Supporting Information for

Structure and absolute configuration of liquid molecules based on adamantane derivative cocrystallization

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Table S1 Crystal data and structure refinement

Compound	1a	1b	1c	1d
Empirical formula	$C_{58}H_{74}O_9$	$C_{58}H_{73}FO_9$	$C_{58}H_{73}ClO_9$	$C_{58}H_{74}O_9$
Formula weight	915.17	933.16	949.61	915.17
Temperature (K)	296.0(2)	296.0(2)	296.0(2)	296.0(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Trigonal	Triclinic
Space group	P-1	P-1	P-31c	P-1
a / Å	14.473(3)	14.545(13)	23.363(17)	14.606(6)
b / Å	14.587(3)	14.729(13)	23.363(17)	14.673(6)
c / Å	15.394(3)	15.409(13)	18.709(14)	15.496(6)
α / °	66.398(3)	66.675(11)	90	66.376(5)
β / °	80.934(3)	81.233(12)	90	80.644(5)
γ / °	62.894(2)	62.481(11)	120	62.069(5)
V / Å^3	2649.7(10)	2686.0(4)	8844.0(15)	2686.9(19)
Z	2	2	6	2
D_c / Mg cm^{-3}	1.147	1.154	1.070	1.131
μ / mm^{-1}	0.076	0.079	0.114	0.075
F (000)	988	1004	3060	988
Crystal size (mm)	0.48×0.26×0.23	0.20×0.20×0.10	0.42×0.26×0.22	0.42×0.26×0.23
θ range	1.44 to 27.42	1.44 to 25.63	1.48 to 27.81	1.44 to 27.66
Reflections collected	30064	27184	98785	30499
Independent reflections	11735 (0.0385)	10084 (0.0358)	6889 (0.0735)	11982 (0.0340)
Data/restraints/parameters	11735/30/614	10084/0/621	6889/1173/420	11982/642/672
Goodness-of-fit on F^2	1.015	1.011	1.022	1.022
Final R indices [$I>2\sigma(I)$]	0.0644, 0.1564	0.0602, 0.1595	0.0808, 0.2053	0.0744, 0.1701
R indices (all data)	0.1216, 0.1864	0.1180, 0.1967	0.1697, 0.2748	0.1453, 0.2022
Max. peak/hole (e. Å^{-3})	0.238/-0.205	0.260/-0.243	0.234/-0.310	0.560/-0.606
Flack parameter				

Compound	1e	2a	2b	2c
Empirical formula	$C_{116}H_{144}Cl_2O_{18}$	$C_{59}H_{76}O_9$	$C_{59}H_{76}O_9$	$C_{59}H_{76}O_9$
Formula weight	1897.20	929.20	929.19	929.19
Temperature (K)	149.9(10)	296.0(2)	149.9(10)	149.9(10)
Wavelength (Å)	1.54184	0.71073	1.54184	1.54184
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P1	P-1	P1	P1
a / Å	14.4591(7)	14.634(10)	14.494(9)	14.494(2)
b / Å	14.5057(5)	14.681(10)	14.691(8)	14.714(18)
c / Å	15.3163(5)	15.413(11)	15.176(2)	15.162(2)
α / °	66.263(3)	66.757(9)	66.838(12)	66.851(12)
β / °	80.241(3)	81.050(10)	81.233(11)	81.242(11)
γ / °	63.042(4)	62.720(10)	63.018(13)	63.018(13)
V / Å^3	2620.8(2)	2703.0(3)	2646.1(7)	2648.3(7)
Z	1	2	2	2
D_c / Mg cm^{-3}	1.202	1.142	1.166	1.165
μ / mm^{-1}	1.086	0.075	0.611	0.611
F (000)	1018	1004	1004	1004
Crystal size (mm)	0.35×0.24×0.21	0.48×0.36×0.25	0.19×0.07×0.06	0.35×0.25×0.20
θ range	6.30 to 148.89	1.44 to 27.42	6.34 to 152.27	6.34 to 147.71
Reflections collected	41735	30680	79146	49460
Independent reflections	18813 (0.0539)	12044(0.0256)	20430 (0.0245)	18715 (0.0163)
Data/restraints/parameters	18813/2747/1215	12044/31/623	20430/3/1222	18715/3/1245
Goodness-of-fit on F^2	1.043	0.997	1.059	1.034
Final R indices [$I > 2\sigma(I)$]	0.0963, 0.2531	0.0658, 0.1924	0.0452, 0.1256	0.0405, 0.1138
R indices (all data)	0.1033, 0.2607	0.1217, 0.2351	0.0463, 0.1269	0.0410, 0.1147
Max. peak/hole (e. Å^{-3})	1.150/-1.060	0.547/-0.340	0.790/-0.350	0.750/-0.300
Flack parameter	0.124(14)		-0.01(4)	0.04(3)

Compound	2d	3a	3b	3c
Empirical formula	$C_{68.83}H_{89.66}O_{10}$	$C_{59}H_{77}O_8N$	$C_{59}H_{77}O_8N$	$C_{118}H_{154}O_{16}N_2$
Formula weight	1077.03	928.21	928.21	1856.42
Temperature (K)	296.0(2)	296.0(2)	149.9(10)	149.9(10)
Wavelength (Å)	0.71073	0.71073	1.54184	1.54184
Crystal system	Trigonal	Triclinic	Triclinic	Triclinic
Space group	P-31c	P-1	P1	P1
a / Å	24.169(7)	14.615(2)	14.479(2)	14.4846(4)
b / Å	24.169(7)	14.871(3)	14.669(3)	14.6777(5)
c / Å	18.917(8)	15.668(3)	15.343(3)	15.3743(5)
α / °	90	66.701(2)	66.856(18)	66.810(3)
β / °	90	80.933(2)	80.780(14)	80.771(3)
γ / °	120	61.155(2)	62.305(16)	62.298(3)
V / Å^3	9570.0(7)	2737.3(8)	2652.2(9)	2659.08(17)
Z	6	2	2	1
D_c / Mg cm^{-3}	1.121	1.126	1.162	1.159
μ / mm^{-1}	0.074	0.074	0.600	0.599
F (000)	3496	1004	1004	1004
Crystal size (mm)	0.36×0.22×0.20	0.42×0.23×0.20	0.38×0.27×0.22	0.20×0.10×0.05
θ range	1.45 to 25.37	1.42 to 27.57	3.13 to 73.86	6.256 to 148.544
Reflections collected	92494	30970	44949	69076
Independent reflections	5853 (0.0964)	12177 (0.0223)	19817 (0.0213)	20308 (0.0585)
Data/restraints/parameters	5853/550/440	12177/693/689	18783/444/1322	20308/372/1225
Goodness-of-fit on F^2	0.989	1.058	1.039	1.076
Final *R* indices [$I > 2\sigma(I)$]	0.0713, 0.2012	0.0766, 0.2423	0.0482, 0.0503	0.0670, 0.1897
R indices (all data)	0.1444, 0.2676	0.1101, 0.2710	0.1295, 0.1321	0.0701, 0.1943
Max. peak/hole (e. Å^{-3})	0.246/-0.344	0.625/-0.363	0.501/-0.316	0.780/-0.690
Flack parameter			0.06(5)	0.03(8)

Compound	4a	4b	5	6
Empirical formula	$C_{55}H_{68}O_8ClN$	$C_{55}H_{68}O_8ClN$	$C_{60}H_{76}O_{10}$	$C_{104}H_{133}O_{18}$
Formula weight	906.55	906.55	957.21	1671.10
Temperature (K)	296.0(2)	296.0(2)	296.0(2)	296.0(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1
a / Å	14.435(8)	14.412(9)	14.571(10)	14.490(7)
b / Å	14.541(8)	14.557(2)	14.891(11)	14.479(7)
c / Å	15.528(8)	15.542(2)	15.392(11)	15.489(7)
α / °	66.197(6)	66.340(2)	102.473(8)	81.001(6)
β / °	81.269(7)	81.457(2)	96.914(8)	66.274(5)
γ / °	61.464(6)	61.084(2)	119.118(7)	62.645(5)
V / Å^3	2616.0(2)	2636.0(6)	2747.0(3)	2641.0(2)
Z	2	2	2	2
D_c / Mg cm^{-3}	1.151	1.142	1.157	1.051
μ / mm^{-1}	0.125	0.124	0.077	0.071
F (000)	972	972	1032	901
Crystal size (mm)	0.42×0.23×0.20	0.35×0.21×0.18	0.45×0.42×0.36	0.42×0.26×0.21
θ range	1.44 to 27.52	1.43 to 25.01	1.40 to 25.01	1.44 to 27.54
Reflections collected	29644	25426	26435	27919
Independent reflections	11615 (0.0274)	9282 (0.0211)	9676 (0.0219)	11454 (0.0327)
Data/restraints/parameters	11615/609/634	9282/801/647	9676/44/641	11454/569/642
Goodness-of-fit on F^2	1.047	1.062	1.041	1.060
Final R indices [$I>2\sigma(I)$]	0.0636, 0.1777	0.0688, 0.2038	0.0651, 0.1940	0.0972, 0.3007
R indices (all data)	0.1129, 0.2081	0.0885, 0.2317	0.0860, 0.2188	0.1333, 0.3339
Max. peak/hole (e. Å^{-3})	0.376/-0.443	0.505/-0.533	0.492/-0.338	0.613/-0.280
Flack parameter				

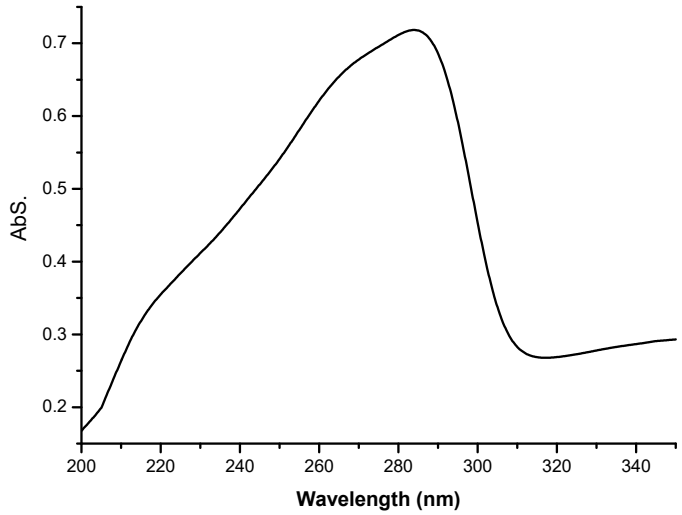

Fig. S1 The solid UV-vis. spectra of **3b.**