

Electronic Supplementary Information (ESI)

Enantioselective [4+4] photodimerisation of anthracene-2,6-dicarboxylic acid mediated by a C_2 -symmetric chiral template

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1) Equipment and general methods

Solvents: Dimethylformamide (DMF, *Acros Organics*, 99.9%, < 0.005% water)
Dichloromethane (CH₂Cl₂, *Wako*, spectroscopic grade)
Acetonitrile (MeCN, *Wako*, HPLC grade)

The technical solvents [Chloroform (CHCl₃) and Methanol (MeOH)] for preparative column chromatography were purified by simple distillation.

Flash column chromatography was performed on silica gel 60 (230–400 mesh) with the eluent mixtures given at the corresponding procedure. Thin layer chromatography (TLC) was performed on silica coated glass plates (silica gel 60 F₂₅₄). Compounds were detected by UV ($\lambda = 254$ nm and 366 nm).

HPLC analyses were performed using a *Shimadzu* system (PU 2089 pump, DG-980-50 degasser, MX-2080-32 mixer, FP-2025 fluorescence detector, excitation wavelength of $\lambda_{\text{exc.}} = 254$ nm, emission detected at a wavelength of $\lambda_{\text{em.}} = 420$ nm) with a *GL Science* CO-7050 column oven. As stationary phases a *Nacalai Tesque* Cosmosil 5C18-AR-II (4.6 × 250 mm) and a *Daicel* Chiralcel OD-RH (4.6 × 150 mm) were connected in series. As mobile phase a mixture of water (0.1% TFA)/acetonitrile (73/27) was used with a flow rate of 0.5 mL/min at a temperature of 40 °C.

As a **temperature control** element for all photochemical experiments and for all photo physical studies an *Unisoku* USP-203HP cryostat was used.

UV-Vis spectra were recorded on a *JASCO* V550 or V560 spectrometer.

CD spectra were recorded on a *JASCO* J-820S at 25 °C.

Fluorescence spectra were recorded on a *JASCO* FP6500 spectrometer.

Fluorescence decay spectrum of the chiral template **6** was recorded on an *Edinburgh Instrument* OB 920 single photon counters (hydrogen-filled ns-flash lamp) in a d = 1 cm quartz cuvette at 25 °C with an excitation wavelength of $\lambda_{\text{exc.}} = 310$ nm and an emission wavelength of $\lambda_{\text{em.}} = 380$ nm in a 20 ns range. The bandwidth was set to 16 nm for both the excitation and the emission monochromators. The instrument response function (IRF) was determined with an aqueous suspension of silica gel.

As **light sources** for the irradiation experiments either an *Ushio* Optical Modulex H500 (500 W ultrahigh-pressure Hg lamp) with an UV37 filter or an *Asahi Spectra* MAX 301 (300 W monochromatic xenon light source) with the respective band-pass filter was used.

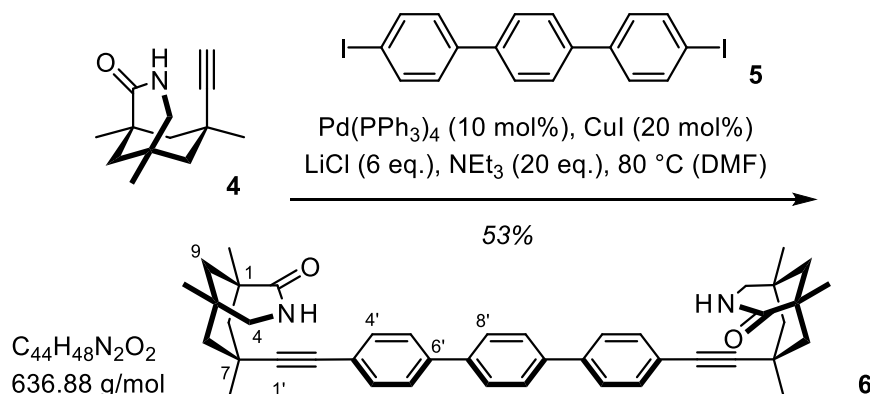
IR spectra were recorded on a *JASCO* IR-4100 (ATR).

¹H and **¹³C-NMR**-spectra were recorded on a *Bruker* AVHD 300 and AVDH 400 spectrometer. The NMR spectra were calibrated to the residual solvent signals of CDCl₃ (CHCl₃ δ (¹H) = 7.26 ppm) and to the ¹³C-D triplet (δ (¹³C) = 77.16 ppm). Multiplicities of ¹³C-NMR signals due to ¹H-coupling were determined by DEPT and 2D HMQC experiments. The proton assignment for the 1,5,7-trimethyl-3-azabicyclo[3.3.1]nonan-2-one skeleton was done as follows: *CHH-X* for nuclei in an equatorial position and *CHH-X* for nuclei in an axial position.

HRMS data were recorded by electron spray ionization (ESI) on a *Thermo Finnigan* LTQ FT Ultra.

2) Synthesis and analytical data of the chiral template **6**

(1*S*,1'*S*,5*R*,5'*R*,7*S*,7'*S*)-7,7'-([1,1':4',1''-terphenyl]-4,4''-diylbis[ethyn-2,1-diyl])bis(1,5,7-trimethyl)-3-azabicyclo[3.3.1]nonan-2-one (**6**)



A solution of **4**^[1] (35.0 mg, 171 μmol , 2.05 eq., >99% *ee*), 4,4''-diiodoterphenyl (**5**, 40.1 mg, 83.2 μmol , 1.0 eq.), Pd(PPh₃)₄ (9.61 mg, 8.32 μmol , 10 mol%), CuI (3.17 mg, 16.6 μmol , 20 mol%), LiCl (21.2 mg, 499 μmol , 6.0 eq.) and triethylamine (232 μL , 168 mg, 1.66 mmol, 20 eq.) in DMF (4 mL) were degassed by three *freeze-pump-thaw* cycles and stirred for three days at 80 °C under argon atmosphere. The reaction mixture was subjected to column chromatography (column diameter = 2.5 cm, 15 g SiO₂, CHCl₃/MeOH = 100/0 → 99.5/0.5 → 99/1) which delivered the chiral template **6** (27.9 g, 43.4 μmol , 53%) as a colourless solid.

TLC: R_f = 0.40 (CHCl₃/MeOH = 97/3) [UV].

¹H-NMR (500 MHz, CDCl₃, 300 K): δ (ppm) = 7.63 (s, 4H, H-8'), 7.54 (d, ³*J* = 8.1 Hz, 4H, H-4')*, 7.48 (d, ³*J* = 8.1 Hz, 1H, H-5')*, 5.63 (s, 2H, NH), 3.46 (d, ²*J* = 11.8 Hz, 2H, CHH-4), 3.18 (d, ²*J* = 11.8 Hz, 2H, CHH-4), 2.25 (d, ²*J* = 13.6 Hz, 2H, CHH-6), 2.00 (d, ²*J* = 13.7 Hz, 2H, CHH-9), 1.83 (d, ²*J* = 12.8 Hz, 2H, CHH-8), 1.35 (s, 6H, C7-CH₃), 1.33 (d, 2H, CHH-9), 1.25-1.20 (m, 8H, CHH-8/C1-CH₃), 1.19 (d, ²*J* = 13.6 Hz, 2H, CHH-6), 1.04 (s, 6H, C5-CH₃).

* The signal assignment is interconvertible.

¹³C-NMR (126 MHz, CDCl₃, 300 K): δ (ppm) = 176.7 (s, C2), 139.7 (s, C-3')*, 139.1 (s, C-6')*, 132.1 (d, C-8'), 127.5 (d, C-4')**, 126.9 (d, C-5')**, 123.1 (s, C-7'), 96.7 (s, C-1'), 79.7 (s, C-2'), 52.6 (t, C-4), 51.7 (t, C-9), 48.6 (t, C-6), 44.5 (t, C-8), 38.6 (s, C-1), 33.9 (q, C7-CH₃), 31.1 (s, C-5), 30.8 (s, C-7), 30.1 (q, C5-CH₃), 25.8 (q, C1-CH₃).

, The signal assignment is interconvertible.

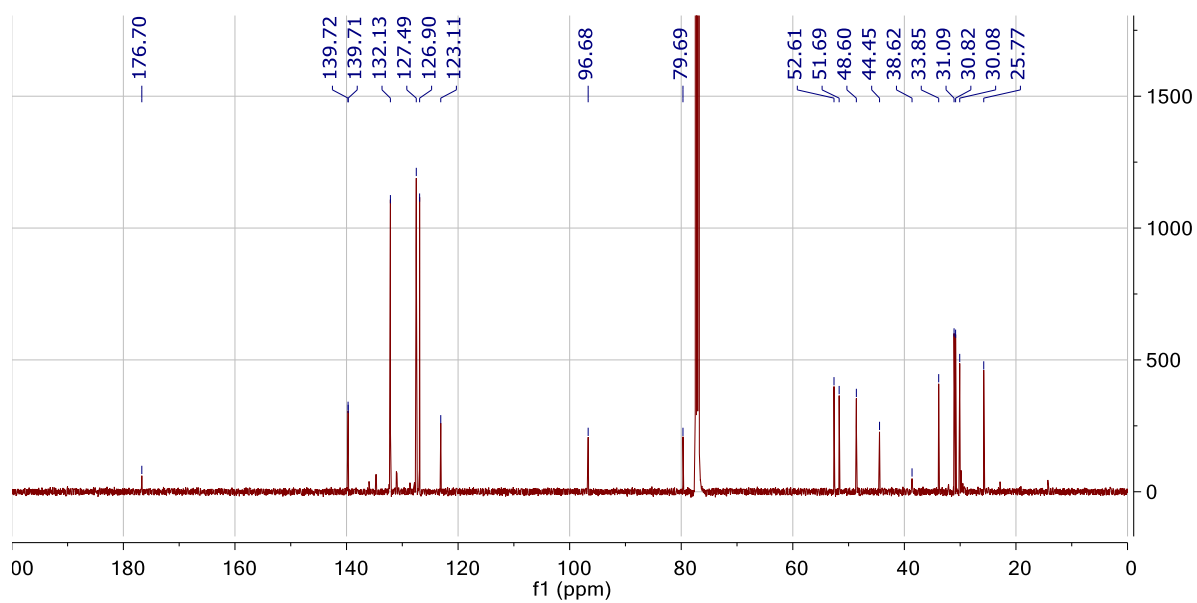
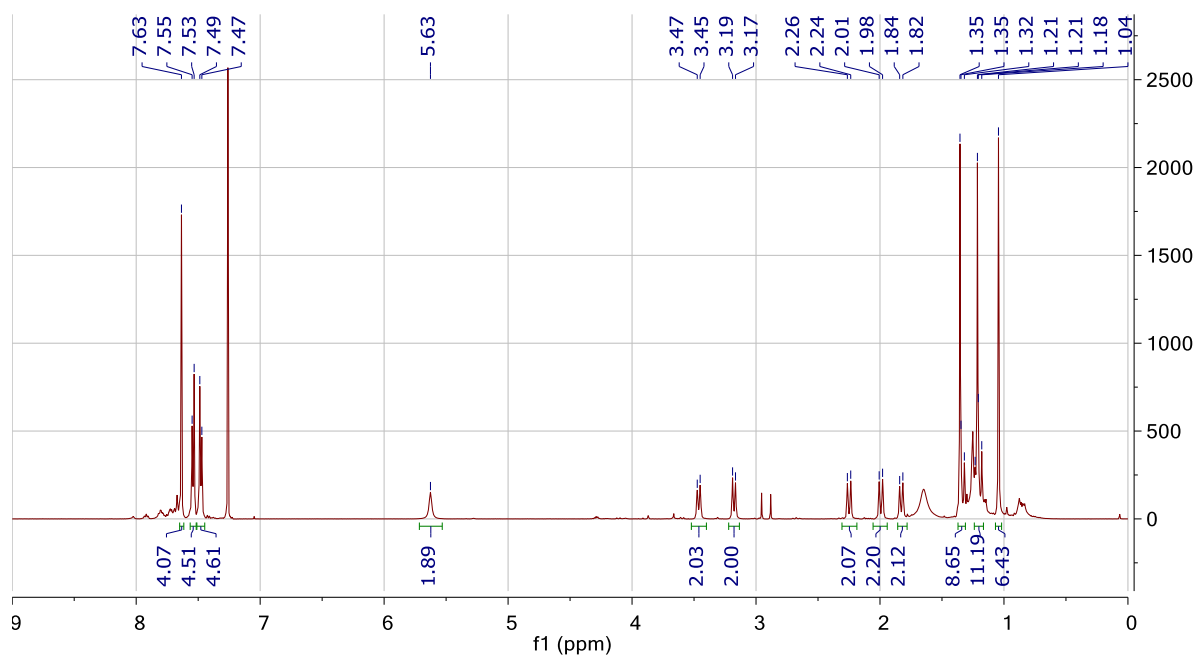
UV-Vis (CH₂Cl₂, *c* = 1.0 mmol/L): λ (nm) = 341 (ϵ = 40000 cm⁻¹ M⁻¹).

HRMS (ESI) ($C_{44}H_{48}N_2O_2$): calc.: $[(M + H)^+]$ 637.3789; found.: $[(M + H)^+]$ 637.3784.

($C_{44}H_{48}N_2O_2$): calc.: $[(M + 2H)^{2+}]$ 638.3861; found.: $[(M + 2H)^{2+}]$ 638.3818.

Optical rotation: $[\alpha]_D^{RT} = -14.5$ ($c = 1.0$ CH_2Cl_2).

1H and ^{13}C -NMR spectra:



3) General procedure for the irradiation experiments

A solution of the chiral template **6** (4.0 mL, 1.0 mM) in CH₂Cl₂ was treated with 2-3 mg of 1,6-anthracene dicarboxylic acid (**1**). The sealed tube was sonicated in an ultrasonic bath for 8-10 hours, filtered and transferred to a quartz cuvette (d = 1 cm), which was sealed with a septum. The colourless solution was purged with nitrogen at 0 °C for 3-5 minutes. The solution was irradiated at the given temperature (*Unisoku* USP-203HP cryostat) for the given time.

The concentration of **1** (prior to irradiation) as well as the conversion was determined by UV-Vis spectroscopy (0-0' transition of the ¹L_b band, ε = 4250 cm⁻¹ M⁻¹).

After the irradiation experiment, the solvent was evaporated and the residue was treated with 1mL of a 1/1 mixture of aq. NaOH (1 mM) and acetonitrile. An aliquot was taken, diluted by a factor of 10 with the same solvent mixture and subjected to HPLC analysis.

Recycling of the chiral template **6**: After 2-3 irradiation experiments, the residues as well as the aqueous solutions were combined, treated with CH₂Cl₂ (15 mL) and the phases were separated. The aqueous layer was extracted with CH₂Cl₂ (3 × 15 mL). The organic layers were combined, the solvent was evaporated and the residue purified by column chromatography (column diameter = 2.5 cm, 15 g SiO₂, CHCl₃/MeOH = 100/0 → 99.5/0.5 → 99/1).

4) Representative HPLC traces

Elution order: **2** ($t_R = 38$ min), **3** ($t_R = 46$ min), *ent-2* ($t_R = 51$ min)

Table 1, Entry 4: $\lambda > 370$ nm, conv. 10%, 55% *ee*.

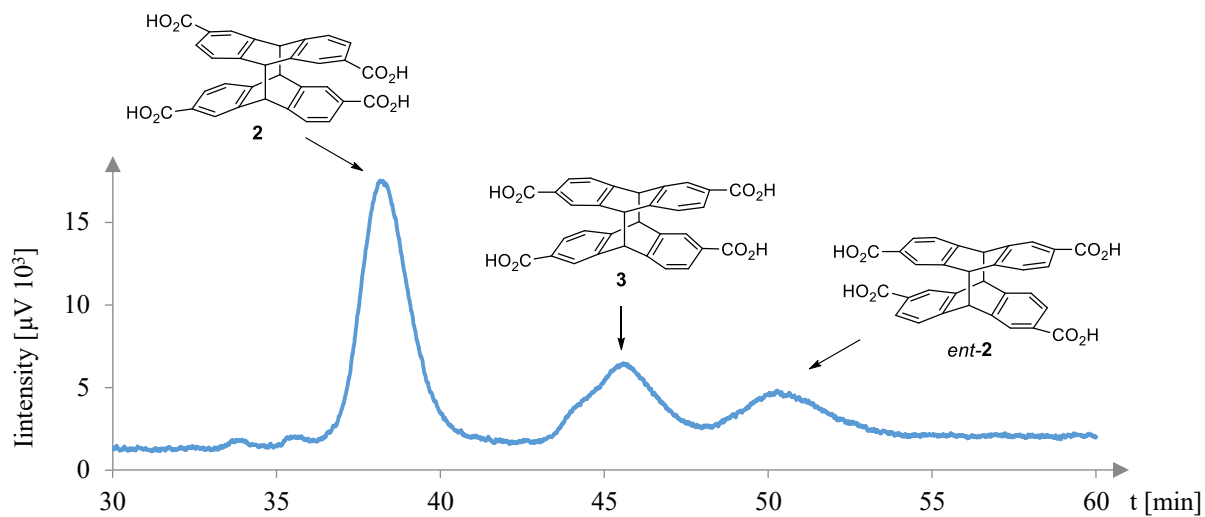


Table 2, Entry 1: $\lambda = 390$ nm, conv. 24%, 7% *ee*.

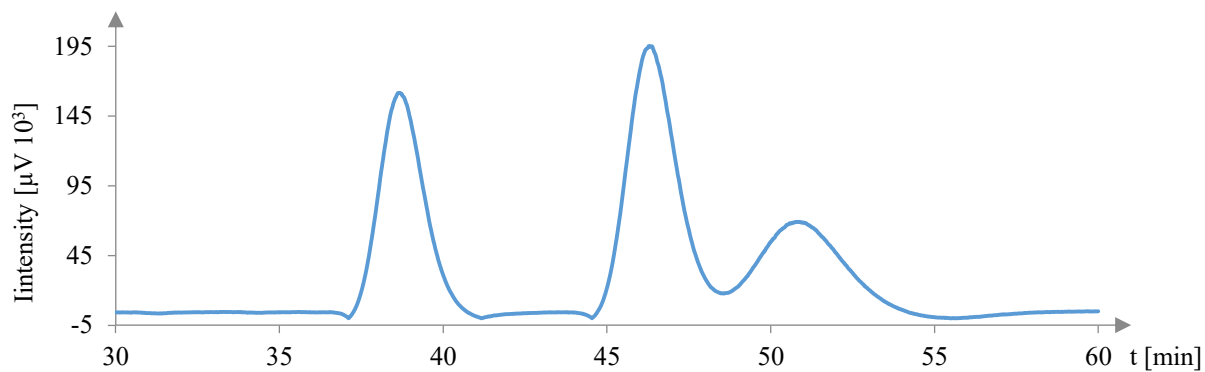


Table 2, Entry 2: $\lambda = 410$ nm, conv. 26%, 6% *ee*.

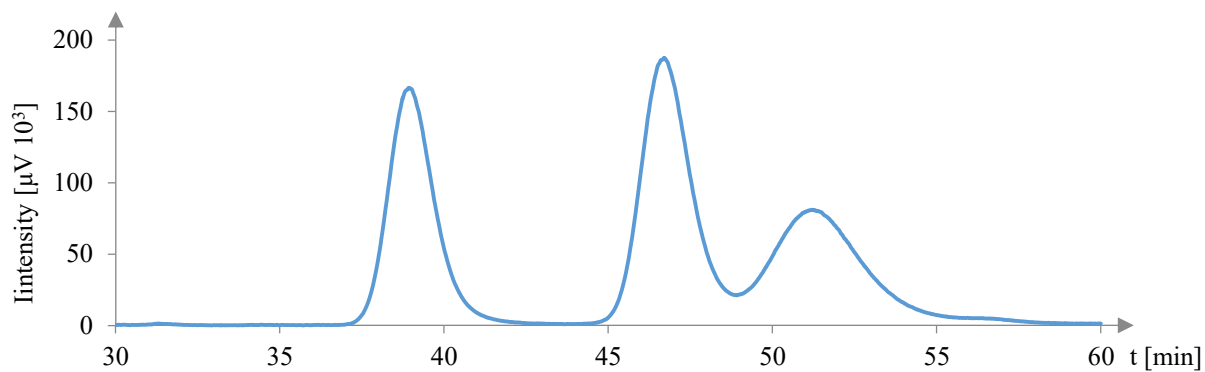
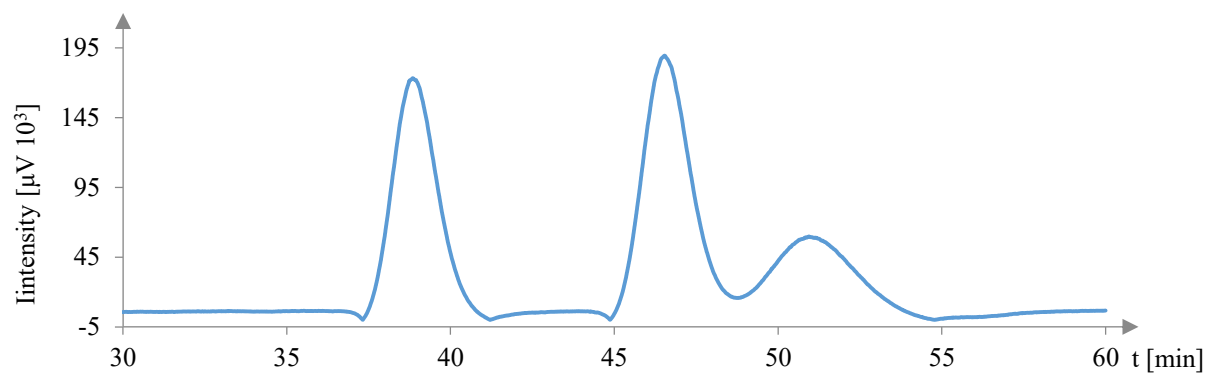
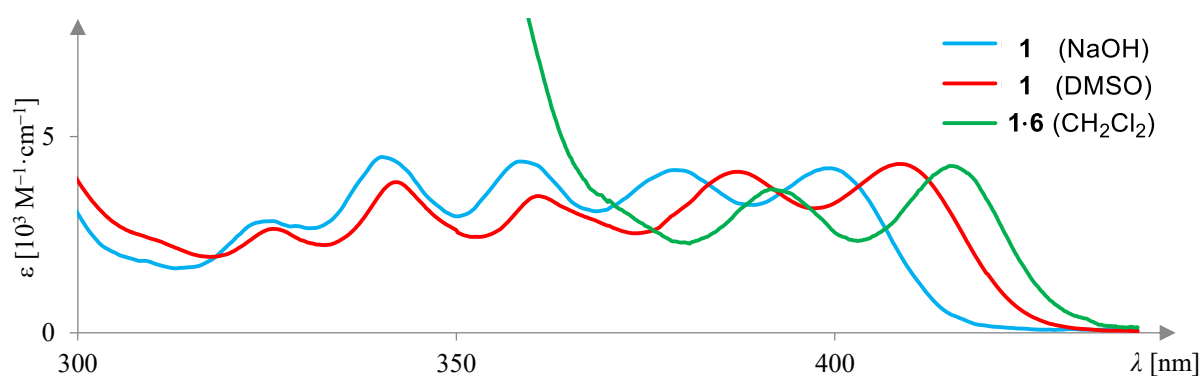


Table 2, Entry 3: $\lambda = 420$ nm, conv. 35%, 16% *ee*.

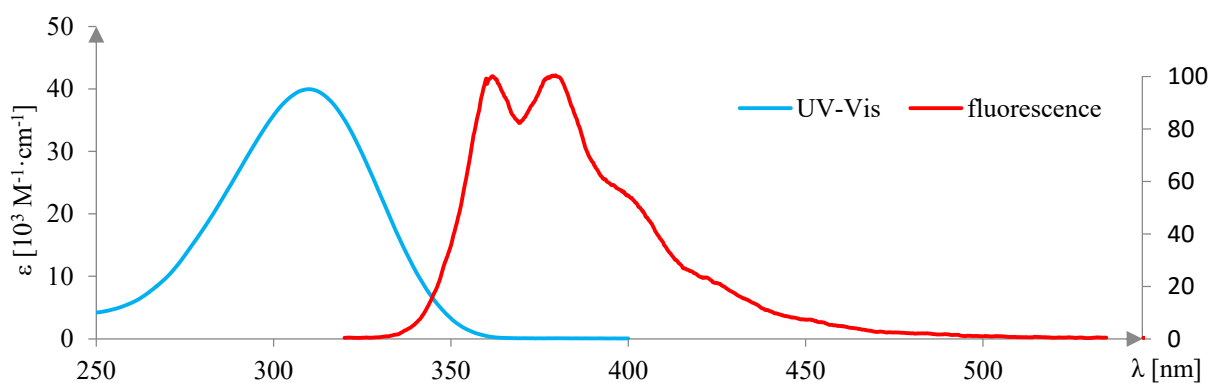


5) UV-Vis and fluorescence spectra

UV-Vis: The molar extinction coefficient ϵ of **1** ($0-0'$ transition of the 1L_b) in the complex **1·6** was estimated at $\epsilon = 4250 \text{ cm}^{-1}\cdot\text{M}^{-1}$ (green), due to the fact, that the same transition of **1** exhibits nearly the same molar extinction coefficient in an alkaline solution (NaOH, $\epsilon = 4190 \text{ cm}^{-1}\cdot\text{M}^{-1}$, blue) as well as in DMSO ($\epsilon = 4300 \text{ cm}^{-1}\cdot\text{M}^{-1}$, red).



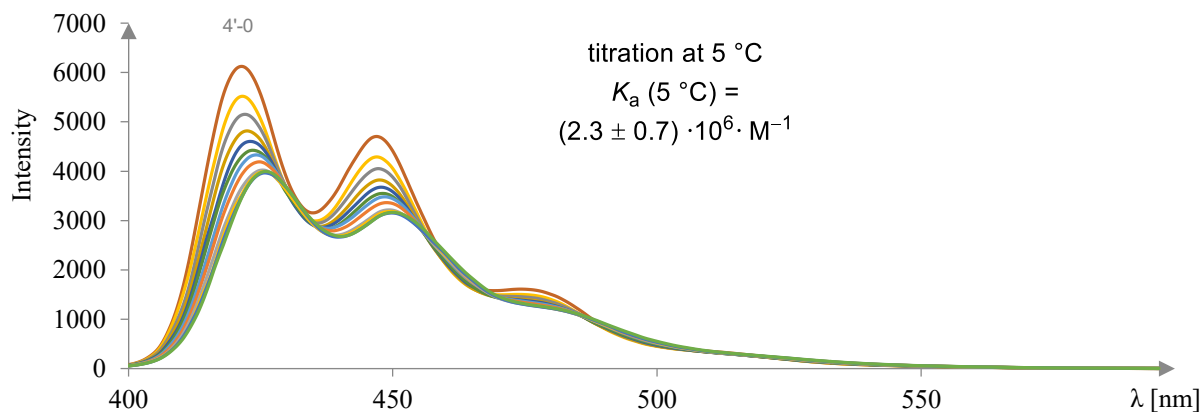
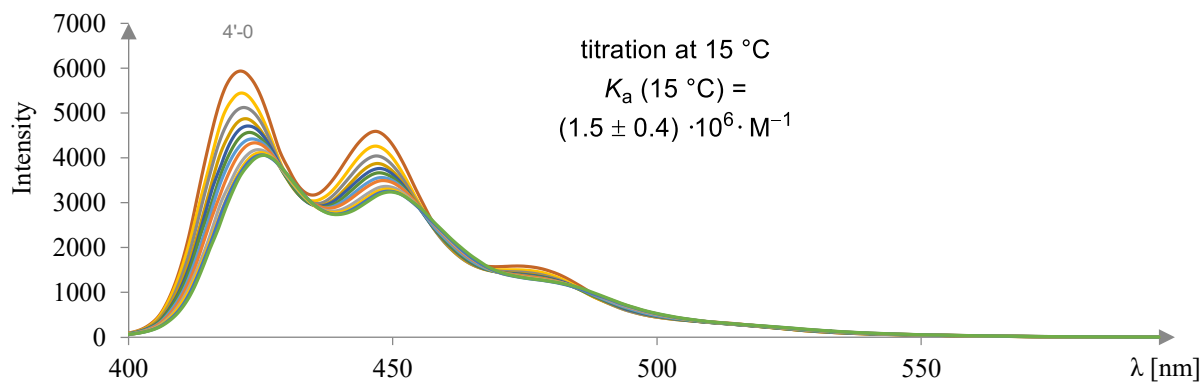
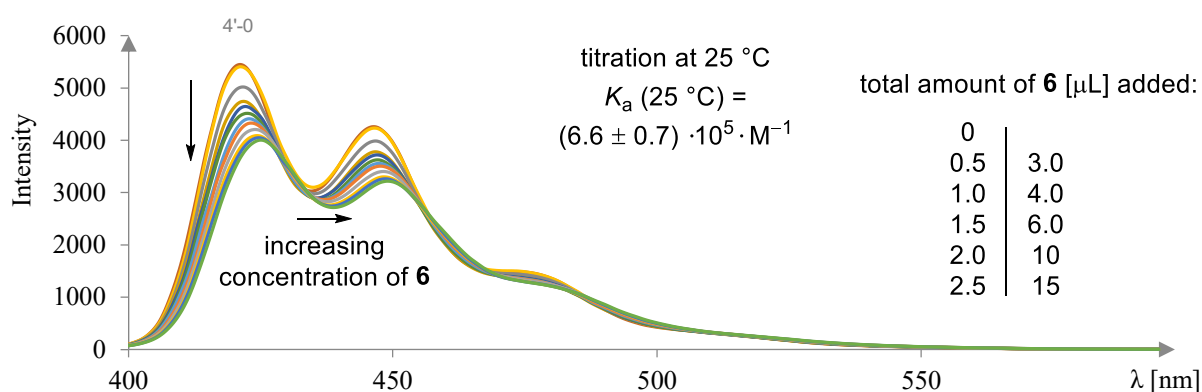
UV-Vis spectrum of the template **6** (blue) and normalized fluorescence spectrum (red) in CH_2Cl_2 .



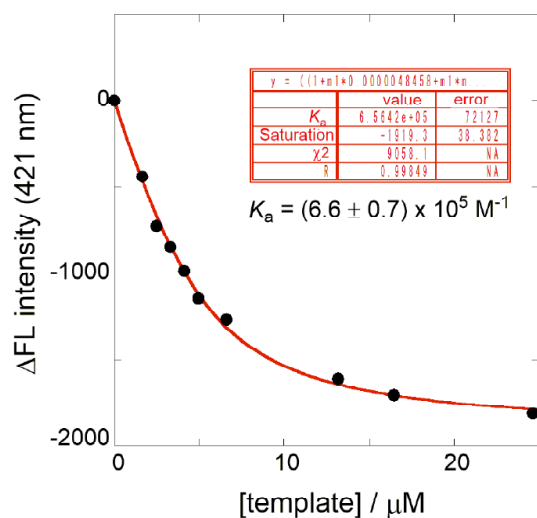
6) Titration experiments, K_a calculations and van't Hoff plot

Fluorescence titration were performed using a stock solution of the template **6** ($c = 4.95 \text{ mM}$, in CH_2Cl_2). The titrant solution was obtained by diluting a concentrated DMSO solution of anthracene dicarboxylic acid **1** with CH_2Cl_2 . The resulting solution of **1** ($V = 3.00 \text{ mL}$, $c = 4.85 \text{ }\mu\text{M}$) had therefore negligible amount of DMSO (approximately 0.02% DMSO v/v). The excitation wavelength was set to $\lambda_{\text{exc.}} = 388 \text{ nm}$ (slit width 2.5 nm) and fluorescence quenching was monitored from 400-600 nm (slit width 5 nm).

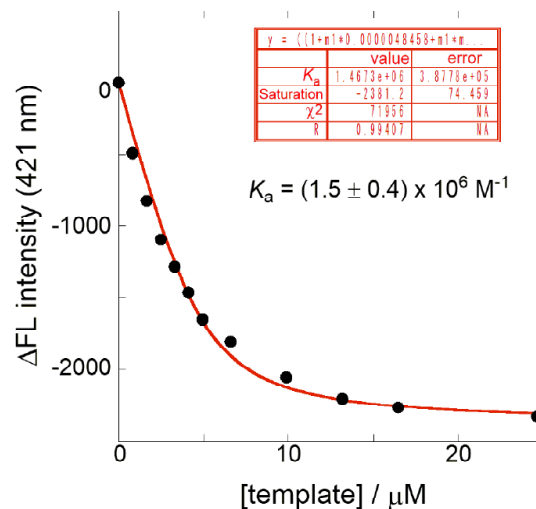
The total amount of stock solution of template **6** added to the titrant solution ranged from 0-15 μL . Therefore the concentration range of **6** was $c = 0\text{-}24.6 \text{ }\mu\text{mol/L}$.



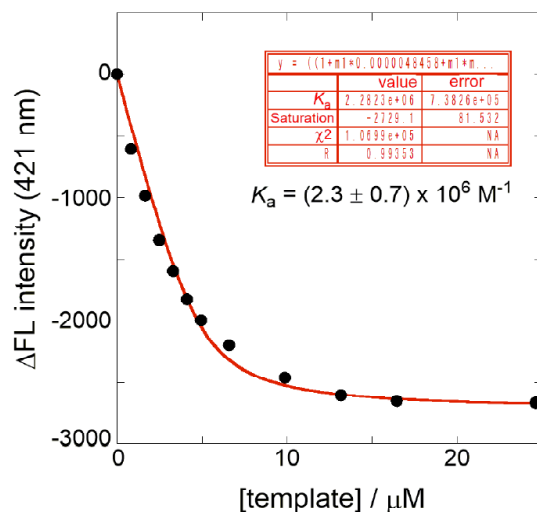
(a) 25 °C



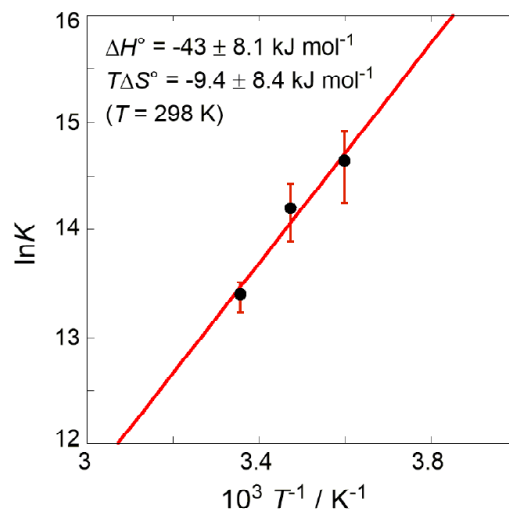
(b) 15 °C



(c) 5 °C



(d) van't Hoff plot



(a) at 25 °C, (b) at 15 °C, and (c) at 5 °C: association constant K_a for the complex **1**·**6** calculated by least-squares-fit analyses of the fluorescence intensity changes of the 4'-0 transition ($\lambda_{\text{em}} = 421 \text{ nm}$) upon addition of template **6** to the above described solution of 2,6-anthracenedicarboxylic acid (**1**) assuming a 1:1 stoichiometry.

(d): van't Hoff plot of the temperature-dependent K_a . The thermodynamic parameters were calculated from the slope and the intercept of the regression line as $\Delta H^\circ = -43 \pm 8 \text{ kJ mol}^{-1}$ and $T\Delta S^\circ = -9 \pm 8 \text{ kJ mol}^{-1}$ ($T = 298 \text{ K}$).

7) Relative energies (ΔE) of the four possible complexes **1·6**

Complex	ΔE (gas phase)	ΔE (in CH ₂ Cl ₂)
1·6-I	0.0018	0.0742
1·6-I'	0.0000	0.0833
1·6-II	0.0486	0.0000
1·6-II'	0.0672	0.0395

Energies were calculated at the DFT-D3-TPSS-BJ/def2-TZVP level in kcal/mol.

8) Atomic coordinates of all four possible complexes 1·6

1·6-I

C	11.074522	0.895970	0.566039	C	33.250583	0.608938	-3.180796
C	11.799022	0.295308	1.774909	H	32.689953	0.100673	-3.974387
C	11.761929	-1.244021	1.661644	H	33.365522	1.661163	-3.463766
C	12.288907	-1.857117	0.337200	H	34.247051	0.156878	-3.128708
H	10.709367	-1.545656	1.756649	C	33.269719	1.912165	1.701192
H	12.302562	-1.693368	2.503179	H	34.297778	1.552338	1.820796
C	11.771143	0.467123	-0.732601	H	33.303553	2.973657	1.434498
H	10.029924	0.556847	0.548146	H	32.742219	1.816509	2.652462
H	11.061779	1.991285	0.639313	C	31.115741	1.566700	0.486748
C	11.702632	-1.072244	-0.865802	C	31.126712	1.103409	-1.977842
H	10.641724	-1.342754	-0.956852	N	30.563509	1.615973	-0.730236
H	12.206669	-1.383072	-1.786320	H	29.551876	1.842159	-0.739383
C	11.092887	1.105600	-1.952762	C	25.002258	1.892013	-0.398440
H	11.607318	0.819232	-2.872344	C	23.586173	1.896341	-0.301653
H	10.048815	0.777265	-2.005852	C	25.789937	2.183196	0.691056
H	11.108875	2.197912	-1.878251	C	25.188220	2.511213	1.943769
C	11.094801	0.687601	3.082516	C	23.825248	2.565029	2.062461
H	10.080882	0.274044	3.112669	C	22.975207	2.260190	0.956624
H	11.641439	0.306238	3.953245	H	23.365855	2.832021	3.011180
H	11.023983	1.777159	3.173921	H	25.479964	1.635072	-1.338818
C	11.812784	-3.328542	0.248463	C	21.580595	2.268902	1.054885
H	10.717564	-3.366361	0.267618	C	20.766081	1.907247	-0.026828
H	12.166791	-3.788328	-0.678691	H	21.113823	2.542030	1.999170
H	12.202070	-3.907687	1.090951	C	21.379187	1.526250	-1.279106
C	13.227923	0.875348	1.810434	C	22.771832	1.536564	-1.383163
N	13.791564	1.159653	0.492185	H	23.239077	1.247600	-2.322028
C	13.236906	0.895681	-0.696001	C	20.535879	1.149936	-2.366897
C	13.753699	-1.863751	0.306264	C	19.348915	1.878574	0.073574
C	14.965551	-1.932551	0.279095	C	19.174267	1.149390	-2.238445
H	14.797007	1.407997	0.461051	H	21.001353	0.862703	-3.306445
C	16.385450	-1.942768	0.247886	C	18.567195	1.513370	-0.998027
C	17.083379	-1.997006	-0.974018	H	18.865957	2.143268	1.009863
C	18.470262	-1.974231	-0.997493	O	16.545500	1.721408	0.254865
C	19.222633	-1.895347	0.187293	O	27.799293	2.041040	-0.582558
C	17.133470	-1.875648	1.439052	C	25.757072	-1.490745	1.254529
C	18.519504	-1.853694	1.404295	H	27.698931	-1.345140	2.163331
H	16.521667	-2.024936	-1.901749	C	25.009703	-1.576377	0.066936
H	16.610815	-1.842477	2.389972	H	25.165889	-1.581810	-2.085826
H	19.070331	-1.821493	2.339549	H	25.244396	-1.510205	2.211355
H	18.980792	-1.971584	-1.955202	C	23.538885	-1.672222	0.097081
C	25.715506	-1.558471	-1.149157	C	20.695364	-1.833060	0.156891
C	27.141595	-1.408907	1.234455	C	22.797862	-1.106548	1.147887
C	27.844043	-1.414147	0.013687	C	22.822934	-2.324068	-0.921685
C	27.100282	-1.479564	-1.180301	C	21.413470	-1.184563	1.175664
C	29.263627	-1.363826	-0.009919	H	23.311870	-0.552599	1.926764
H	27.624251	-1.459238	-2.130729	C	21.436592	-2.402371	-0.892611
C	30.476554	-1.306995	-0.027620	H	23.363284	-2.806801	-1.731086
C	33.277875	1.259694	-0.741142	H	20.920570	-2.942957	-1.680732
C	32.563749	1.099114	0.607831	H	20.874714	-0.689568	1.977342
C	32.559877	-0.394696	1.011346	H	31.177467	1.937112	-2.690501
C	31.941970	-1.354549	-0.039660	H	30.428371	0.362169	-2.385963
H	32.040129	-0.513796	1.967192	O	30.478534	1.890397	1.517724
H	33.606771	-0.692918	1.159668	O	13.880036	1.006919	-1.767220
C	32.530055	0.483369	-1.830186	H	13.218799	1.814447	2.378733
H	33.337021	2.322880	-1.008558	H	13.902775	0.181995	2.328093
H	34.307428	0.886635	-0.654627	C	27.267778	2.128853	0.529901
C	32.501598	-1.010844	-1.445091	O	27.930853	2.177959	1.675880
H	31.946538	-1.580537	-2.199906	H	25.832264	2.726331	2.789018
H	33.540751	-1.367716	-1.471252	H	28.952921	2.091031	1.529566
C	32.355402	-2.805201	0.315539	C	17.087815	1.486384	-0.830553
H	33.448166	-2.889848	0.316777	H	18.533316	0.865876	-3.065206
H	31.977887	-3.077428	1.305315	O	16.434701	1.189398	-1.944602
H	31.945977	-3.508812	-0.415179	H	15.409902	1.156416	-1.794404

1-6-I'

C	11.175741	0.603094	0.718478	C	33.364088	1.488880	-2.964493
C	11.950728	-0.187258	1.778003	H	32.836944	1.135989	-3.858922
C	12.049777	-1.659740	1.326374	H	33.384170	2.584073	-2.989554
C	12.633278	-1.913876	-0.088376	H	34.396235	1.125470	-3.015465
H	11.027855	-2.064115	1.327778	C	33.340657	1.600322	2.086857
H	12.625459	-2.237242	2.059502	H	34.398819	1.318154	2.124047
C	11.905546	0.536236	-0.630036	H	33.273940	2.693222	2.078642
H	10.164870	0.188211	0.606089	H	32.839152	1.235085	2.985396
H	11.066455	1.649289	1.032976	C	31.210046	1.367089	0.811156
C	11.979265	-0.936054	-1.100275	C	31.223166	1.500000	-1.691909
H	10.947784	-1.273690	-1.270551	N	30.644551	1.674672	-0.361192
H	12.509847	-0.988522	-2.056140	H	29.627949	1.870864	-0.319393
C	11.170692	1.365568	-1.691704	C	25.059377	2.047541	0.059290
H	11.707910	1.336706	-2.641899	C	23.642634	1.984179	0.148466
H	10.160628	0.965978	-1.835909	C	25.856104	1.669348	1.115169
H	11.087487	2.411351	-1.377956	C	25.265741	1.198662	2.327426
C	11.216088	-0.155862	3.126498	C	23.905953	1.109679	2.443764
H	10.241755	-0.649899	3.045323	C	23.047134	1.495614	1.371561
H	11.794043	-0.673522	3.901358	H	23.453791	0.741370	3.361259
H	11.051166	0.876166	3.455487	H	25.530342	2.394300	-0.856069
C	12.288656	-3.364130	-0.511869	C	21.655946	1.414922	1.463360
H	11.200918	-3.498099	-0.525737	C	20.827169	1.785397	0.396526
H	12.684125	-3.573832	-1.509829	H	21.202082	1.044810	2.380015
H	12.725330	-4.080878	0.189712	C	21.421616	2.257870	-0.833263
C	13.323283	0.488463	1.965909	C	22.813547	2.357321	-0.918175
N	13.870604	1.082896	0.747905	H	23.267952	2.712783	-1.840851
C	13.329754	1.063512	-0.474999	C	20.560719	2.573070	-1.927724
C	14.094772	-1.798003	-0.086907	C	19.413561	1.687810	0.479522
C	15.309034	-1.792134	-0.099947	C	19.203060	2.428165	-1.825185
H	14.870094	1.356361	0.776739	H	21.008125	2.922397	-2.855194
C	16.729199	-1.762448	-0.118892	C	18.615666	1.991937	-0.598952
C	17.432132	-1.644535	-1.333701	H	18.947314	1.347636	1.399010
C	18.819045	-1.642189	-1.351243	O	16.611386	1.654732	0.645705
C	19.568098	-1.752237	-0.166694	O	27.866897	2.076672	-0.105343
C	17.473372	-1.854987	1.072966	C	26.117440	-1.805607	0.910059
C	18.860476	-1.849337	1.044525	H	28.063648	-1.795492	1.820764
H	16.873574	-1.559336	-2.260109	C	25.364069	-1.699963	-0.271999
H	16.947471	-1.921994	2.020193	H	25.516389	-1.483604	-2.414697
H	19.408879	-1.895530	1.981056	H	25.605815	-1.892846	1.863189
H	19.333689	-1.573997	-2.304790	C	23.890234	-1.731918	-0.246730
C	26.066008	-1.540020	-1.479873	C	21.042046	-1.754787	-0.194442
C	27.503203	-1.743535	0.893314	C	23.134673	-1.069730	-1.229001
C	28.199298	-1.573084	-0.318921	C	23.184203	-2.409333	0.762027
C	27.450938	-1.476335	-1.507845	C	21.748073	-1.081197	-1.204947
C	29.616486	-1.481515	-0.341869	H	23.642539	-0.494075	-1.996219
H	27.972573	-1.353190	-2.451905	C	21.795585	-2.420522	0.787492
C	30.823225	-1.348703	-0.358826	H	23.731576	-2.962997	1.519311
C	33.371612	1.544940	-0.439941	H	21.285172	-2.984269	1.563261
C	32.694197	1.006379	0.827635	H	21.201772	-0.514716	-1.952256
C	32.833762	-0.533462	0.867601	H	31.189626	2.472199	-2.200540
C	32.286183	-1.270235	-0.383094	H	30.582128	0.809920	-2.254917
H	32.343510	-0.922540	1.765514	O	30.561042	1.382791	1.884596
H	33.905946	-0.759693	0.946451	O	13.958178	1.463269	-1.484483
C	32.677293	0.985748	-1.685899	H	13.229770	1.285407	2.715357
H	33.333488	2.642095	-0.446798	H	14.052125	-0.238255	2.345867
H	34.430848	1.254202	-0.438406	C	27.335065	1.740679	0.958584
C	32.785477	-0.554188	-1.665929	O	28.000029	1.411482	2.056339
H	32.267070	-0.976117	-2.535173	H	25.918344	0.907069	3.142172
H	33.850958	-0.800619	-1.775057	H	29.025771	1.446712	1.911979
C	32.830888	-2.720474	-0.381641	C	17.142998	1.837527	-0.455039
H	33.926684	-2.705666	-0.398736	H	18.551843	2.651152	-2.662873
H	32.497860	-3.251655	0.514618	O	16.484991	1.910237	-1.602673
H	32.470137	-3.265095	-1.259118	H	15.469203	1.753207	-1.471066

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C	-11.31065	-0.433305	0.620267	C	-34.17972	-0.138470	-2.864144
C	-11.98788	0.494868	1.634166	H	-33.81511	0.624669	-3.562106
C	-12.23337	1.867794	0.971913	H	-34.23119	-1.093573	-3.398535
C	-12.97991	1.868840	-0.388153	H	-35.19463	0.139682	-2.559861
H	-11.24567	2.313796	0.790081	C	-33.24192	-2.598078	1.449472
H	-12.76020	2.529229	1.670030	H	-34.27040	-2.440672	1.793243
C	-12.20579	-0.608313	-0.614136	H	-33.19777	-3.552801	0.915146
H	-10.34399	-0.012595	0.311871	C	-32.57889	-2.661020	2.314822
H	-11.11056	-1.410030	1.079887	C	-31.37366	-1.651877	0.095111
C	-12.39315	0.762245	-1.303627	C	-31.84497	-0.607048	-2.135075
H	-11.40261	1.095641	-1.642224	N	-31.04065	-1.344076	-1.163683
H	-13.02769	0.644811	-2.187595	H	-30.04006	-1.478656	-1.396317
C	-11.57853	-1.592246	-1.611435	C	-25.23833	-2.087356	0.271319
H	-12.23334	-1.734207	-2.473683	C	-23.82453	-2.039286	0.123350
H	-10.61202	-1.204134	-1.951980	C	-26.07030	-1.815132	-0.790821
H	-11.41369	-2.567928	-1.142501	C	-25.52164	-1.472859	-2.063273
C	-11.08609	0.717147	2.857670	C	-24.16793	-1.403484	-2.238732
H	-10.16105	1.226507	2.566479	C	-23.27202	-1.684022	-1.163725
H	-11.58974	1.335269	3.610464	H	-23.74846	-1.133601	-3.204685
H	-10.81985	-0.238452	3.322855	H	-25.66561	-2.339449	1.236779
C	-12.75691	3.242890	-1.069546	C	-21.88455	-1.626076	-1.313734
H	-11.68514	3.408537	-1.228089	C	-21.01819	-1.891825	-0.245584
H	-13.26742	3.275734	-2.036275	H	-21.46353	-1.359524	-2.280737
H	-13.15146	4.048557	-0.443542	C	-21.56986	-2.223497	1.048049
C	-13.28037	-0.193264	2.113946	C	-22.95814	-2.302557	1.192851
N	-13.94048	-0.997810	1.089141	H	-23.37939	-2.555154	2.163921
C	-13.57691	-1.131977	-0.191359	C	-20.67140	-2.430133	2.138614
C	-14.42731	1.704359	-0.219470	C	-19.60649	-1.826981	-0.394327
C	-15.63917	1.662110	-0.152218	C	-19.31868	-2.318467	1.968063
H	-14.88764	-1.352775	1.315563	H	-21.08662	-2.670972	3.114293
C	-17.05835	1.618388	-0.099022	C	-18.77267	-2.029508	0.681397
C	-17.81567	1.559080	-1.285490	H	-19.18278	-1.596046	-1.365863
C	-19.20185	1.566523	-1.241528	O	-16.55979	-1.889758	1.539184
C	-19.89635	1.630423	-0.020363	O	-28.28991	-1.667959	-1.629629
C	-17.74813	1.654780	1.127997	C	-26.38521	1.643531	1.355088
C	-19.13520	1.661884	1.160889	H	-28.28560	1.550192	2.353110
H	-17.29829	1.499358	-2.237547	C	-25.69096	1.676008	0.132627
H	-17.18118	1.688481	2.052858	H	-25.94796	1.655970	-2.009754
H	-19.63994	1.717990	2.120529	H	-25.82997	1.678452	2.287499
H	-19.76088	1.497232	-2.170298	C	-24.21719	1.687068	0.094674
C	-26.45249	1.667267	-1.048978	C	-21.36957	1.657478	0.019485
C	-27.76944	1.584227	1.399044	C	-23.50991	2.229819	-0.991878
C	-28.52604	1.560523	0.211247	C	-23.46249	1.134386	1.143161
C	-27.83831	1.611908	-1.016012	C	-22.12189	2.214493	-1.029052
C	-29.94136	1.455118	0.264115	H	-24.05510	2.699126	-1.805532
H	-28.40297	1.572978	-1.941721	C	-22.07606	1.121411	1.108615
C	-31.14394	1.300568	0.326799	H	-23.97161	0.661088	1.976593
C	-33.72998	-1.369179	-0.705267	H	-21.53120	0.640633	1.914651
C	-32.82342	-1.441009	0.531525	H	-21.60965	2.673285	-1.870015
C	-32.92952	-0.112290	1.315113	H	-31.92773	-1.225376	-3.038347
C	-32.59317	1.157816	0.488339	H	-31.30098	0.306165	-2.408701
H	-32.28426	-0.153927	2.198207	O	-30.53853	-2.123355	0.903279
H	-33.96820	-0.022256	1.662040	O	-14.32369	-1.681951	-1.035824
C	-33.25999	-0.248705	-1.638717	H	-13.04346	-0.852936	2.958900
H	-33.71788	-2.330664	-1.234976	H	-13.99580	0.558018	2.472407
H	-34.76486	-1.183650	-0.387191	C	-27.55126	-1.856131	-0.655074
C	-33.32155	1.094219	-0.879511	O	-27.98133	-2.104175	0.571761
H	-32.94992	1.902241	-1.520975	H	-26.21228	-1.265805	-2.873517
H	-34.38303	1.301190	-0.684038	H	-29.01516	-2.111369	0.621967
C	-33.10002	2.400943	1.260940	C	-17.29635	-1.925948	0.545389
H	-34.18252	2.326445	1.415530	H	-18.62896	-2.456809	2.793967
H	-32.60730	2.471179	2.234943	O	-16.86848	-1.878712	-0.706344
H	-32.88458	3.314445	0.698924	H	-15.83638	-1.813824	-0.759829

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C	11.178487	0.554232	0.654380	C	33.946767	0.379319	-2.739572
C	11.709137	-0.604594	1.504903	H	33.493006	-0.180950	-3.565790
C	11.741384	-1.885058	0.642829	H	34.156370	1.395827	-3.090581
C	12.485162	-1.795118	-0.715240	H	34.899200	-0.100426	-2.489220
H	10.697403	-2.142932	0.416381	C	33.253833	2.137891	1.948233
H	12.158062	-2.715617	1.225063	H	34.238377	1.774438	2.263379
C	12.091102	0.779473	-0.559375	H	33.362809	3.167948	1.593051
H	10.160735	0.330079	0.307232	H	32.579996	2.142562	2.807499
H	11.124238	1.469990	1.257457	C	31.305902	1.714084	0.448709
C	12.076312	-0.487612	-1.445437	C	31.689759	1.061042	-1.940875
H	11.048503	-0.614646	-1.812562	N	30.966295	1.700858	-0.845228
H	12.725491	-0.336799	-2.313613	H	29.999722	2.015510	-1.048209
C	11.609624	1.976948	-1.390484	C	25.242193	1.982547	0.620091
H	12.277162	2.150062	-2.237107	C	23.831089	1.964658	0.453578
H	10.597404	1.782704	-1.762548	C	26.071162	2.349410	-0.415107
H	11.586124	2.887105	-0.782199	C	25.520032	2.727907	-1.676089
C	10.785640	-0.868121	2.703841	C	24.164787	2.761436	-1.859053
H	9.793678	-1.184491	2.363400	C	23.271454	2.384809	-0.810571
H	11.190841	-1.659334	3.345901	H	23.744156	3.069225	-2.813352
H	10.667983	0.036965	3.310034	H	25.670658	1.684822	1.571140
C	12.065784	-3.003200	-1.589222	C	21.882704	2.381793	-0.971562
H	10.982234	-2.985001	-1.752928	C	21.025461	1.954366	0.051235
H	12.571021	-2.965756	-2.558615	H	21.455310	2.700039	-1.920398
H	12.333820	-3.942636	-1.096876	C	21.587581	1.512258	1.306842
C	13.093139	-0.198245	2.049178	C	22.974009	1.535138	1.474897
N	13.859113	0.661023	1.150003	H	23.402157	1.203362	2.418299
C	13.520256	1.045213	-0.086009	C	20.701992	1.065842	2.333189
C	13.939184	-1.857440	-0.546077	C	19.613549	1.918361	-0.116726
C	15.149080	-1.935631	-0.482658	C	19.348761	1.058665	2.141347
H	14.847223	0.837348	1.406997	H	21.128876	0.731429	3.275406
C	16.568052	-1.946673	-0.424792	C	18.791334	1.485588	0.898670
C	17.328440	-1.796724	-1.600907	H	19.180181	2.234177	-1.060506
C	18.713171	-1.762047	-1.548574	O	16.578402	1.111393	1.682221
C	19.403922	-1.868120	-0.328317	O	28.297117	2.455584	-1.242887
C	17.253535	-2.072662	0.798274	C	25.863377	-1.438331	1.119529
C	18.639639	-2.032435	0.840109	H	27.753401	-1.340577	2.138432
H	16.814343	-1.702485	-2.552012	C	25.180130	-1.428571	-0.109627
H	16.684368	-2.167611	1.717174	H	25.451169	-1.284174	-2.245640
H	19.138794	-2.082317	1.802487	H	25.296986	-1.499899	2.044360
H	19.272455	-1.663328	-2.473943	C	23.712668	-1.554708	-0.167918
C	25.946644	-1.289505	-1.279571	C	20.874573	-1.778320	-0.276071
C	27.245443	-1.340511	1.179456	C	22.973666	-0.965861	-1.207030
C	28.010238	-1.230214	0.001403	C	22.998097	-2.263766	0.813083
C	27.329834	-1.190918	-1.230727	C	21.591811	-1.073486	-1.257463
C	29.428878	-1.184780	0.066900	H	23.485700	-0.371279	-1.956682
H	27.901714	-1.094010	-2.148059	C	21.614933	-2.373533	0.759808
C	30.640338	-1.155731	0.147399	H	23.538648	-2.765791	1.610486
C	33.622098	1.255476	-0.392971	H	21.101816	-2.957816	1.517979
C	32.703279	1.234350	0.836225	H	21.053364	-0.558185	-2.046336
C	32.597253	-0.213957	1.365496	H	31.893664	1.825826	-2.701669
C	32.093659	-1.245682	0.321998	H	31.028973	0.311666	-2.395313
H	31.946508	-0.236701	2.245207	O	30.515253	2.117396	1.334990
H	33.603460	-0.520033	1.683152	O	14.332186	1.629718	-0.842311
C	33.018079	0.406071	-1.516300	H	12.961777	0.341391	2.996095
H	33.763974	2.288212	-0.737405	H	13.691258	-1.094094	2.259937
H	34.610270	0.864521	-0.115120	C	27.549503	2.334988	-0.264121
C	32.853670	-1.045110	-1.015593	O	27.966569	2.184989	0.983159
H	32.378375	-1.655657	-1.792598	H	26.207175	2.996372	-2.471515
H	33.865921	-1.446090	-0.866520	H	28.999983	2.182653	1.047706
C	32.397918	-2.670629	0.850291	C	17.312738	1.437364	0.741406
H	33.476370	-2.784819	1.009063	H	18.665631	0.725426	2.915024
H	31.879879	-2.843979	1.797840	O	16.880050	1.765849	-0.465474
H	32.063557	-3.424341	0.131434	H	15.849168	1.703366	-0.534026