Supporting Information to

Formation of a supramolecular chromophore: a spectroscopic and theoretical study

Andreas Bernet,[a,b] Rodrigo Q. Albuquerque,*[b,c] Marina Behr,[a,b] Sebastian T. Hoffmann,[d] and Hans-Werner Schmidt*[a,b]

Macromolecular Chemistry I,[a] Bayreuth Institute for Macromolecular Research (BIMF),[b] Theoretical Physics IV,[c] Experimental Physics I,[d] University of Bayreuth, Bayreuth 95440, Germany

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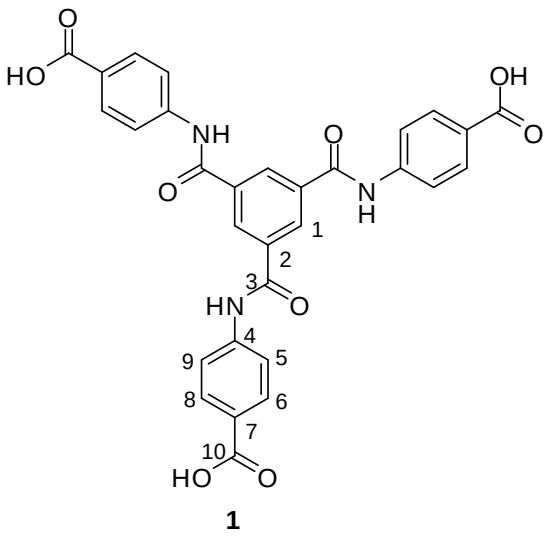
Synthesis of N, N', N''-tris(4-Carboxyphenylene)-1, 3, 5-benzenetricarboxamide 1



1

Figure S1. Chemical structure of trisamide **1**

All chemicals were used as received. Solvents were distilled prior to usage. Water was desalted by a standard ion exchange setup. For UV-Vis absorption measurements, spectroscopic grade solvents were used.

To a mixture of 4.94 g of 4-aminobenzoic acid (36.00 mmol), 5.0 mL of triethylamine (3.64 g, 36.00 mmol) and 100 mL of acetone a solution of 3.19 g of trimesic acid trichloride (12.00 mmol) in 20 mL of acetone was slowly added. After stirring the white suspension for 1 h at room temperature it was poured into 100 mL of ice water under vigorous stirring. After stirring for another hour the white precipitate was filtered and washed with 400 mL of desalted water. Drying at the rotary evaporator at 60 °C for 3 h and under high vacuum (4 x 10^{-3} mbar) over night yielded 6.04 g (10.64 mmol, 89 %) of a slightly hygroscopic white powder. Recrystallization from DMSO/H_2O (2:1) resulted in 5.03 g (8.86 mmol, 74 %) of **1**.

Molecular characterization of 1 (NMR, EA, MS)

Nuclear magnetic resonance spectroscopy

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AC 300 MHz spectrometer at 298 K at 300 and 100 MHz, respectively. All samples were dissolved in DMSO-d_6, which also acted as internal reference.

^{1}H-NMR (300 MHz, DMSO-d_6): δ [ppm] = 12.82 (3 H, br_s, COOH), 10.87 (3 H, s, NH), 8.75 (3 H, s, H-1), 7.98 (12 H, m, H-5, H-6, H-8, H-9).

^{13}C-NMR (100 MHz, DMSO-d_6): δ [ppm] = 167.4 (C-10), 165.2 (C-3), 143.4 (C-4), 135.7 (C-2), 130.8 (C-6, C-8, C-1), 126.4 (C-7), 120.1 (C-5, C-9).

Elemental analysis

To remove traces of DMSO, **1** was rinsed with acetone in a Soxlett apparatus. Elemental analysis (C, H, N) was carried out with an EA 3000 (HEKAtech) at the Department of Chemical Engineering laboratory (Prof. A. Jess) of the University of Bayreuth. The amount of oxygen was calculated assuming that the difference between the measured amounts of carbon, hydrogen and nitrogen and 100 % was the amount of oxygen. For comparison, the theoretical amount of all four elements for compound **1** x 1.5 H_2O was calculated using MDL ISIS^{TM} /Draw 2.5.

Found (Calculated for **1** x 1.5 H_2O): C 60.75 % (60.61 %); H 4.34 % (4.07 %); N 6.96 % (7.07 %); O 28.00 % (28.26 %).

Mass spectroscopy

Mass spectroscopy was carried out on a Finnigan MAT 8500 apparatus (EI, 70 eV) using direct injection mode.

MS, EI^{+}: *m/z* (%)=403 (1), 329 (22), 193 (100), 165 (19), 120 (18), 65 (16).

UV-Vis spectroscopy of 1 and 1Na in solution and of 1 as film from DMSO

*UV-Vis absorption measurements of **1** and **1Na** in solution*

The UV-Vis spectra in solution were recorded using a U-3000 Spectrophotometer (Fa. Hitachi) with a 10 mm quartz glass cuvette (Hellma QS-100).

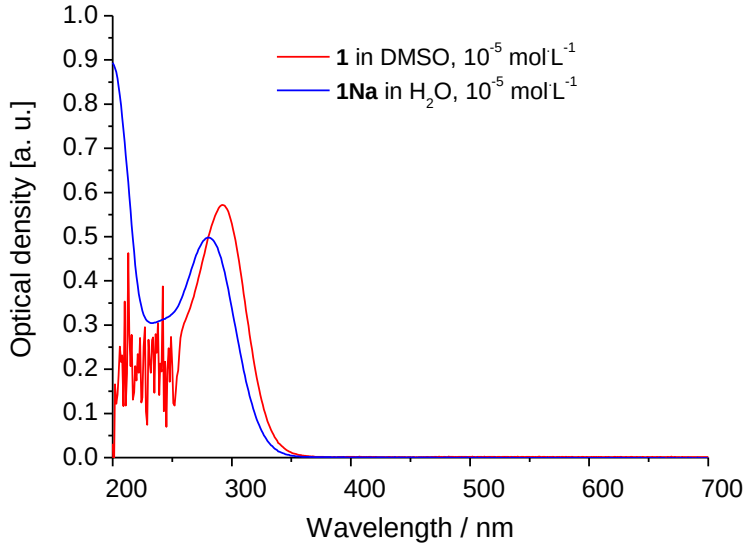


Figure S2. UV-Vis absorption spectra of **1** in DMSO and **1Na** in H_2O (c = 10^{-5} mol·L^{-1})

Note: In agreement to the work of Markovitsi et al., absorption spectra with increasing concentration of **1** in DMSO solution show a slight blue shift.
C. Ecoffet, D. Markovitsi, P. Millié and J.-P. Lemaistre, *Chem. Phys.*, 1993, **177**, 629.

*UV-Vis absorption measurements of **1** in solid state (film)*

A thin film of **1** was drop casted from DMSO solution (40 g·L^{-1} of **1**) onto quartz substrates (Spectrosil B) followed by evaporation of the solvent in an oven at 80 °C for at least 1 h. Films were typically of 150 nm to 200 nm thickness as measured using a Dektak 150 Systems profilometer from Veeco. A Cary5000 UV-Vis-NIR spectrometer was used to take the absorption spectra of the films.

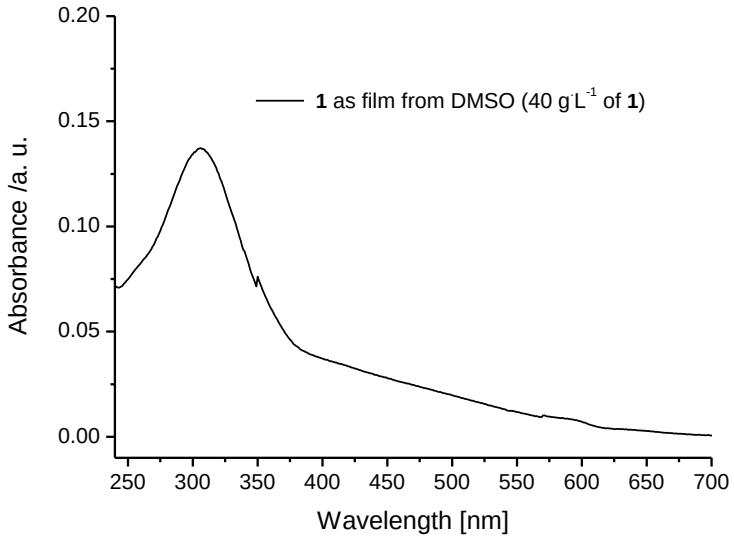


Figure S3. UV-Vis absorption spectrum of **1** in solid state (film casted from 40 g·L^{-1} of **1** in DMSO).

Sample preparation for photoluminescence (PL) investigations of 1 as hydrogel and as film from DMSO

*Preparation of hydrogel samples of **1** for PL investigations*

3.00 g (5.29 mmol) of **1** were dispersed in 25 mL of water. By addition of 0.65 g of NaOH beads in 10 mL of water, **1** was transferred into its water-soluble sodium salt **1Na**. Precipitation by the addition of 200 mL of 2-propanol followed by filtration and drying under reduced pressure (6×10^{-3} mbar) yielded 2.75 g of **1Na** as a white powder (4.34 mmol, 82 %).

Gel samples were prepared by dissolving 30 mg of **1Na** in 3 mL of desalted water (10 $g \cdot L^{-1}$ of **1Na**). This solution was mixed with 4 mol-eq. Glucono-δ-lactone (GdL) (33.7 mg of GdL). Afterwards the solution was immediately filled in a quartz glass cuvette (Hellma 111-QS 10 mm path length) for PL investigations during the gel formation process. The PL spectra during the gel formation were recorded on a Spectrofluorometer RF-5301 (Fa. Shimadzu) at an excitation wavelength of 300 nm.

*Preparation of film samples of **1** for PL investigations*

A thin film of **1** was drop casted from DMSO solution (20 $g \cdot L^{-1}$ of **1**) onto quartz substrates followed by evaporation of the solvent in an oven at 80 °C for 1 h. Films were typically of 1-2 µm thickness as measured using a Dektak 3030 Systems profilometer from Veeco. The PL spectra were recorded on a Spectrofluorometer RF-5301 (Fa. Shimadzu) at an excitation wavelength of 330 nm.

Sample preparation for scanning electron microscopy

*Film of **1** from DMSO solution*

A drop of a solution of **1** (40 $g \cdot L^{-1}$ of **1**) in DMSO was put on top of aluminium plate (diameter approx. 10 mm). The sample was dried in an oven at 100 °C for at least 1 h.

*Dried hydrogels of **1***

A mixture of 30 mg of **1Na**, 33.7 mg of GdL and 3 mL of desalted water was poured in 10 moulds (each 0.3 mL) of an Ambrose Mesa Mold (97 x 38 x 11 mm). After 8 h gel samples were removed, immersed three times with 3 mL of desalted water for at least 24 h to remove the formed sodium gluconate. Afterwards the water was blotted with a piece of paper, the samples were left to dry at room temperature under normal pressure, and dried under high vaccum (6×10^{-3} mbar).

All samples were mounted on a SEM stub using conductive adhesive tape and sputtered with platinum prior to SEM experiments. SEM images were taken using a Zeiss LEO 1530 (FE-SEM with Schottky-field-emission cathode; in-lens detector) operating at an acceleration voltage of 3 kV.

Note: Although a comparatively large amount of GdL is used for the gelation experiments, the resulting gluconic acid sodium salt is not incorporated in the gel fibers, but completely removed by the applied washing steps with water (GdL has a very high water solubility). This was checked by preparing several washed hydrogel samples, which were dried in high vacuum. The absence of the characteristic signals of gluconic acid and / or GdL in the ^{1}H-NMR spectrum (DMSO-d_6) prove that no GdL is incorporated or adsorbed on the fiber surface.

X-Ray investigation of 1 as dried hydrogel and as film from DMSO solution

Dried hydrogel samples and film samples from DMSO solution that were prepared as described for the SEM measurements were powdered and filled into Mark tubes (diameter 1 mm, wall thickness 0.01 mm). XRD analysis was performed on a Huber Guinier-Diffraktometer 6000, equipped with a Huber Quarz-Monochromator 611, a Cu-anode ($CuK_{\alpha 1}$-beam, λ = 154,051 pm, x-ray generator from Seifert Company (Germany)), a Huber SMC 9000 stepping motor controller and a self-developed gate system, primary beam stopper and sample oven. The data was collected from 1-30 ° (2 Theta) with a scan step of 0.02 ° (2 Theta) and a count time of 50 s.

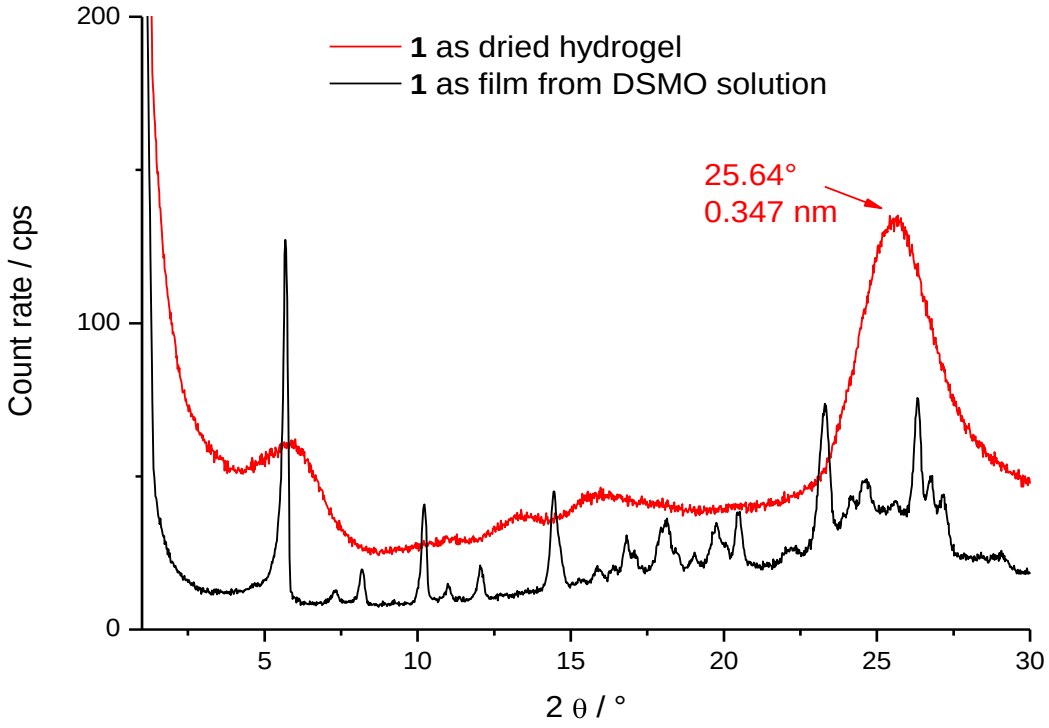


Figure S4. X-Ray powder diffractogram of **1** as dried hydrogel and as film from DMSO solution.

It is clearly visible that the film sample shows a much higher crystallinity and therefore long-range order than the dried hydrogel sample. Note: It was not possible to grow a single crystal of **1**, as it tends to precipitate in very voluminous and sponge-like mesocrystalline aggregates.

FT-IR spectra of 1 as obtained from synthesis and as dried gel

IR spectra were recorded with a Perkin-Elmer Spectrum 100 FT-IR spectrometer in ATR mode. The samples were powdered prior to the measurements.

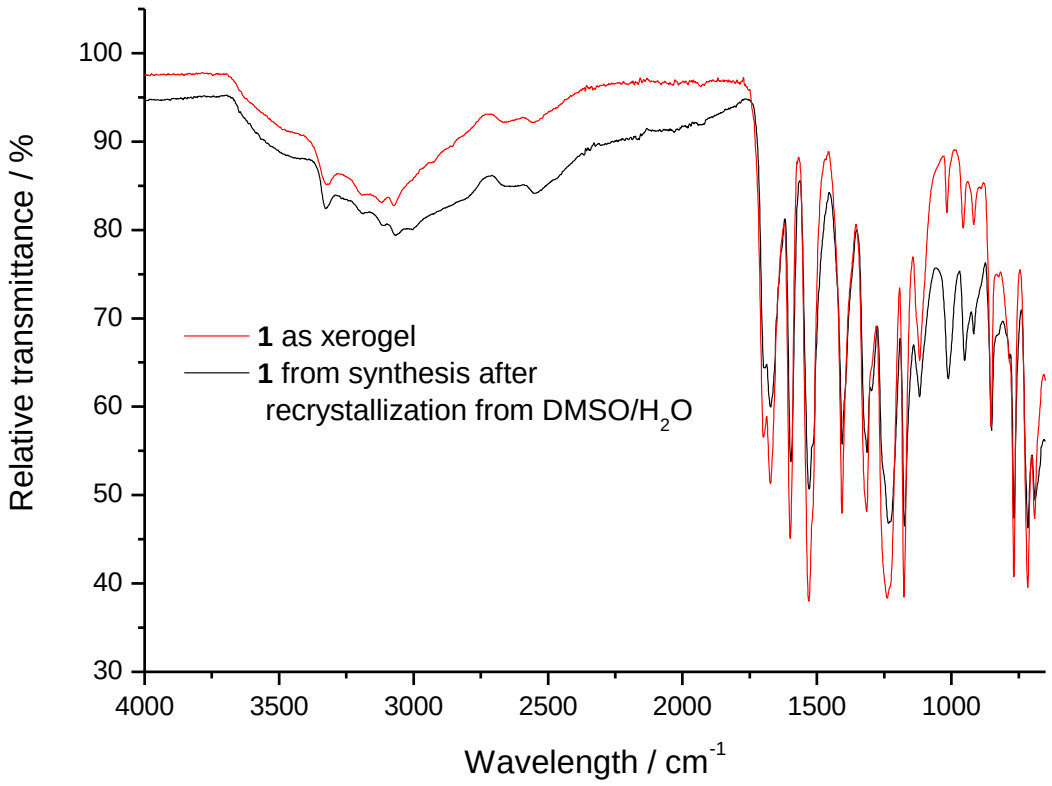


Figure S5. FT-IR spectra of **1** as obtained from synthesis and as dried gel.

Note: The measurement of the IR absorption spectra in the wet gel state is not trivial and substraction mode measurements gave only unsatisfactory results. Substitution of water by D_2O was omitted as it is known that there are huge differences of hydrogen binding strengths in H_2O and in D_2O.

DFT optimized geometries of 1 as monomer, "side-by-side" dimer, "on-top"-dimer, trimer and tetramer

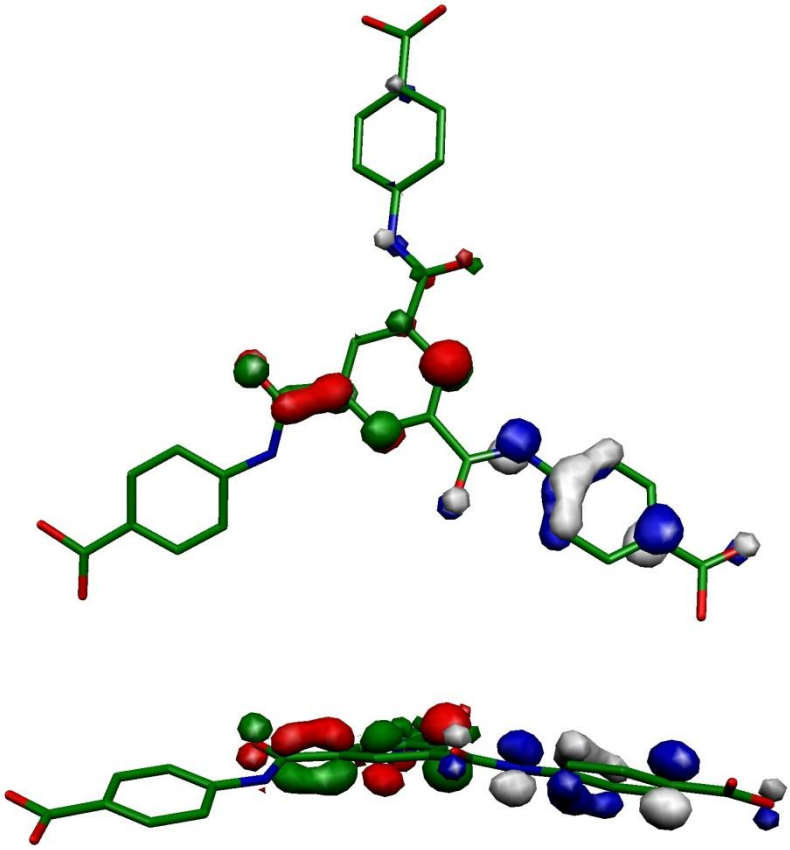


Figure S6. DFT-Optimized geometries and electron densities of the HOMO (blue/white) and LUMO (red/green) orbitals of the monomer of **1** (top and side view). The atom labels are: carbon (green), nitrogen (blue), oxygen (red). The hydrogens are omitted for clarity.

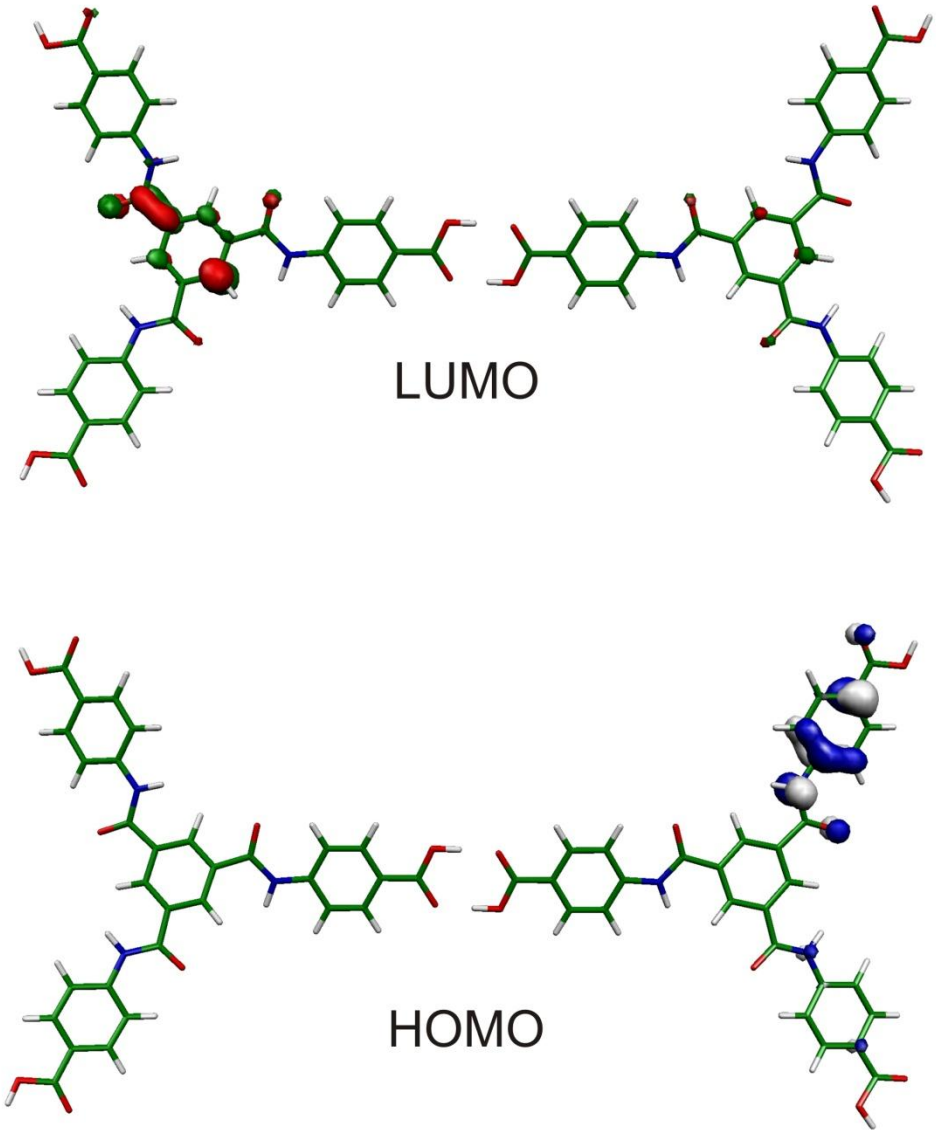


Figure S7. DFT-Optimized geometries and electron densities of the HOMO (blue/white) and LUMO (red/green) orbitals of the "side-by-side" dimer of **1**. The atom labels are: carbon (green), nitrogen (blue), oxygen (red), hydrogen (white).

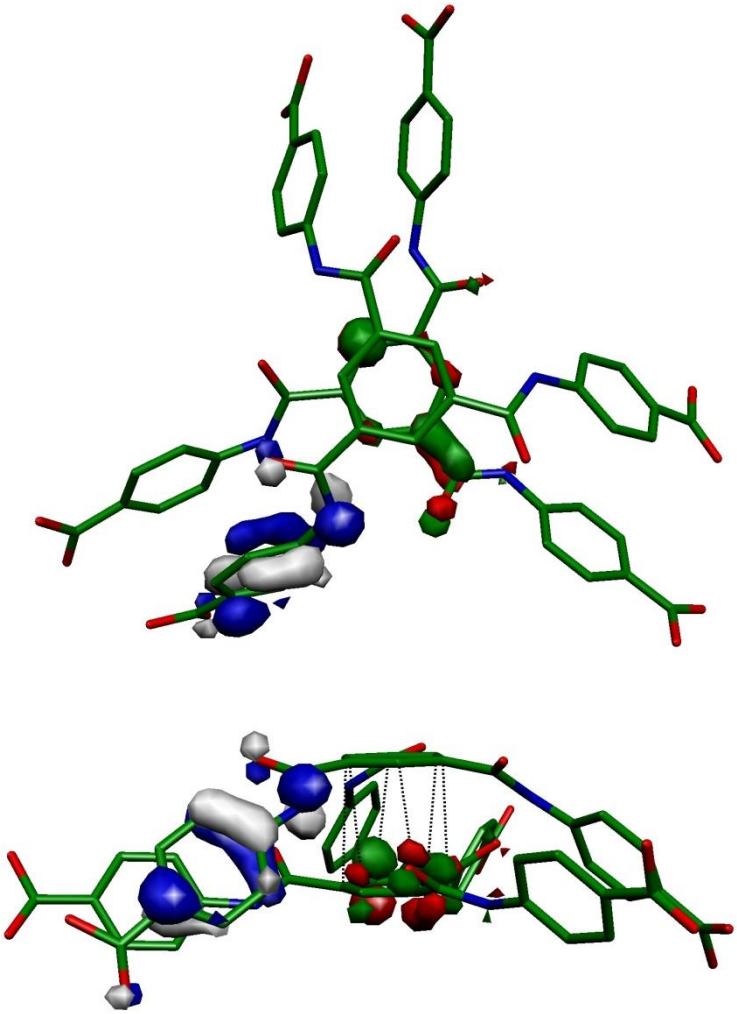


Figure S8. DFT-Optimized geometries and electron densities of the HOMO (blue/white) and LUMO (red/green) orbitals of the "on-top" dimer of **1** (top and side view). The atom labels are: carbon (green), nitrogen (blue), oxygen (red). The hydrogens are omitted for clarity. The black dotted lines represent the stacking of the aromatic cores.

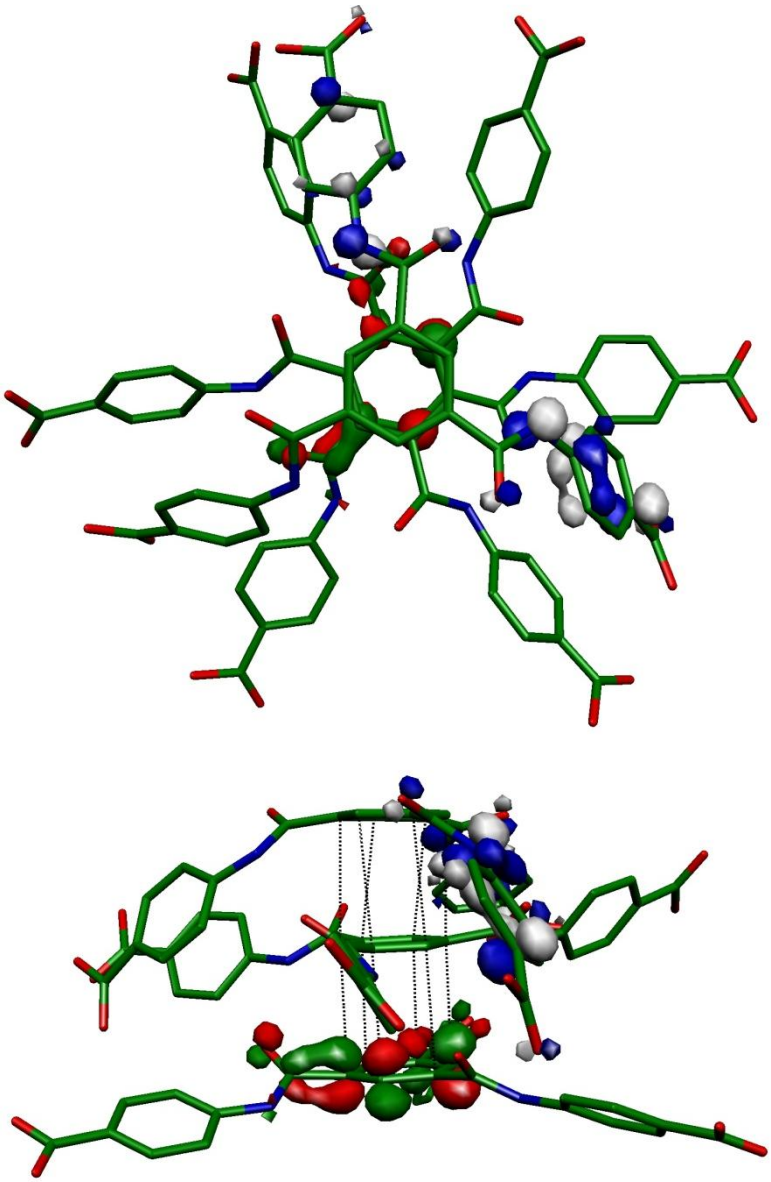


Figure S9. DFT-Optimized geometries and electron densities of the HOMO (blue/white) and LUMO (red/green) orbitals of the trimer of **1** (top and side view). The atom labels are: carbon (green), nitrogen (blue), oxygen (red). The hydrogens are omitted for clarity. The black dotted lines represent the stacking of the aromatic cores.

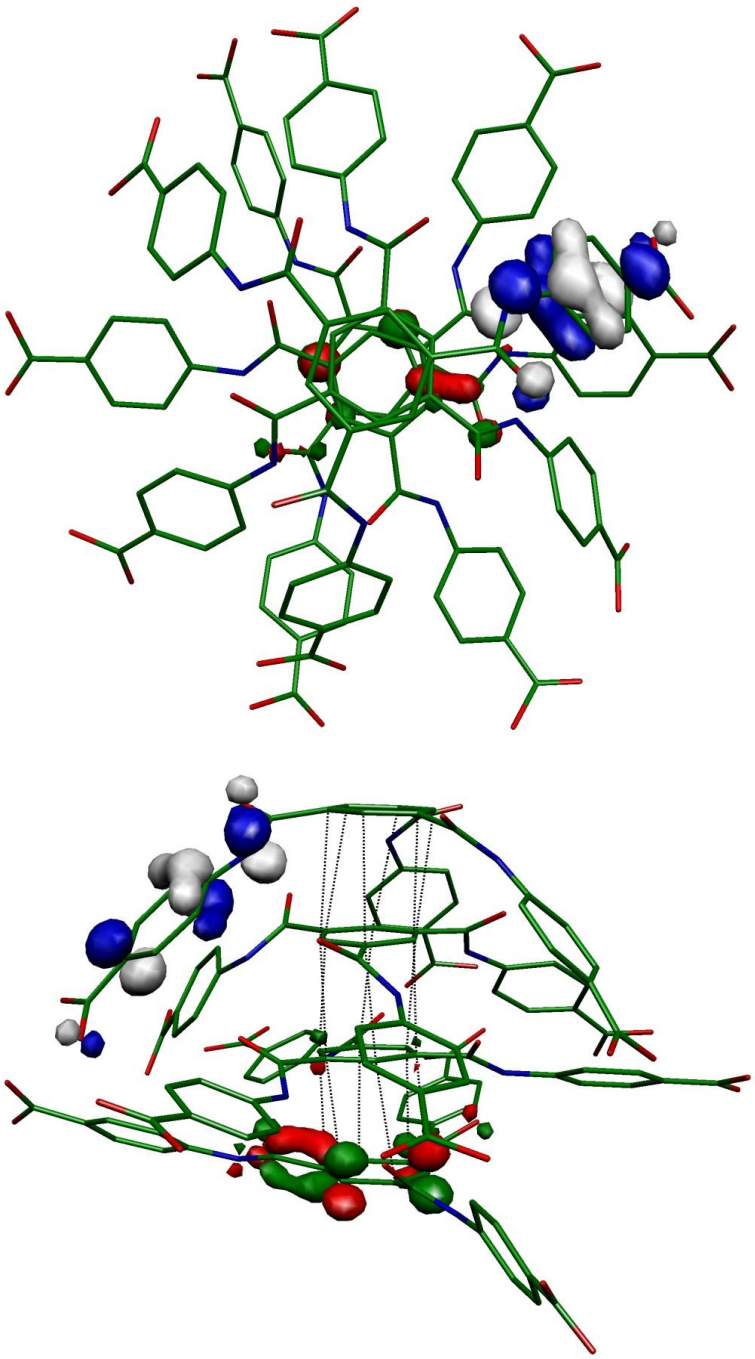


Figure S10. DFT-Optimized geometries and electron densities of the HOMO (blue/white) and LUMO (red/green) orbitals of the tetramer of **1** (top and side view). The atom labels are: carbon (green), nitrogen (blue), oxygen (red). The hydrogens are omitted for clarity. The black dotted lines represent the stacking of the aromatic cores.

Energies of S_1 and T_1 of 1 in different aggregation states

Table S1. Calculated energy values of the lowest excited states of the aggregates of **1**.

n	S_1 energy / eV	T_1 energy / eV
1	3.79	3.02
2[a]	3.67	2.97
2	3.28	2.94
3	2.65	2.63
4	2.45	2.44

[a] This "side-by-side" dimer is held together by double hydrogen bonds between the carboxylic groups, as shown in Fig. S7.

Computational details

The programs Gaussian 03 [1] and Turbomole [2] and was used to carry out the DFT (Density Functional Theory) and TDDFT (Time-Dependent DFT) calculations for the monomer, dimer, trimer and tetramer of **1**, where the three-parameter semi-empirical hybrid functional B3LYP [3], together with the basis set 6-31G** were used for all atoms. No constraints in the geometry optimizations were applied. The reliability of the optimized geometries was checked by calculation of vibrational frequencies. The (ground state) optimized geometries obtained from the DFT calculations were used to compute the energies of the excited states (singlets and triplets) using TDDFT. The xyz coordinates of the optimized structures are shown below:

Monomer (B3LYP/6-31G** - Turbomole)

Atoms	X	Y	Z
C	8.06186	-4.17065	2.55152
C	8.21746	-2.85262	2.08990
C	3.13234	0.43735	3.44155
C	3.72982	1.69797	3.29974
C	5.09084	1.81600	3.01166
C	5.86706	0.65452	2.89044
C	5.28989	-0.60924	3.02846
C	3.92136	-0.70783	3.31751
C	1.65963	0.42824	3.76809
C	-2.98163	-1.93433	4.17457
C	-2.04423	-2.80821	3.60387
C	-0.73507	-2.39687	3.40866
C	-0.33271	-1.09977	3.77869
C	-1.26484	-0.21799	4.35155
C	-2.57648	-0.64395	4.54349
C	-4.36775	-2.42583	4.36035
O	-4.75878	-3.53553	4.05265
O	-5.19032	-1.50101	4.92151
H	-6.06243	-1.93049	4.99480
H	-2.36409	-3.80575	3.32179
H	-0.01052	-3.07909	2.96837
N	1.01538	-0.76838	3.55108
H	-0.95655	0.77797	4.63279
H	-3.29675	0.03534	4.98581
H	1.55665	-1.50348	3.11801
O	1.10400	1.44121	4.17813
H	3.09217	2.56016	3.46824

H	3.52909	-1.70683	3.48029
C	6.04857	-1.90976	2.93318
N	7.27286	-1.83348	2.30950
O	5.56771	-2.94732	3.37496
H	7.17275	-4.44419	3.09994
C	9.05908	-5.10626	2.28908
C	10.21220	-4.75605	1.57286
C	10.35940	-3.43776	1.11621
C	9.37458	-2.49651	1.37192
H	8.94053	-6.12369	2.64498
C	11.29570	-5.72170	1.27132
O	11.05220	-6.96581	1.76081
H	11.82180	-7.50723	1.50587
O	12.30910	-5.45837	0.65257
H	11.25480	-3.17316	0.56368
H	9.49437	-1.47424	1.01855
H	7.51952	-0.94326	1.90022
H	6.93143	0.79535	2.73038
C	5.82205	3.12689	2.85969
N	5.02405	4.22353	2.62546
H	4.03775	4.04780	2.49475
C	5.39868	5.57004	2.46501
O	7.04517	3.17116	2.92683
C	6.72294	6.02868	2.57685
C	4.36554	6.48330	2.18566
C	4.64204	7.83285	2.01750
C	5.96155	8.29762	2.12687
C	6.98648	7.38355	2.40694
H	3.34097	6.12592	2.10315
H	3.83976	8.52962	1.80251
H	7.51669	5.32788	2.78881
H	8.00212	7.75659	2.48936
C	6.32216	9.72547	1.95770
O	7.44881	10.17430	2.04137
O	5.24850	10.51680	1.69172
H	5.60130	11.42120	1.60209

“Side-by-side“ dimer (B3LYP/6-31G** - Gaussian03)

Atoms	X	Y	Z
C	6.212551	-0.200349	-0.160945
C	5.505212	-1.381604	-0.467588
C	4.116428	-1.389349	-0.481424
C	3.403875	-0.213167	-0.186916
C	4.111328	0.961328	0.117369
C	5.504359	0.981465	0.132771
H	6.046115	1.885971	0.362395

H	6.050895	-2.294168	-0.692543
H	3.571621	-2.295100	-0.715874
H	3.552164	1.862043	0.342153
C	1.932876	-0.193374	-0.190653
N	7.622823	-0.286036	-0.163817
C	8.545558	0.703508	0.090574
H	7.985895	-1.196692	-0.406672
O	8.233308	1.895314	0.323438
C	9.990843	0.294533	0.062719
C	10.930898	1.338640	0.053321
C	12.301621	1.064723	0.047732
C	12.735904	-0.271152	0.026660
C	11.813697	-1.321637	0.034033
C	10.439871	-1.029253	0.069984
H	10.530184	2.346214	0.037100
H	9.771598	-1.881659	0.129118
C	12.180322	-2.778871	0.036414
O	11.305923	-3.646761	0.270814
N	13.492541	-3.083101	-0.246551
H	14.099110	-2.312137	-0.487121
H	13.809398	-0.424860	0.025156
C	13.377798	2.112520	0.039550
O	14.559659	1.798350	-0.238270
N	12.989467	3.391808	0.367349
H	12.027639	3.518600	0.649033
C	13.771562	4.568509	0.406885
C	15.142625	4.602633	0.088176
C	15.829785	5.814401	0.151999
C	15.176233	6.998554	0.529770
C	13.806986	6.956820	0.847560
C	13.112397	5.756533	0.786614
H	12.053896	5.732637	1.031600
H	13.307685	7.873882	1.138068
C	15.872817	8.292725	0.607346
H	16.884287	5.846622	-0.091686
H	15.646764	3.692371	-0.197589
C	14.115819	-4.351103	-0.283504
C	13.445316	-5.556537	-0.000673
C	14.147970	-6.759793	-0.057223
C	15.511355	-6.787146	-0.392505
C	16.174375	-5.579493	-0.674491
C	15.485545	-4.375591	-0.620299
H	16.005348	-3.446251	-0.837520
H	17.226674	-5.606780	-0.932516
H	12.396815	-5.537009	0.253460
H	13.637588	-7.689763	0.159653
C	16.281690	-8.039275	-0.461844
O	17.483945	-8.131346	-0.750975

O	15.528738	-9.161104	-0.166000
O	17.212653	8.212522	0.273345
H	17.621036	9.101469	0.342938
O	15.356217	9.371837	0.933087
H	16.094023	-9.960158	-0.227587
O	1.272337	0.851646	0.072714
O	1.348441	-1.361614	-0.492254
H	0.325618	-1.322414	-0.483607
H	-0.302781	0.999236	0.110467
O	-1.325431	1.035555	0.121580
C	-1.907709	-0.133555	-0.176109
O	-1.245753	-1.177280	-0.444405
C	-3.378739	-0.122949	-0.169800
C	-4.103538	1.043152	0.126731
C	-5.497602	1.042322	0.128421
C	-6.187337	-0.148748	-0.170140
C	-5.461783	-1.321647	-0.467552
C	-4.073757	-1.308372	-0.468174
H	-3.509548	-2.204881	-0.695937
H	-5.992841	-2.241710	-0.696625
H	-3.563655	1.953578	0.355530
H	-6.053685	1.940165	0.349908
N	-7.596458	-0.251758	-0.186794
H	-7.947126	-1.167234	-0.430858
C	-8.533325	0.731663	0.039412
O	-8.239092	1.931536	0.253150
C	-9.972220	0.303854	-0.003168
C	-10.403986	-1.022922	0.079938
C	-10.923604	1.331965	-0.108953
H	-10.530912	2.341178	-0.167331
H	-9.722934	-1.858623	0.197753
C	-11.773008	-1.335467	0.034425
C	-12.289577	1.038296	-0.155996
C	-12.705400	-0.302738	-0.100119
C	-12.122549	-2.794420	0.115785
H	-13.772412	-0.475171	-0.191146
C	-13.380752	2.062925	-0.290885
O	-14.558681	1.699591	-0.522364
N	-13.013147	3.379394	-0.130613
H	-12.049700	3.559742	0.112779
C	-13.816928	4.537969	-0.228597
O	-11.224792	-3.662953	0.005882
N	-13.448261	-3.097740	0.328420
H	-14.077936	-2.320315	0.466841
C	-14.060242	-4.368843	0.412503
C	-13.357411	-5.582029	0.276606
C	-15.451461	-4.389299	0.642334
H	-15.994840	-3.453713	0.745362

H	-12.292302	-5.566361	0.104676
C	-15.191029	4.508789	-0.534595
C	-15.899925	5.707116	-0.613817
H	-15.680156	3.561637	-0.701682
C	-13.176655	5.775119	-0.005591
H	-12.116044	5.800085	0.230018
C	-13.892732	6.961526	-0.086243
H	-13.408173	7.916036	0.083465
C	-15.265162	6.939961	-0.392086
H	-16.956601	5.690838	-0.849463
C	-15.984304	8.221848	-0.467806
O	-15.484253	9.341431	-0.283766
O	-17.325378	8.078526	-0.774602
H	-17.748859	8.962352	-0.811513
C	-14.053346	-6.785076	0.371051
C	-15.438893	-6.809659	0.600257
C	-16.134870	-5.595536	0.736098
H	-13.527129	-7.727255	0.268429
C	-16.115731	-8.113322	0.691056
O	-15.570530	-9.220885	0.580990
O	-17.476727	-8.005241	0.920525
H	-17.871583	-8.901502	0.971207
H	-17.202814	-5.608555	0.912718

“On-top“ dimer (B3LYP/6-31G** - Turbomole)

Atoms	X	Y	Z
C	9.30490	2.85230	0.48369
C	8.28938	3.11820	-0.44299
C	3.64223	-0.85643	0.54465
C	2.65323	0.11437	0.72737
C	2.96953	1.46914	0.63306
C	4.28434	1.85714	0.34968
C	5.27954	0.89555	0.17444
C	4.94765	-0.46134	0.26025
C	3.30967	-2.28183	0.87055
C	4.43327	-7.36570	0.52478
C	4.65897	-6.71526	-0.69497
C	4.49299	-5.34336	-0.79013
C	4.09253	-4.60471	0.33234
C	3.83315	-5.24347	1.55147
C	4.00534	-6.62298	1.63712
C	4.72771	-8.81647	0.59135
O	5.24495	-9.46390	-0.30370
O	4.37625	-9.38056	1.77128
H	4.63427	-10.31900	1.71111

H	5.00075	-7.28870	-1.54854
H	4.70201	-4.83449	-1.72727
N	4.04563	-3.20226	0.18242
H	3.55381	-4.65873	2.41773
H	3.83825	-7.12527	2.58337
H	4.62457	-2.84567	-0.56640
O	2.45243	-2.55351	1.71557
H	1.66004	-0.20244	1.02078
H	5.74172	-1.19369	0.18814
C	6.73866	1.24140	0.11956
N	7.03400	2.46906	-0.39245
O	7.58071	0.44675	0.55190
H	9.15221	2.11295	1.25599
C	10.48620	3.58488	0.41793
C	10.66440	4.57695	-0.55803
C	9.63735	4.83856	-1.47575
C	8.45835	4.10853	-1.42047
H	11.27460	3.39433	1.13720
C	11.91240	5.37507	-0.66637
O	12.80360	5.10178	0.32286
H	13.57500	5.67255	0.15069
O	12.14200	6.18988	-1.53726
H	9.77334	5.63160	-2.20233
H	7.65015	4.32056	-2.11598
H	6.27445	2.98385	-0.81868
H	4.52119	2.91421	0.34972
C	1.98549	2.52422	1.04160
N	0.68395	2.21859	0.76596
H	0.52686	1.40304	0.18884
C	-0.49383	2.89610	1.14788
O	2.36072	3.55548	1.60570
C	-0.57062	3.68450	2.30362
C	-1.62865	2.68233	0.35314
C	-2.84866	3.23493	0.71440
C	-2.94683	4.00142	1.88294
C	-1.80018	4.22900	2.65980
H	-1.55774	2.05924	-0.53448
H	-3.72652	3.04354	0.10946
H	0.30389	3.81732	2.92620
H	-1.89716	4.81828	3.56554
C	-4.23768	4.55139	2.35956
O	-4.37982	5.24178	3.34821
O	-5.29807	4.20266	1.57239
H	-6.07136	4.64116	1.97360
C	7.21146	-4.46825	2.20293
C	7.27919	-3.18918	1.63052
C	3.33723	0.62839	3.99574
C	4.05339	1.81908	3.82605

C	5.41074	1.78395	3.50658
C	6.06967	0.55156	3.41143
C	5.36059	-0.63701	3.58397
C	3.99611	-0.59561	3.89558
C	1.85022	0.77296	4.10472
C	-2.81397	0.19808	2.18181
C	-1.93143	-0.69275	1.55198
C	-0.65512	-0.89498	2.06285
C	-0.23191	-0.17586	3.19875
C	-1.13745	0.65640	3.87438
C	-2.41665	0.83641	3.36301
C	-4.08868	0.53569	1.50910
O	-4.38440	0.20807	0.37446
O	-4.89074	1.32090	2.27081
H	-5.61320	1.63390	1.69683
H	-2.25665	-1.19796	0.64800
H	0.03209	-1.59257	1.58931
N	1.12007	-0.28059	3.57881
H	-0.82173	1.18971	4.75767
H	-3.09875	1.51536	3.85996
H	1.63816	-1.01955	3.10719
O	1.34622	1.80717	4.52834
H	3.50454	2.75114	3.89933
H	3.47173	-1.53832	4.00380
C	5.91384	-1.99818	3.28940
N	6.92778	-2.02795	2.34742
O	5.40534	-3.00150	3.77812
H	6.95228	-4.57793	3.24470
C	7.41575	-5.58805	1.40632
C	7.69138	-5.45785	0.03984
C	7.83640	-4.17558	-0.51087
C	7.64885	-3.04645	0.27816
H	7.31524	-6.57618	1.83826
C	7.68554	-6.63289	-0.86477
O	7.63237	-7.80508	-0.18996
H	7.38371	-8.50751	-0.82002
O	7.65916	-6.56782	-2.08020
H	8.06803	-4.08532	-1.56751
H	7.76840	-2.04834	-0.13701
H	7.16089	-1.15179	1.88143
H	7.12078	0.55426	3.14675
C	6.19221	2.98511	3.06282
N	5.42789	3.98247	2.48211
H	4.43149	3.80203	2.38118
C	5.91305	4.98839	1.62751
O	7.41676	3.00399	3.11415
C	7.23706	5.45965	1.66459
C	5.01410	5.49819	0.66867

C	5.44814	6.42244	-0.27477
C	6.78293	6.85536	-0.27474
C	7.65685	6.37934	0.71254
H	3.98070	5.16099	0.67780
H	4.75780	6.80269	-1.01984
H	7.92488	5.07456	2.40141
H	8.68525	6.72224	0.70199
C	7.32895	7.76061	-1.31062
O	8.50098	8.06764	-1.41828
O	6.38306	8.21644	-2.17585
H	6.85620	8.78895	-2.80759

Trimer (B3LYP/6-31G** - Turbomole)

Atoms	X	Y	Z
C	9.56323	1.97961	-0.97468
C	8.35503	2.66265	-1.17265
C	3.65950	-0.91940	0.59735
C	2.70122	0.09039	0.76143
C	3.06678	1.43018	0.63990
C	4.39597	1.76885	0.35406
C	5.35095	0.76914	0.17760
C	4.97978	-0.57549	0.31150
C	3.23898	-2.32995	0.88572
C	3.55356	-7.49147	0.21261
C	4.57710	-6.84400	-0.49505
C	4.65683	-5.45931	-0.49295
C	3.71023	-4.69997	0.21564
C	2.67568	-5.33728	0.91535
C	2.60980	-6.72977	0.91365
C	3.52325	-8.97708	0.18113
O	4.31528	-9.67033	-0.42723
O	2.50785	-9.50051	0.90997
H	2.58262	-10.46870	0.82273
H	5.30223	-7.44475	-1.03361
H	5.45861	-4.95818	-1.03173
N	3.86237	-3.29264	0.15470
H	1.93733	-4.77443	1.46588
H	1.81204	-7.20670	1.47061
H	4.52991	-2.96902	-0.53353
O	2.37563	-2.55735	1.73842
H	1.69512	-0.18669	1.06094
H	5.75741	-1.33177	0.26229

C	6.80860	1.06299	-0.01627
N	7.09276	2.14245	-0.79294
O	7.66032	0.33451	0.50117
H	9.59251	1.01477	-0.49178
C	10.75570	2.57037	-1.38971
C	10.75490	3.82495	-2.01287
C	9.53950	4.49456	-2.21823
C	8.34833	3.91995	-1.79998
H	11.68200	2.03683	-1.21222
C	11.99970	4.49326	-2.47464
O	13.11570	3.77180	-2.21052
H	13.86470	4.29715	-2.54783
O	12.03640	5.57257	-3.03291
H	9.55232	5.46602	-2.70079
H	7.40710	4.44564	-1.94824
H	6.29776	2.63969	-1.17355
H	4.67501	2.81851	0.34881
C	2.11571	2.54431	0.94827
N	0.83384	2.36195	0.51535
H	0.67698	1.57539	-0.10215
C	-0.22743	3.29565	0.60738
O	2.50003	3.54936	1.54975
C	-0.31615	4.21683	1.65936
C	-1.20962	3.26641	-0.39438
C	-2.25981	4.17774	-0.37043
C	-2.33457	5.12938	0.65811
C	-1.36612	5.12671	1.67017
H	-1.13641	2.54066	-1.20132
H	-3.01167	4.16237	-1.15129
H	0.41456	4.22455	2.45586
H	-1.45722	5.83678	2.48016
C	-3.40094	6.16184	0.71729
O	-3.46465	7.05944	1.53814
O	-4.32724	6.02119	-0.26150
H	-4.96691	6.74702	-0.13837
C	9.25626	-3.06575	3.69479
C	8.74986	-2.27142	2.65534
C	3.33911	0.32991	4.04778
C	3.78545	1.64431	3.88859
C	5.12495	1.90402	3.59618
C	6.02268	0.84044	3.46082
C	5.58479	-0.47214	3.63152
C	4.24104	-0.72675	3.92255
C	1.93042	0.09729	4.50322
C	-2.06470	-3.21379	5.05930
C	-1.43760	-3.39438	3.81938
C	-0.33079	-2.63659	3.47911
C	0.17077	-1.67939	4.37785

C	-0.46888	-1.45967	5.60656
C	-1.58156	-2.22997	5.93714
C	-3.17059	-4.13309	5.40599
O	-3.51096	-5.09765	4.73916
O	-3.78766	-3.81825	6.57022
H	-4.47051	-4.50057	6.70770
H	-1.80549	-4.16026	3.14622
H	0.17984	-2.80759	2.53878
N	1.36979	-1.04186	4.00555
H	-0.06659	-0.73536	6.30210
H	-2.06109	-2.09053	6.89978
H	1.87436	-1.51536	3.25416
O	1.37350	0.88960	5.27138
H	3.08653	2.45686	4.03964
H	3.91533	-1.74711	4.08523
C	6.56035	-1.60767	3.67632
N	7.56958	-1.51048	2.76348
O	6.42277	-2.51878	4.49987
H	8.70462	-3.15781	4.62055
C	10.49220	-3.68780	3.53170
C	11.22710	-3.53267	2.34550
C	10.68850	-2.77027	1.30058
C	9.46385	-2.14397	1.45113
H	10.90520	-4.27688	4.34321
C	12.58820	-4.08129	2.16115
O	12.97690	-4.90658	3.16211
H	13.88830	-5.18013	2.94942
O	13.32120	-3.82621	1.21809
H	11.25880	-2.64369	0.38757
H	9.07148	-1.51774	0.65889
H	7.48673	-0.77549	2.05889
H	7.06860	1.04841	3.26763
C	5.66587	3.30038	3.61651
N	4.79140	4.25244	3.19039
H	3.96306	3.91729	2.69744
C	4.81844	5.64514	3.40542
O	6.81038	3.52049	4.03484
C	5.75517	6.27640	4.23792
C	3.78469	6.38721	2.80964
C	3.66180	7.74495	3.06946
C	4.57992	8.38195	3.91783
C	5.62408	7.63774	4.48591
H	3.05464	5.88058	2.18564
H	2.83615	8.30699	2.64761
H	6.54176	5.70022	4.70201
H	6.32273	8.14504	5.14286
C	4.47530	9.81991	4.26585
O	5.26266	10.42770	4.96518

O	3.37826	10.41230	3.72702
H	3.39162	11.33740	4.03370
C	11.46820	-0.23632	3.80910
H	12.17210	-1.03746	3.99867
C	10.56050	0.12166	4.79797
H	10.55410	-0.38622	5.74945
C	9.59900	1.11209	4.52991
N	8.54734	1.42194	5.40927
C	8.06060	0.57549	6.38778
O	8.66274	-0.40206	6.81722
C	6.64375	0.84471	6.79817
C	6.03937	2.10218	6.77181
C	4.66130	2.22473	6.99030
C	4.05115	3.57147	6.72376
O	4.71518	4.60061	6.79039
N	2.73480	3.52090	6.31248
C	1.92051	4.57535	5.86983
C	2.32895	5.92027	5.81505
H	3.32666	6.19315	6.12511
C	1.44907	6.87740	5.32011
H	1.76420	7.91181	5.23529
C	0.15821	6.53345	4.89736
C	-0.70512	7.58528	4.30847
O	-0.33783	8.70296	4.00342
O	-1.97524	7.14478	4.09593
H	-2.43464	7.77615	3.51024
C	-0.24901	5.19038	4.97558
H	-1.24513	4.90943	4.65401
C	0.62463	4.21938	5.44288
H	0.31997	3.17687	5.48247
H	2.32801	2.59950	6.16456
C	3.90822	1.08875	7.29022
H	2.84094	1.13704	7.47052
C	4.50603	-0.17621	7.29391
C	3.56512	-1.33837	7.37760
O	2.48656	-1.23911	7.95132
N	3.95639	-2.45277	6.65255
C	3.07698	-3.45250	6.19858
C	1.86582	-3.75067	6.84498
H	1.61634	-3.25787	7.77132
C	0.96795	-4.62482	6.24578
H	0.01054	-4.80899	6.71710
C	1.25293	-5.21671	5.00827
C	0.21298	-5.94786	4.25318
O	-0.85851	-6.26091	5.01444
H	-1.60092	-6.50159	4.42872
O	0.26316	-6.19501	3.05743
C	2.50167	-4.98364	4.41273

H	2.73626	-5.46094	3.46960
C	3.41486	-4.12400	5.00648
H	4.37964	-3.93358	4.54342
H	4.81617	-2.37584	6.11266
H	6.59920	2.99834	6.53007
C	5.87544	-0.29465	7.06710
H	6.37079	-1.25957	7.04978
H	7.91705	2.14842	5.06689
C	9.62706	1.79313	3.29585
C	10.53450	1.41802	2.31633
H	10.53070	1.91160	1.35321
H	8.91055	2.58888	3.11179
C	11.44610	0.37786	2.54978
C	12.25040	-0.14700	1.42603
O	13.22080	-0.99459	1.83202
H	13.53960	-1.50208	1.06147
O	12.03920	0.09249	0.24596

Tetramer (B3LYP/6-31G** - Turbomole)

Atoms	X	Y	Z
C	9.14006	2.88247	0.11857
C	8.00369	3.42983	0.73277
C	3.66026	-0.96071	1.19812
C	2.57170	-0.10974	1.44182
C	2.74635	1.27355	1.35660
C	3.99808	1.80807	1.02305
C	5.09097	0.97490	0.80229
C	4.89984	-0.40849	0.87475
C	3.57244	-2.41533	1.57137
C	6.16268	-6.88882	2.10039
C	6.89240	-5.95260	1.35573
C	6.30260	-4.75688	0.98171
C	4.97435	-4.48307	1.34576
C	4.22902	-5.41713	2.07344
C	4.83112	-6.62020	2.44488
C	6.86341	-8.13201	2.49259
O	7.89266	-8.54673	2.01343
O	6.21410	-8.81465	3.49746
H	6.74853	-9.61364	3.66690
H	7.92722	-6.16252	1.11160
H	6.88272	-4.01091	0.44414
N	4.46748	-3.22452	0.93611
H	3.20561	-5.20670	2.35156
H	4.24613	-7.35116	2.99434
H	5.00210	-2.79509	0.19325

O	2.79655	-2.80168	2.45126
H	1.63674	-0.53590	1.79297
H	5.78239	-1.02906	0.78418
C	6.52130	1.43058	0.68498
N	6.75111	2.77187	0.75967
O	7.42465	0.59375	0.58146
H	9.09784	1.90555	-0.34039
C	10.33200	3.60138	0.13323
C	10.40470	4.85239	0.76314
C	9.25605	5.40409	1.35002
C	8.06120	4.69958	1.32537
H	11.21880	3.17057	-0.31891
C	11.67350	5.60649	0.86051
O	12.63200	5.16254	0.02585
H	13.42790	5.69920	0.20094
O	11.86960	6.54909	1.61736
H	9.29924	6.37334	1.83427
H	7.17673	5.12512	1.78733
H	5.98168	3.36601	1.03987
H	4.08308	2.88844	1.01458
C	1.72476	2.26670	1.82289
N	0.42675	1.98670	1.51503
H	0.28186	1.19866	0.89592
C	-0.69512	2.83399	1.69054
O	2.09311	3.26953	2.44320
C	-0.74091	3.83289	2.67310
C	-1.78038	2.64878	0.81913
C	-2.88753	3.48595	0.89225
C	-2.91752	4.52356	1.83673
C	-1.84761	4.67343	2.72827
H	-1.74213	1.86227	0.06842
H	-3.71771	3.35079	0.20827
H	0.06842	3.95609	3.37788
H	-1.89862	5.45488	3.47503
C	-4.03674	5.49763	1.91638
O	-4.05242	6.49280	2.61675
O	-5.07291	5.17738	1.10205
H	-5.73758	5.88149	1.21847
C	8.88468	-3.67245	2.92947
C	8.66862	-2.40428	2.36767
C	3.57499	0.23686	4.53805
C	4.00747	1.55291	4.37909
C	5.31934	1.83280	4.00236
C	6.22189	0.78516	3.79478
C	5.79126	-0.53357	3.94140
C	4.47487	-0.80609	4.32677
C	2.15313	0.03369	4.96793
C	-2.08991	-2.96072	5.39750

C	-1.04081	-3.67412	4.79780
C	0.16207	-3.04359	4.52028
C	0.34001	-1.68893	4.85322
C	-0.70268	-0.96482	5.44984
C	-1.91038	-1.60673	5.71569
C	-3.35321	-3.68670	5.67511
O	-3.55391	-4.85764	5.41472
O	-4.29759	-2.90647	6.26304
H	-5.07041	-3.48390	6.40391
H	-1.17649	-4.72911	4.58560
H	0.98550	-3.59531	4.07863
N	1.60264	-1.13978	4.54994
H	-0.56454	0.07331	5.71311
H	-2.71324	-1.04376	6.17774
H	2.15809	-1.71693	3.91551
O	1.56677	0.90084	5.62858
H	3.30165	2.35052	4.56751
H	4.17884	-1.84112	4.45121
C	6.69009	-1.71233	3.73700
N	7.59096	-1.56724	2.71932
O	6.55881	-2.71650	4.43810
H	8.17694	-4.10321	3.62057
C	10.03970	-4.37544	2.59235
C	10.97290	-3.82919	1.69717
C	10.69770	-2.60218	1.07706
C	9.55683	-1.89080	1.40653
H	10.21530	-5.34076	3.05501
C	12.29640	-4.43594	1.44593
O	12.37890	-5.73278	1.80851
H	13.29960	-6.00940	1.64352
O	13.25490	-3.83620	0.97457
H	11.40810	-2.18671	0.37266
H	9.37164	-0.91750	0.96379
H	7.54779	-0.70428	2.18066
H	7.24852	1.00891	3.52296
C	5.79198	3.24560	3.88479
N	4.84864	4.11577	3.40965
H	3.94342	3.71686	3.15655
C	4.84012	5.53337	3.46462
O	6.94825	3.55673	4.19427
C	5.98282	6.30829	3.70841
C	3.59209	6.14946	3.26891
C	3.48032	7.53137	3.34233
C	4.61679	8.31572	3.59367
C	5.86114	7.69451	3.76108
H	2.71194	5.53966	3.09223
H	2.51013	8.00140	3.22649
H	6.94523	5.84896	3.87356

H	6.74637	8.29587	3.93686
C	4.54793	9.79551	3.70786
O	5.50060	10.52310	3.90286
O	3.28217	10.27080	3.58139
H	3.34218	11.23800	3.68671
C	11.57600	-0.25093	4.44456
H	12.24940	-1.05183	4.72817
C	10.65590	0.23197	5.36996
H	10.61650	-0.17258	6.36943
C	9.73603	1.22208	4.98089
N	8.63684	1.60658	5.77508
C	8.12784	0.90041	6.82871
O	8.74892	0.05122	7.47549
C	6.67023	1.09639	7.09508
C	5.99978	2.31714	7.07981
C	4.63122	2.35214	7.36946
C	3.93359	3.67145	7.29063
O	4.49674	4.71152	7.63482
N	2.67569	3.58919	6.75513
C	1.78103	4.62714	6.43528
C	2.16916	5.96759	6.28565
H	3.19292	6.25776	6.47463
C	1.22747	6.89736	5.85411
H	1.51748	7.92853	5.68012
C	-0.10038	6.52178	5.60622
C	-1.03476	7.52977	5.04342
O	-0.71831	8.64246	4.67012
O	-2.29708	7.04383	4.93525
H	-2.82624	7.64596	4.38021
C	-0.49021	5.18778	5.81188
H	-1.52087	4.88737	5.67204
C	0.45054	4.24435	6.19849
H	0.16514	3.20656	6.33359
H	2.33120	2.65956	6.51765
C	3.94351	1.17856	7.67040
H	2.88458	1.19157	7.88838
C	4.60761	-0.04725	7.64155
C	3.79137	-1.27615	7.86490
O	2.81673	-1.26821	8.62173
N	4.16526	-2.34647	7.10000
C	3.43313	-3.50375	6.78535
C	2.15800	-3.79115	7.29917
H	1.71708	-3.14254	8.04129
C	1.46334	-4.89509	6.81166
H	0.46017	-5.09519	7.16991
C	2.03266	-5.72991	5.83888
C	1.30868	-6.85143	5.20239
O	0.03909	-6.99467	5.66017

H	-0.35243	-7.73926	5.16727
O	1.76597	-7.56830	4.32813
C	3.33226	-5.46555	5.38766
H	3.79065	-6.13246	4.67522
C	4.02604	-4.35937	5.84125
H	5.01873	-4.14182	5.46437
H	5.00871	-2.24233	6.54536
H	6.51227	3.23710	6.82565
C	5.96560	-0.08291	7.34728
H	6.50308	-1.02164	7.30953
H	8.02391	2.30237	5.34374
C	9.82617	1.79459	3.69657
C	10.75930	1.30722	2.79144
H	10.80620	1.70512	1.78703
H	9.14424	2.59141	3.41240
C	11.61970	0.25740	3.14042
C	12.44700	-0.35762	2.07079
O	13.14670	-1.42563	2.50170
H	13.44370	-1.95548	1.72955
O	12.43830	0.01184	0.90746
C	7.87937	2.96077	9.82980
O	9.05983	2.64696	9.92194
C	6.79717	2.06193	10.36350
C	7.12164	0.69959	10.40000
H	8.14581	0.42559	10.17070
C	6.13393	-0.25786	10.63560
C	6.31071	-1.73106	10.38490
O	5.55372	-2.55502	10.88270
N	7.27655	-2.04449	9.44129
C	7.30024	-3.18538	8.61645
C	6.43003	-4.28074	8.77314
H	5.75905	-4.31363	9.61817
C	6.41509	-5.28417	7.81040
H	5.71166	-6.10276	7.90872
C	7.26979	-5.24068	6.69779
C	7.19660	-6.23896	5.60753
O	6.18271	-7.11641	5.76091
H	6.18915	-7.72676	4.98959
O	7.94521	-6.27077	4.63909
C	8.17843	-4.17892	6.58441
H	8.84360	-4.14200	5.73000
C	8.19349	-3.16011	7.52578
H	8.86202	-2.31423	7.40380
H	7.81893	-1.27131	9.06431
C	4.81990	0.15481	10.89440
H	4.06974	-0.61369	11.04660
C	4.48605	1.50995	10.85800
C	3.07556	2.03342	10.83430

O	2.81985	3.18581	11.16140
N	2.15237	1.16057	10.28850
C	0.91354	1.49510	9.71461
C	0.40699	2.80799	9.64587
H	0.93728	3.61264	10.13320
C	-0.75104	3.05279	8.91790
H	-1.12389	4.06588	8.81416
C	-1.43903	2.01450	8.27093
C	-2.59243	2.35881	7.41802
O	-2.97696	3.48772	7.17089
O	-3.20576	1.26853	6.87114
H	-3.93145	1.62113	6.32411
C	-0.96452	0.69975	8.40053
H	-1.49135	-0.11842	7.92672
C	0.20016	0.44316	9.10639
H	0.59014	-0.56633	9.16328
H	2.50202	0.25931	9.96540
C	5.48327	2.46244	10.61100
H	5.18139	3.50438	10.56590
N	7.43563	4.05947	9.11931
C	8.14055	4.73362	8.09983
C	9.39385	4.31673	7.61559
H	9.92247	3.51619	8.11114
C	9.92208	4.91913	6.47774
H	10.86760	4.56887	6.07876
C	9.23585	5.94976	5.82004
C	9.71178	6.53026	4.54266
O	10.91350	6.07430	4.16316
H	11.14870	6.45024	3.27990
O	9.05732	7.32058	3.87101
C	8.01789	6.40075	6.34918
H	7.49413	7.20880	5.85416
C	7.47150	5.80089	7.47277
H	6.50293	6.11574	7.84447
H	6.43294	4.21154	9.06673

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