	4557	3075	1452	36
H(36E)	5063	3263	958	36
H(36F)	4300	2620	918	36
H(38D)	534	2457	1156	41
H(38E)	-259	2613	621	41
H(38F)	509	3209	879	41
H(39D)	1038	3342	17	61
H(39E)	296	2730	-240	61
H(39F)	1458	2684	-257	61
H(40D)	1477	1489	176	62
H(40E)	312	1598	166	62
H(40F)	1056	1412	712	62

Table S6. Torsion angles [°] for **2** (THInd1ABS).

C(1)-C(2)-C(3)-C(3A)	0.02(14)
C(1)-C(2)-C(3)-C(15)	175.14(10)
C(1)-C(9)-C(10)-C(11)	-175.90(11)
C(1)-C(9)-C(14)-C(13)	175.51(11)
C(2)-C(1)-C(8B)-C(3A)	-0.33(12)
C(2)-C(1)-C(8B)-C(8A)	121.09(11)
C(2)-C(1)-C(9)-C(10)	141.72(12)
C(2)-C(1)-C(9)-C(14)	-34.65(17)
C(2)-C(3)-C(3A)-C(4)	179.62(11)
C(2)-C(3)-C(3A)-C(8B)	-0.24(13)
C(2)-C(3)-C(15)-C(16)	-38.16(16)
C(2)-C(3)-C(15)-C(20)	139.50(12)
C(3)-C(3A)-C(4)-C(5)	135.22(12)

C(3)-C(3A)-C(4)-C(33)	-96.50(14)
C(3)-C(3A)-C(8B)-C(1)	0.35(12)
C(3)-C(3A)-C(8B)-C(8A)	-128.30(10)
C(3)-C(15)-C(16)-C(17)	176.86(11)
C(3)-C(15)-C(20)-C(19)	-176.60(12)
C(3A)-C(3)-C(15)-C(16)	135.59(14)
C(3A)-C(3)-C(15)-C(20)	-46.8(2)
C(3A)-C(4)-C(5)-C(6A)	38.43(13)
C(3A)-C(4)-C(5)-C(37)	-90.41(11)
C(3A)-C(4)-C(33)-C(34)	48.19(14)
C(3A)-C(4)-C(33)-C(35)	165.12(10)
C(3A)-C(4)-C(33)-C(36)	-73.68(13)
C(4)-C(3A)-C(8B)-C(1)	-179.52(10)
C(4)-C(3A)-C(8B)-C(8A)	51.83(13)
C(4)-C(5)-C(6A)-C(6)	124.64(12)
C(4)-C(5)-C(6A)-C(8A)	-49.75(14)
C(4)-C(5)-C(37)-C(38)	50.82(13)
C(4)-C(5)-C(37)-C(39)	-71.27(12)
C(4)-C(5)-C(37)-C(40)	170.23(10)
C(5)-C(4)-C(33)-C(34)	175.50(11)
C(5)-C(4)-C(33)-C(35)	-67.57(13)
C(5)-C(4)-C(33)-C(36)	53.63(14)
C(5)-C(6A)-C(8A)-C(8)	-179.47(10)
C(5)-C(6A)-C(8A)-C(8B)	55.71(13)
C(6)-C(6A)-C(8A)-C(8)	5.16(12)
C(6)-C(6A)-C(8A)-C(8B)	-119.66(10)
C(6)-C(7)-C(8)-C(8A)	0.83(13)
C(6)-C(7)-C(8)-C(27)	-171.11(10)
C(6)-C(21)-C(22)-C(23)	-175.78(12)
C(6)-C(21)-C(26)-C(25)	176.76(13)

C(6A)-C(5)-C(37)-C(38)	-76.81(13)
C(6A)-C(5)-C(37)-C(39)	161.09(10)
C(6A)-C(5)-C(37)-C(40)	42.60(14)
C(6A)-C(6)-C(7)-C(8)	2.58(14)
C(6A)-C(6)-C(21)-C(22)	34.2(2)
C(6A)-C(6)-C(21)-C(26)	-142.90(13)
C(6A)-C(8A)-C(8B)-C(1)	-168.46(10)
C(6A)-C(8A)-C(8B)-C(3A)	-50.04(12)
C(7)-C(6)-C(6A)-C(5)	-179.75(11)
C(7)-C(6)-C(6A)-C(8A)	-4.83(13)
C(7)-C(6)-C(21)-C(22)	-151.67(12)
C(7)-C(6)-C(21)-C(26)	31.24(17)
C(7)-C(8)-C(8A)-C(6A)	-3.50(12)
C(7)-C(8)-C(8A)-C(8B)	113.88(11)
C(7)-C(8)-C(27)-C(28)	-23.33(17)
C(7)-C(8)-C(27)-C(32)	154.85(12)
C(8)-C(8A)-C(8B)-C(1)	76.33(13)
C(8)-C(8A)-C(8B)-C(3A)	-165.24(9)
C(8)-C(27)-C(28)-C(29)	-179.63(11)
C(8)-C(27)-C(32)-C(31)	178.42(11)
C(8A)-C(8)-C(27)-C(28)	166.13(11)
C(8A)-C(8)-C(27)-C(32)	-15.68(17)
C(8B)-C(1)-C(2)-C(3)	0.21(13)
C(8B)-C(1)-C(9)-C(10)	-26.30(18)
C(8B)-C(1)-C(9)-C(14)	157.34(11)
C(8B)-C(3A)-C(4)-C(5)	-44.93(14)
C(8B)-C(3A)-C(4)-C(33)	83.35(13)
C(9)-C(1)-C(2)-C(3)	-169.98(10)
C(9)-C(1)-C(8B)-C(3A)	169.13(11)
C(9)-C(1)-C(8B)-C(8A)	-69.45(15)

C(9)-C(10)-C(11)-C(12)	0.22(19)
C(10)-C(9)-C(14)-C(13)	-1.01(17)
C(10)-C(11)-C(12)-C(13)	-0.52(19)
C(11)-C(12)-C(13)-C(14)	0.04(19)
C(12)-C(13)-C(14)-C(9)	0.74(19)
C(14)-C(9)-C(10)-C(11)	0.53(17)
C(15)-C(3)-C(3A)-C(4)	5.4(2)
C(15)-C(3)-C(3A)-C(8B)	-174.51(11)
C(15)-C(16)-C(17)-C(18)	0.2(2)
C(16)-C(15)-C(20)-C(19)	1.07(18)
C(16)-C(17)-C(18)-C(19)	0.5(2)
C(17)-C(18)-C(19)-C(20)	-0.4(2)
C(18)-C(19)-C(20)-C(15)	-0.4(2)
C(20)-C(15)-C(16)-C(17)	-0.98(18)
C(21)-C(6)-C(6A)-C(5)	-5.0(2)
C(21)-C(6)-C(6A)-C(8A)	169.90(11)
C(21)-C(6)-C(7)-C(8)	-172.74(10)
C(21)-C(22)-C(23)-C(24)	-1.2(2)
C(22)-C(21)-C(26)-C(25)	-0.6(2)
C(22)-C(23)-C(24)-C(25)	0.3(2)
C(23)-C(24)-C(25)-C(26)	0.5(2)
C(24)-C(25)-C(26)-C(21)	-0.4(2)
C(26)-C(21)-C(22)-C(23)	1.35(19)
C(27)-C(8)-C(8A)-C(6A)	168.43(10)
C(27)-C(8)-C(8A)-C(8B)	-74.20(14)
C(27)-C(28)-C(29)-C(30)	0.59(19)
C(28)-C(27)-C(32)-C(31)	-3.34(17)
C(28)-C(29)-C(30)-C(31)	-2.16(19)
C(29)-C(30)-C(31)-C(32)	0.96(19)
C(30)-C(31)-C(32)-C(27)	1.84(18)

C(32)-C(27)-C(28)-C(29)	2.13(17)
C(33)-C(4)-C(5)-C(6A)	-90.47(11)
C(33)-C(4)-C(5)-C(37)	140.68(10)
C(37)-C(5)-C(6A)-C(6)	-106.29(14)
C(37)-C(5)-C(6A)-C(8A)	79.33(13)
C(1')-C(2')-C(3')-C(3A')	-1.25(14)
C(1')-C(2')-C(3')-C(15')	174.75(10)
C(1')-C(9')-C(10')-C(11')	179.65(11)
C(1')-C(9')-C(14')-C(13')	-179.29(11)
C(2')-C(1')-C(8B')-C(3A')	5.32(12)
C(2')-C(1')-C(8B')-C(8A')	-110.89(11)
C(2')-C(1')-C(9')-C(10')	-155.56(12)
C(2')-C(1')-C(9')-C(14')	23.07(18)
C(2')-C(3')-C(3A')-C(4')	177.34(11)
C(2')-C(3')-C(3A')-C(8B')	4.74(13)
C(2')-C(3')-C(15')-C(16')	-33.24(16)
C(2')-C(3')-C(15')-C(20')	147.20(12)
C(3')-C(3A')-C(4')-C(5')	-121.39(13)
C(3')-C(3A')-C(4')-C(33')	110.25(13)
C(3')-C(3A')-C(8B')-C(1')	-6.15(12)
C(3')-C(3A')-C(8B')-C(8A')	116.93(10)
C(3')-C(15')-C(16')-C(17')	-178.41(11)
C(3')-C(15')-C(20')-C(19')	177.87(12)
C(3A')-C(3')-C(15')-C(16')	141.73(13)
C(3A')-C(3')-C(15')-C(20')	-37.8(2)
C(3A')-C(4')-C(5')-C(6A')	-37.71(12)
C(3A')-C(4')-C(5')-C(37')	91.87(11)
C(3A')-C(4')-C(33')-C(34')	-45.11(13)
C(3A')-C(4')-C(33')-C(35')	-162.95(10)
C(3A')-C(4')-C(33')-C(36')	75.29(12)

C(4')-C(3A')-C(8B')-C(1')	-179.42(10)
C(4')-C(3A')-C(8B')-C(8A')	-56.34(13)
C(4')-C(5')-C(6A')-C(6')	-136.57(12)
C(4')-C(5')-C(6A')-C(8A')	43.51(14)
C(4')-C(5')-C(37')-C(38')	-53.06(14)
C(4')-C(5')-C(37')-C(39')	68.55(13)
C(4')-C(5')-C(37')-C(40')	-174.09(11)
C(5')-C(4')-C(33')-C(34')	-172.35(10)
C(5')-C(4')-C(33')-C(35')	69.81(12)
C(5')-C(4')-C(33')-C(36')	-51.95(13)
C(5')-C(6A')-C(8A')-C(8')	-179.41(10)
C(5')-C(6A')-C(8A')-C(8B')	-50.70(13)
C(6')-C(6A')-C(8A')-C(8')	0.65(12)
C(6')-C(6A')-C(8A')-C(8B')	129.36(10)
C(6')-C(7')-C(8')-C(8A')	0.11(13)
C(6')-C(7')-C(8')-C(27')	172.52(10)
C(6')-C(21')-C(22')-C(23')	177.72(11)
C(6')-C(21')-C(26')-C(25')	-178.69(12)
C(6A')-C(5')-C(37')-C(38')	74.75(13)
C(6A')-C(5')-C(37')-C(39')	-163.63(11)
C(6A')-C(5')-C(37')-C(40')	-46.27(14)
C(6A')-C(6')-C(7')-C(8')	0.33(14)
C(6A')-C(6')-C(21')-C(22')	53.88(19)
C(6A')-C(6')-C(21')-C(26')	-127.94(14)
C(6A')-C(8A')-C(8B')-C(1')	163.85(10)
C(6A')-C(8A')-C(8B')-C(3A')	49.57(11)
C(7')-C(6')-C(6A')-C(5')	179.46(11)
C(7')-C(6')-C(6A')-C(8A')	-0.61(13)
C(7')-C(6')-C(21')-C(22')	-133.45(12)
C(7')-C(6')-C(21')-C(26')	44.73(16)

C(7')-C(8')-C(8A')-C(6A')	-0.45(12)
C(7')-C(8')-C(8A')-C(8B')	-122.28(11)
C(7')-C(8')-C(27')-C(28')	37.22(17)
C(7')-C(8')-C(27')-C(32')	-140.50(12)
C(8')-C(8A')-C(8B')-C(1')	-77.43(13)
C(8')-C(8A')-C(8B')-C(3A')	168.29(9)
C(8')-C(27')-C(28')-C(29')	-177.22(11)
C(8')-C(27')-C(32')-C(31')	178.45(11)
C(8A')-C(8')-C(27')-C(28')	-152.00(11)
C(8A')-C(8')-C(27')-C(32')	30.28(18)
C(8B')-C(1')-C(2')-C(3')	-2.81(13)
C(8B')-C(1')-C(9')-C(10')	14.88(17)
C(8B')-C(1')-C(9')-C(14')	-166.49(11)
C(8B')-C(3A')-C(4')-C(5')	50.40(13)
C(8B')-C(3A')-C(4')-C(33')	-77.96(13)
C(9')-C(1')-C(2')-C(3')	169.06(11)
C(9')-C(1')-C(8B')-C(3A')	-166.53(10)
C(9')-C(1')-C(8B')-C(8A')	77.26(14)
C(9')-C(10')-C(11')-C(12')	-0.61(18)
C(10')-C(9')-C(14')-C(13')	-0.61(17)
C(10')-C(11')-C(12')-C(13')	-0.17(19)
C(11')-C(12')-C(13')-C(14')	0.55(19)
C(12')-C(13')-C(14')-C(9')	-0.15(19)
C(14')-C(9')-C(10')-C(11')	0.99(17)
C(15')-C(3')-C(3A')-C(4')	1.9(2)
C(15')-C(3')-C(3A')-C(8B')	-170.71(11)
C(15')-C(16')-C(17')-C(18')	-0.05(19)
C(16')-C(15')-C(20')-C(19')	-1.69(18)
C(16')-C(17')-C(18')-C(19')	-0.6(2)
C(17')-C(18')-C(19')-C(20')	0.1(2)

C(18')-C(19')-C(20')-C(15')	1.1(2)
C(20')-C(15')-C(16')-C(17')	1.18(18)
C(21')-C(6')-C(6A')-C(5')	-7.2(2)
C(21')-C(6')-C(6A')-C(8A')	172.70(11)
C(21')-C(6')-C(7')-C(8')	-173.84(10)
C(21')-C(22')-C(23')-C(24')	1.05(19)
C(22')-C(21')-C(26')-C(25')	-0.38(19)
C(22')-C(23')-C(24')-C(25')	-0.78(19)
C(23')-C(24')-C(25')-C(26')	0.0(2)
C(24')-C(25')-C(26')-C(21')	0.6(2)
C(26')-C(21')-C(22')-C(23')	-0.46(18)
C(27')-C(8')-C(8A')-C(6A')	-172.36(11)
C(27')-C(8')-C(8A')-C(8B')	65.80(15)
C(27')-C(28')-C(29')-C(30')	-1.27(18)
C(28')-C(27')-C(32')-C(31')	0.69(17)
C(28')-C(29')-C(30')-C(31')	0.65(19)
C(29')-C(30')-C(31')-C(32')	0.63(19)
C(30')-C(31')-C(32')-C(27')	-1.31(19)
C(32')-C(27')-C(28')-C(29')	0.59(17)
C(33')-C(4')-C(5')-C(6A')	91.11(11)
C(33')-C(4')-C(5')-C(37')	-139.30(10)
C(37')-C(5')-C(6A')-C(6')	94.33(14)
C(37')-C(5')-C(6A')-C(8A')	-85.60(13)

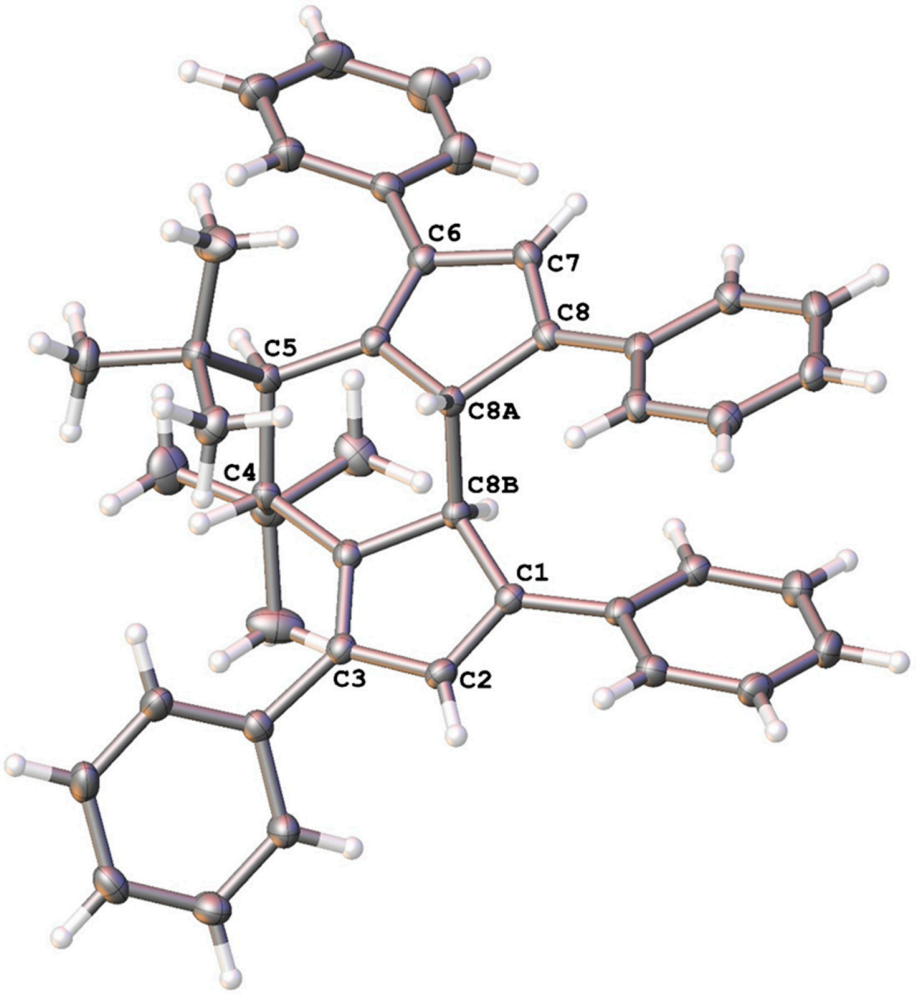
Single Crystal X-ray Diffraction Study - Experimental Summary (Crystals from 2-Butanol)

The single crystal X-ray diffraction studies were carried out on a Rigaku Synergy-i dual source (Cu, Mo) single crystal diffractometer using the Cu K_α radiation source (λ = 1.54184 Å) and a Bantam HyPIX-3000 direct photon counting detector. Crystals of the subject compound were grown from iPrOH solution. A 0.181 x 0.115 x 0.082 mm^3 colorless translucent prism crystal was mounted on a Cryoloop with Paratone-N oil.

Data were collected in a nitrogen gas stream at 100.00(10) K using ϖ scans. Crystal-to-detector distance was 40 mm using exposure times of 1 and 2 seconds with a scan width of 0.50°. Data collection was 99.9 % complete to 68.959° in θ. A total of 64158 reflections were collected. 12117 reflections were found to be symmetry independent, with an R_{int} of 0.0250. Indexing and unit cell refinement indicated a **primitive monoclinic** lattice. The space group was found to be **$P2_1/c$.** The data were integrated using the CrysAlisPro software program (Rigaku Oxford Diffraction, 2019, 1.171.40.53) and scaled using an empirical absorption correction implemented in the SCALE 3 ABSPACK software program as well as a numerical absorption correction based on Gaussian integration over a multifaceted crystal model. Solution by direct methods (SHELXT-2014/5) produced a complete phasing model consistent with the proposed structure.

All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL- 2016/6). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL.

Notes: Excellent data and stable refinement. The asymmetric unit consists of two molecules of 4,5-di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene **2**. The molecule crystallizes out as the racemate.



Selected Bond Distances (Å)

C1-C8B	1.523(2)	C8-C8A	1.520(2)
C1-C2	1.346(2)	C7-C8	1.347(2)
C2-C3	1.462(2)	C6-C7	1.464(2)
C3-C3A	1.357(2)	C6-C6A	1.359(2)
C4-C5	1.567(2)	C5-C6A	1.499(2)
C6A-C8A	1.523(2)	C8A-C8B	1.569(2)
C3A-C8B	1.527(2)	C3A-C4	1.508(2)

Selected Bond Angles (°)

C5-C6A-C8A	121.3(1)	C3A-C8B-C8A	109.0(1)
C4-C3A-C8B	121.6(1)	C6A-C8A-C8B	106.8(1)
C4-C5-C6A	110.9(1)	C3A-C4-C5	110.8(1)

Figure S20. Thermal ellipsoid view of the molecular structure of 4,5-di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene **2 (**crystal obtained from 2-butanol solution). Thermal ellipsoids are shown at the 50% probability level. Compare to Figure S13 and manuscript Figure 1).

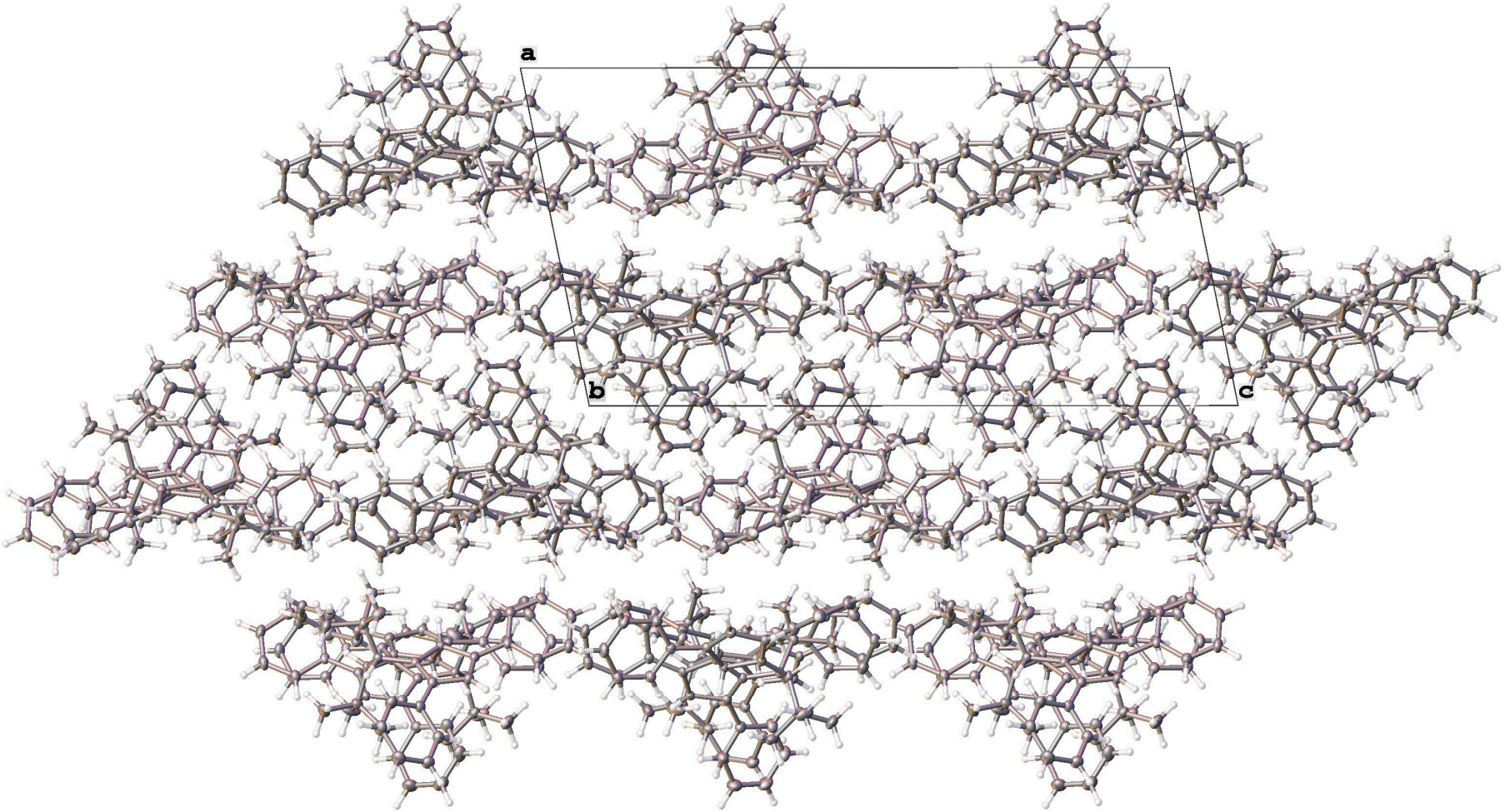


Figure S21. Thermal ellipsoid view of the molecular packing of **2**, view along the b-axis direction (crystal obtained from 2-butanol solution). Thermal ellipsoids are shown at the 50% probability level. Compare to Figure S15.

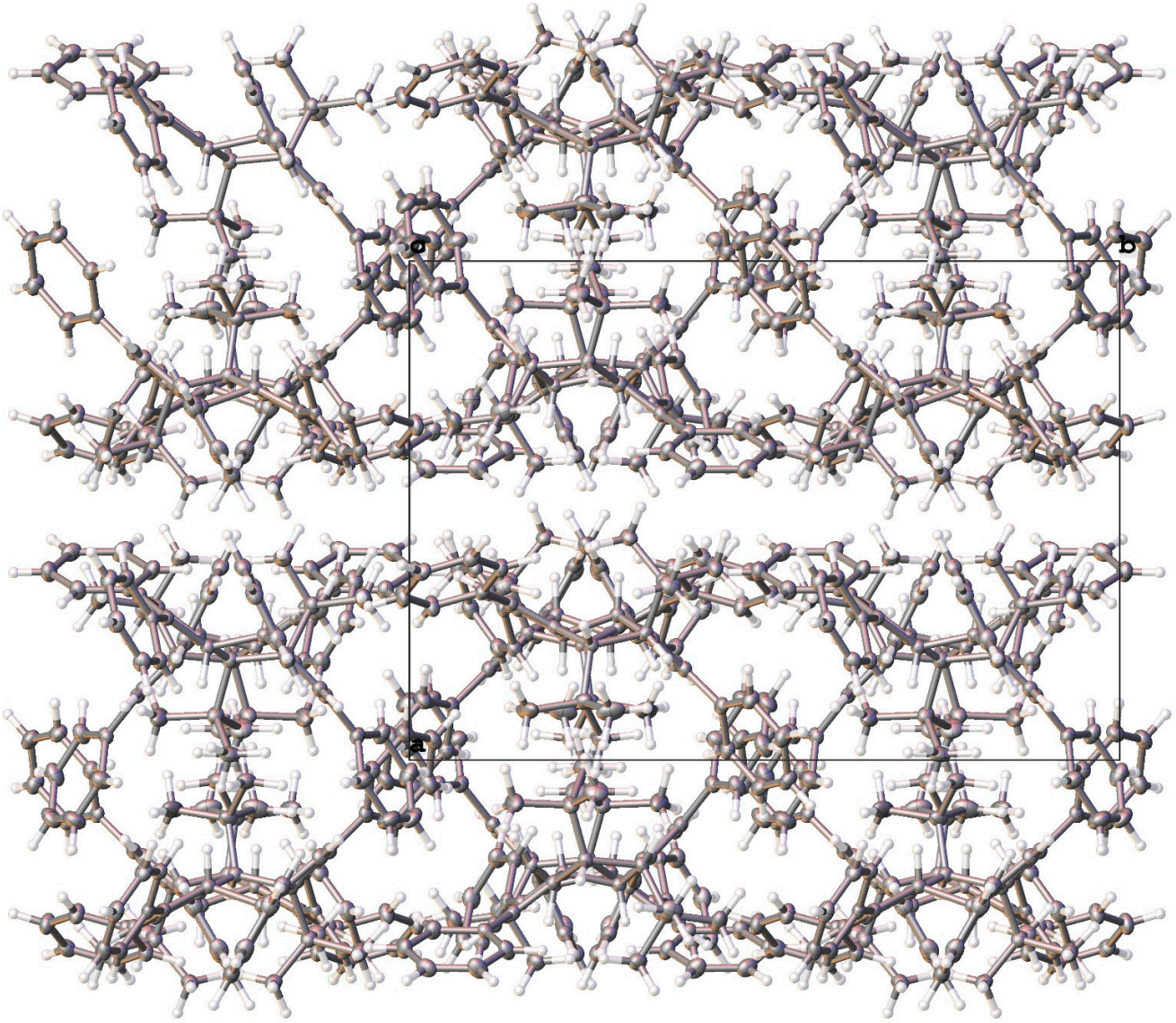


Figure S22. Thermal ellipsoid view of the molecular packing of **2**, view along the c-axis direction (crystal obtained from 2-butanol solution). Thermal ellipsoids are shown at the 50% probability level. Compare to Figure S16.

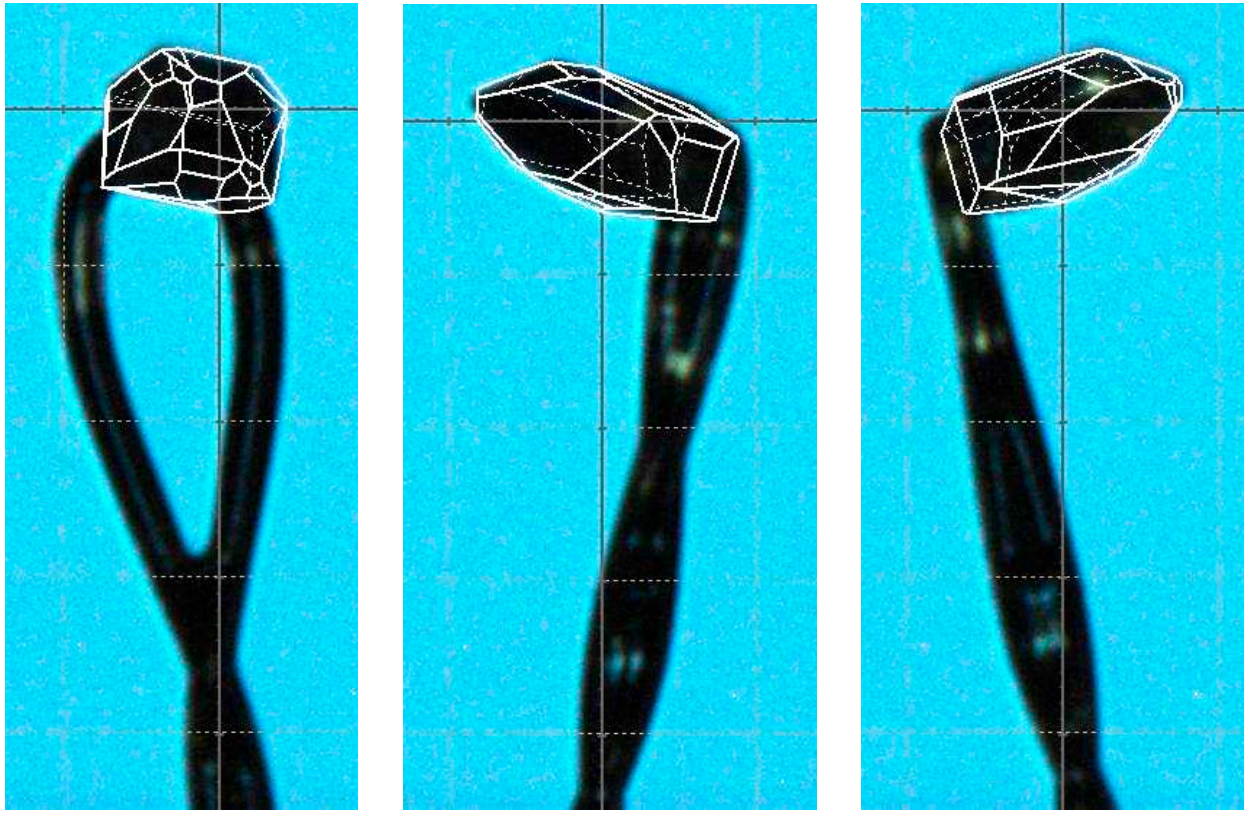


Figure S23. Images of the mounted crystal of **2** (THInd2ABS, crystal from 2-butanol solution). A 0.181 x 0.115 x 0.082 mm^3 translucent colorless prism crystal was selected from crystals that were grown from a hot 2- butanol solution by slow cooling and evaporation.

Table S7. Crystal data and structure refinement for 4,5-di-*tert*-butyl-1,3,6,8-tetraphenyl-4,5,8a,8b-tetrahydro-as-indacene **2** (THInd2ABS, crystal obtained from 2-butanol solution).

Identification code	thind2abs	
Empirical formula	C44 H44	
Formula weight	572.79	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.66160(10) Å	α= 90°.
	b = 19.09420(10) Å	β= 101.4550(10)°.
	c = 25.6524(2) Å	γ = 90°.
Volume	6558.33(8) $Å^3$	
Z	8	
Density (calculated)	1.160 Mg/m^3	
Absorption coefficient	0.486 mm^{-1}	
F(000)	2464	
Crystal size	0.181 x 0.115 x 0.082 mm^3	
Theta range for data collection	2.906 to 68.959°.	
Index ranges	-16<=h<=16, -23<=k<=18, -30<=l<=31	
Reflections collected	64158	
Independent reflections	12117 [R(int) = 0.0250]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.689	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12117 / 0 / 806	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0883	
R indices (all data)	R1 = 0.0417, wR2 = 0.0917	
Extinction coefficient	0.00026(3)	
Largest diff. peak and hole	0.235 and -0.186 e.$Å^{-3}$	