What is the Opto-Electronic Effect of the Capsule on the Guest Molecule in Aqueous Host/Guest Complexes? A Combined Computational and Spectroscopic Perspective

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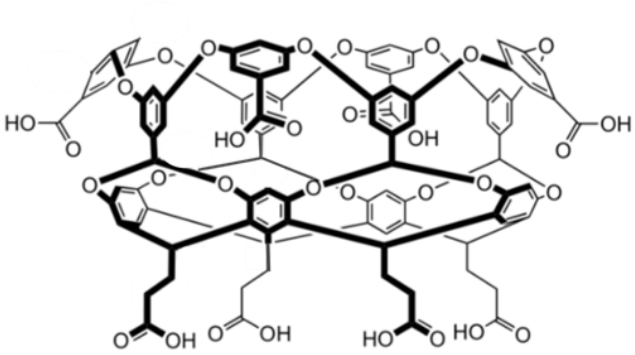

Figure S1. Chemical structure of an octa-acid.

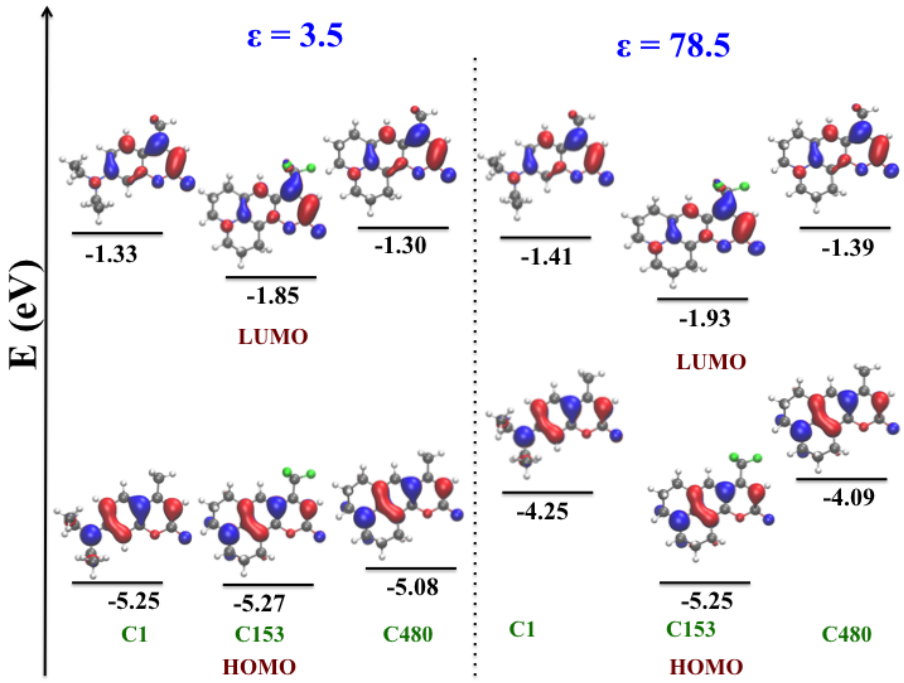

Figure S2. The frontier molecular orbitals (MOs) energies of C1, C153 and C480. The MOs are calculated at the B3LYP/6-31G(d) level.

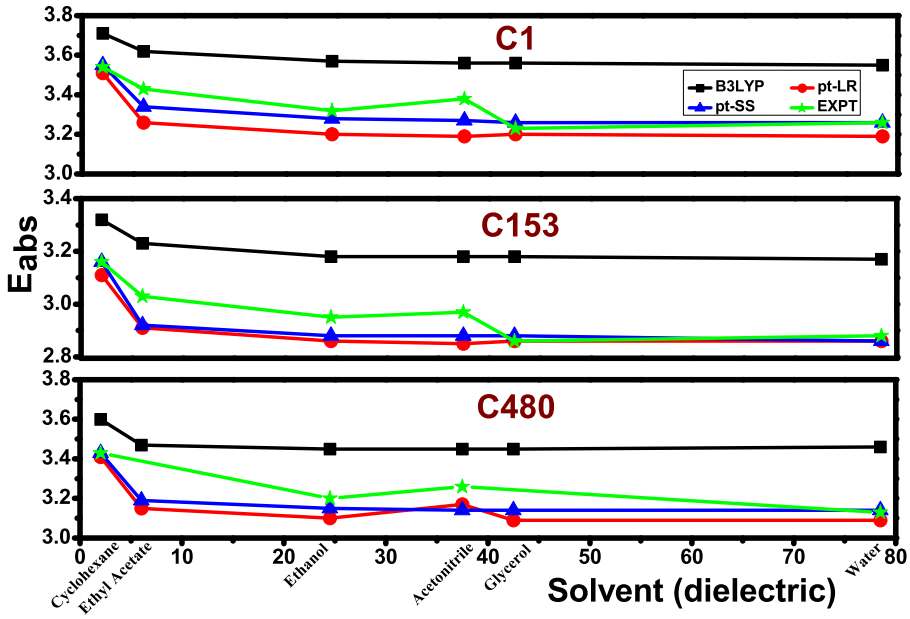

Figure S3. Comparison of measured (green) and calculated absorption spectra at B3LYP (black), pt-LR LRC-ωPBE (red) and pt-SS LRC-ωPBE (blue) .

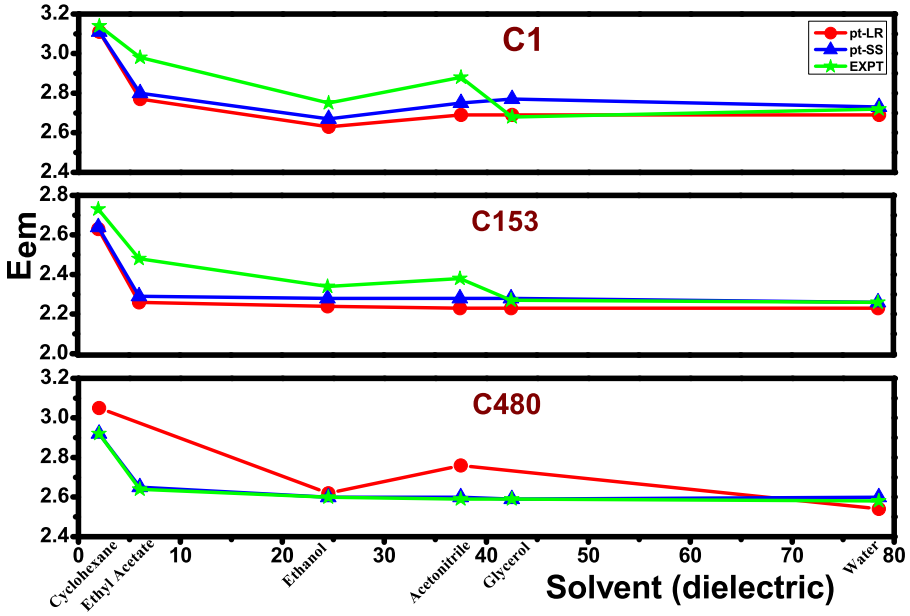

Figure S4. Comparison of measured (green) and calculated emission spectra pt-LR LRC-ωPBE (red) and pt-SS LRC-ωPBE (blue) .

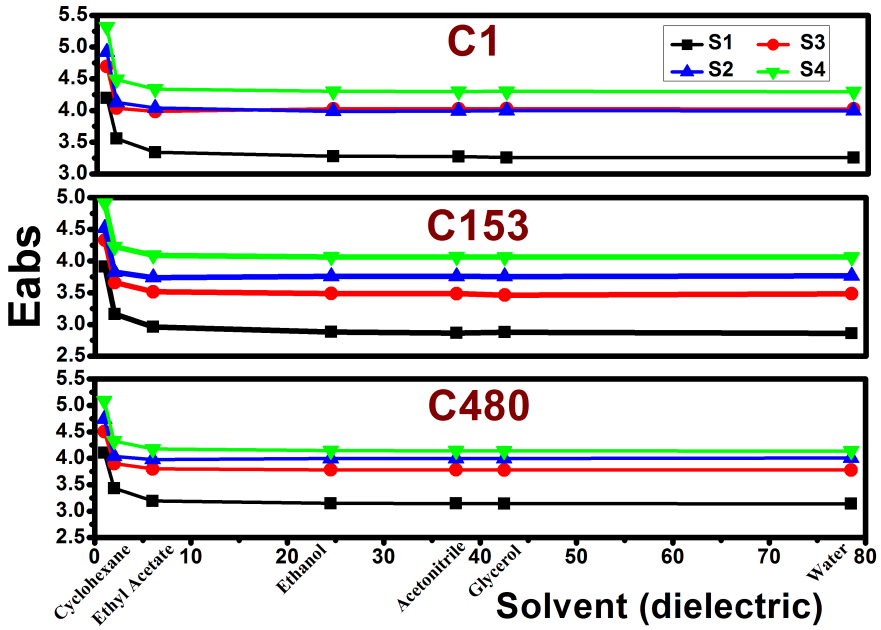

Figure S5. Calculated energies of the first (black), second (blue), third (red) and fourth (green) absorbing excited states at pt-SS LRC-ωPBE .

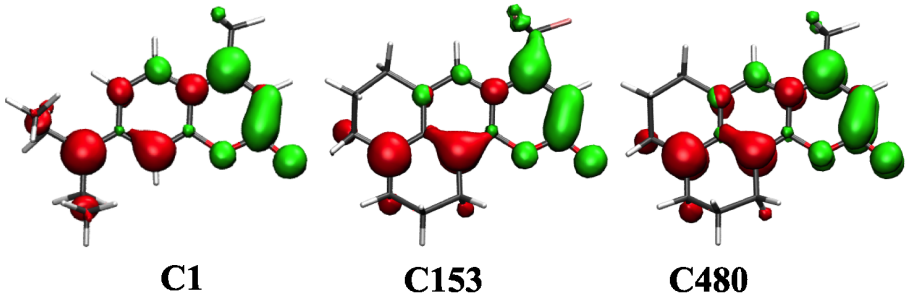

Figure S6. Isosurface plots of the attachment (green) and detachment (red) densities of the lowest excited state. The intramolecular CT character of these states is well evident. The excited states are calculated at the pt-SS LRC-ωPBE/6-31G(d) level.

Table S1. Solvents dielectric (ε) and optical dielectric constant (ε_o).

Solvent	ε	ε_o
Gas	1.00	1.00
Cyclohexane	2.02	2.02
Ethyl acetate	6.02	2.24
Ethanol	24.5	1.85
Acetonitrile	37.5	2.04
Glycerol	42.5	2.16
Water	78.5	1.78

Table S2. Calculated energies [eV] of HOMO, LUMO, Ionization potential (IP) and electron affinity (EA) in different solutions using B3LYP functional and 6-31G(d) basis set.

Solvent	HOMO	LUMO	IP	EA
C1				
Gas	-5.30	-1.25	-7.30	-0.18
Cyclohexane	-5.30	-1.32	-5.97	0.74
Ethyl acetate	-5.31	-1.45	-5.32	-1.20
Ethanol	-5.32	-1.41	-5.21	-1.68
Acetonitrile	-5.32	-1.45	-5.19	-1.71
Glycerol	-5.32	-1.45	-5.18	-1.72
Water	-5.32	-1.46	-5.16	-1.75
C153				
Gas	-5.41	1.81	-6.82	-0.49
Cyclohexane	-5.36	-1.82	-6.02	-1.85
Ethyl acetate	-5.32	-1.91	-5.37	-1.20
Ethanol	-5.30	-1.94	-5.14	-2.24
Acetonitrile	-5.30	-1.94	-5.12	-2.27
Glycerol	-5.30	-1.94	-5.12	-2.27
Water	-5.30	-1.94	-5.09	-2.30
C480				
Gas	-5.14	-1.22	-5.72	0.15
Cyclohexane	-5.13	-1.28	-5.79	-0.76
Ethyl acetate	-5.13	-1.36	-5.17	-1.41
Ethanol	-5.14	-1.40	-4.96	-1.67
Acetonitrile	-5.14	-1.40	-4.92	-1.70
Glycerol	-5.14	-1.41	-4.92	1.71
Water	-5.14	-1.41	-4.92	-1.74

Table S3. Absorption (E_{abs}) and emission (E_{em}) energies calculated using LRC-ωPBE functional and cc-pVTZ basis set with ptSS. Experimental measured values are provided in the parenthesis.

Solvent	E_{abs}	E_{em}
	C1	
Cyclohexane	3.54 (3.54)	-
Ethyl acetate	3.28 (3.34)	-
Ethanol	3.22 (3.32)	-
Acetonitrile	2.21 (3.38)	-
Glycerol	3.21 (3.23)	-
Water	3.20 (3.26)	-
	C153	
Cyclohexane	3.15 (3.16)	-
Ethyl acetate	2.91 (3.03)	-
Ethanol	2.86 (2.95)	-
Acetonitrile	2.86 (2.97)	-
Glycerol	2.86 (2.86)	-
Water	2.86 (2.88)	-
	C480	
Cyclohexane	3.41 (3.43)	2.92 (3.05)
Ethyl acetate	3.16 (n/a)	2.64 (n/a)
Ethanol	3.11 (3.20)	2.58 (2.62)
Acetonitrile	3.11 (3.26)	2.58 (2.76)
Glycerol	3.11 (n/a)	2.57 (n/a)
Water	3.11 (3.13)	2.57 (2.54)

Table S4. Comparison of Mulliken and CHELPG based population analysis at different dielectric constant of C1, C153 and C480.

ε	$\Delta Q_{Mulliken}$	ΔQ_{CHELPG}
	C1	
1.00	0.13	0.08
2.02	0.54	0.55
2.50	0.59	0.60
3.00	0.62	0.64
3.50	0.64	0.66
4.00	0.66	0.68
5.00	0.67	0.69
6.02	0.67	0.69
24.5	0.71	0.73
37.5	0.71	0.73
42.5	0.71	0.74
78.5	0.71	0.74
	C153	
1.00	0.14	0.34
2.02	0.79	0.76
2.50	0.79	0.79
3.00	0.83	0.82
3.50	0.85	0.83
4.00	0.86	0.84
5.00	0.87	0.85
6.02	0.87	0.85
24.5	0.88	0.86
37.5	0.91	0.88
42.5	0.91	0.88
78.5	0.91	0.87
	C480	
1.00	0.13	0.46
2.02	0.63	0.67
2.50	0.68	0.71
3.00	0.71	0.75
3.50	0.73	0.77
4.00	0.74	0.78
5.00	0.75	0.78
6.02	0.72	0.80
24.5	0.76	0.81
37.5	0.79	0.83
42.5	0.80	0.83
78.5	0.80	0.84

Table S5. Absorption energy (E_{abs}), emission energy (E_{em}) and stokes shift (Δ) calculated using LRC-ωPBE functional and 6-31G(d) basis set with ptLR approach of the coumarins in various solvents. Experimental measured values are provided in the parenthesis. All energies are in eV.

Solvent	E_{abs}	E_{em}	Δ
	C1		
Cyclohexane	3.51 (3.54)	3.11 (3.14)	0.40 (0.40)
Ethyl acetate	3.26 (3.34)	2.77 (2.98)	0.49 (0.45)
Ethanol	3.20 (3.32)	2.63 (2.75)	0.57 (0.57)
Acetonitrile	3.19 (3.38)	2.69 (2.88)	0.50 (0.50)
Glycerol	3.20 (3.23)	2.69 (2.68)	0.51 (0.55)
Water	3.19 (3.26)	2.69 (2.72)	0.50 (0.54)
	C153		
Cyclohexane	3.11 (3.16)	2.63 (2.73)	0.48 (0.43)
Ethyl acetate	2.91 (3.03)	2.26 (2.48)	0.65 (0.55)
Ethanol	2.86 (2.95)	2.24 (2.34)	0.62 (0.61)
Acetonitrile	2.85 (2.97)	2.23 (2.38)	0.62 (0.59)
Glycerol	2.86 (2.86)	2.23 (2.27)	0.63 (0.59)
Water	2.86 (2.88)	2.23 (2.26)	0.63 (0.62)
	C480		
Cyclohexane	3.41 (3.43)	2.92 (3.05)	0.49 (0.38)
Ethyl acetate	3.15 (n/a)	2.65 (n/a)	0.50 (n/a)
Ethanol	3.10 (3.20)	2.60 (2.62)	0.50(0.58)
Acetonitrile	3.17 (3.26)	2.60 (2.76)	0.57 (0.50)
Glycerol	3.09 (n/a)	2.59 (n/a)	0.50(n/a)
Water	3.09 (3.13)	2.60 (2.54)	0.49 (0.59)

Table S6. Absorption energies calculated using B3LYP and LRC-ωPBE with 6-31G(d) at the ptSS level. Measured values are provided in the parentheses.

Medium	B3LYP	LRC
	C1	
Gas	3.93 (n/a)	4.24 (n/a)
Cyclohexane	3.71 (3.54)	3.55 (3.54)
Ethyl acetate	3.62 (3.34)	3.34 (3.43)
Ethanol	3.57 (3.28)	3.28 (3.32)
Acetonitrile	3.56 (3.28)	3.27 (3.38)
Glycerol	3.56 (3.27)	3.26 (3.23)
Water	3.55 (3.26)	3.26 (3.26)
	C153	
Gas	3.54 (n/a)	3.91 (n/a)
Cyclohexane	3.32 (3.16)	3.16 (3.16)
Ethyl acetate	3.23 (3.03)	2.92 (3.03)
Ethanol	3.18 (2.95)	2.88 (2.95)
Acetonitrile	3.18 (2.97)	2.88 (2.97)
Glycerol	3.18 (2.86)	2.88 (2.86)
Water	3.17 (2.88)	2.86 (2.88)
	C480	
Gas	3.81 (n/a)	4.10 (n/a)
Cyclohexane	3.60 (3.43)	3.43 (3.43)
Ethyl acetate	3.47 (n/a)	3.19 (n/a)
Ethanol	3.45 (3.20)	3.15 (3.20)
Acetonitrile	3.45 (3.10)	3.14 (3.26)
Glycerol	3.45 (n/a)	3.14 (n/a)
Water	3.46 (3.13)	3.14 (3.13)

Table S7. Capsule effective dielectric constant (ε) and the corresponding RMSD of the calculated absorption energies from the measured values for the encapsulated coumarins using LRC-ωPBE functional and 6-31G(d) basis set with ptSS approach.

ε	RMSD
1.00	0.67
2.02	0.15
2.50	0.07
3.00	0.01
3.50	0.03
4.00	0.05
5.00	0.06
6.02	0.10
24.5	0.13
37.5	0.14
42.5	0.14
78.5	0.14

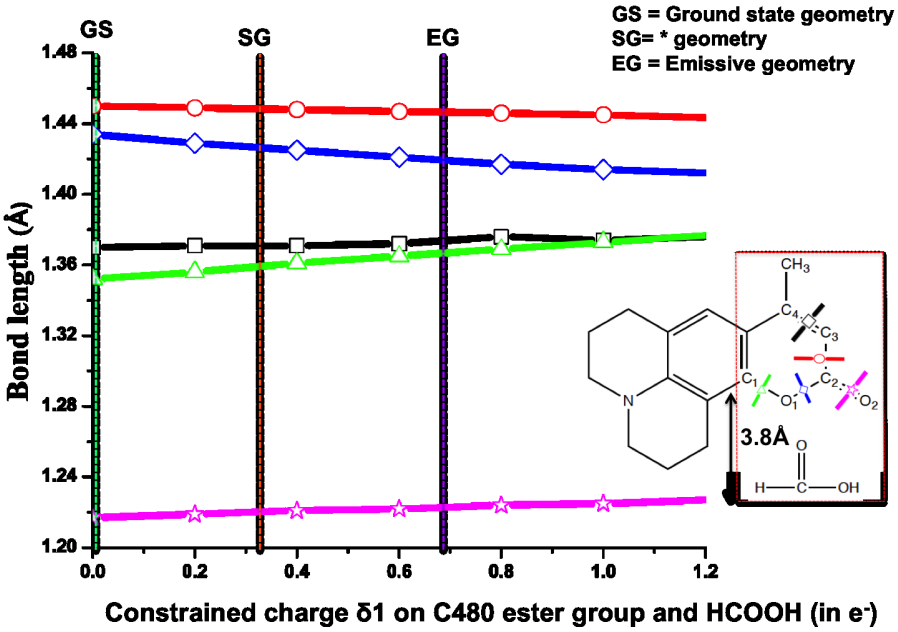

Figure S7. Bond length dependence on charge transfer in the CDFT series of geometries: The bond length in the zero charge CDFT optimized geometry is in good agreement with that of the ground state geometry, and the bond length in the CDFT 0.7e geometry is in good agreement with that of the fully optimized emissive geometry.

Table S8. Bond lengths in C480 geometries in Å.

Bond	GS	EG	0	0.70	0.35(*)
C3-C4	1.367	1.376	1.369	1.372	1.371
C2-C3	1.457	1.446	1.453	1.448	1.450
C2-O2	1.210	1.224	1.212	1.222	1.218
C2-O1	1.436	1.417	1.432	1.423	1.428
C1-O1	1.347	1.369	1.351	1.363	1.357

Table S9. Excitation energies at different CDFT optimized geometries compared to key geometries of the ground state (absorption), free excited state (emission) and of the capsulated excited state (measured) for C480.

Geometries	0-CDFT	0.35-CDFT	0.7-CDFT	Ground State	Measured@Capsule	Excited state
Excitation energy	3.20	2.95	2.70	3.29	2.92	2.75

Table S10. XYZ coordinates of the optimized geometry of an octa-acid capsule at B3LYP/STO-3G level.

O	-4.41801	6.36830 7.03959
C	-3.60691	5.34798 7.44566
O	-3.52481	5.23594 8.66802
C	-2.92969	4.49716 6.44340
H	-2.64693	6.08980 4.97489
C	-2.49954	5.02642 5.22253
C	-2.69229	3.15498 6.76381
H	-3.00181	2.75209 7.74346
C	-1.83420	4.19151 4.31685
C	-2.03195	2.34111 5.83482
O	-1.24180	4.74051 3.17799
C	-1.60126	2.83983 4.59941
O	-1.66400	1.04924 6.21805
C	-2.05473	4.87491 2.05641
H	-3.91759	4.16152 2.93453
H	-1.06633	2.19780 3.88508
C	-2.46622	0.01959 5.73071
C	-3.40932	4.52799 2.03037
C	-1.39425	5.36266 0.91870
H	-4.21119	1.22783 5.23464
H	-0.85951	-1.39890 6.15593
H	-5.43834	2.62842 3.75027
H	-0.32775	5.63794 0.95259
C	-6.41936	2.39348 3.31217
C	-1.88261	-1.25532 5.77407
C	-3.76264	0.22305 5.24475
O	-11.13169	6.84021 1.79888
O	-6.24001	4.33653 1.94651
C	-6.98330	3.22465 2.34089
C	-7.11747	1.24999 3.70771
O	-6.51711	0.43171 4.66276
H	-10.82757	0.76412 4.13560
H	-10.60402	4.12195 1.88024
O	-11.63592	-0.28440 6.55111
C	-4.11782	4.65765 0.83330
C	-2.14212	5.49569 -0.25957
C	-10.48836	6.48470 0.64524
H	-8.71965	-0.56641 4.64871
C	-8.38344	0.94292 3.17409
C	-4.49054	-0.87485 4.78180
C	-8.25246	2.95602 1.79378
H	-8.36932	4.90011 0.91992
C	-2.65557	-2.33682 5.32823
C	-10.57144	-0.20294 3.62356
C	-8.93938	1.82163 2.23885
C	-5.50420	4.09276 0.74384
C	-10.31242	3.99397 0.80256
C	-3.49915	5.15470 -0.31458
C	-9.05600	-0.33581 3.58448
H	-12.32960	-1.35810 4.15100
C	-11.01791	-1.27712 5.84134
C	-8.79801	3.86166 0.72716
C	-5.79145	-0.64933 4.07075
O	-1.43283	6.00304 -1.34393
O	-2.04243	-3.58469 5.42604
H	-11.93318	5.10079 -0.12150
C	-10.81907	5.17270 -0.00440
C	-3.95502	-2.16239 4.83742
O	-6.28188	4.77963 -0.24018
C	-11.22595	-1.35619 4.35702
O	-9.68463	7.32500 0.24763
H	-9.93376	1.60017 1.82030

O -10.34480 -2.03632 6.53431
O -6.67515 -1.75864 4.25477
H -2.89185 7.78099 -2.62033
H -10.81401 3.06245 0.43245
H -10.99512 -0.14971 2.58710
H -5.42422 2.98909 0.52022
H -3.87410 -5.32171 6.18899
H -5.57704 -0.46084 2.97891
H -4.07470 5.27903 -1.24446
C -2.71294 6.85735 -3.19359
H -4.55460 -3.02476 4.50746
C -2.00634 5.80301 -2.60286
C -8.27881 3.42206 -0.61168
C -2.58348 -4.58299 4.61079
C -7.01794 3.89368 -1.02740
C -8.54839 -1.45342 2.71841
H -10.36030 5.15880 -1.02998
C -3.50934 -5.47751 5.16088
C -7.34839 -2.09570 3.08159
H -10.80284 -2.33055 3.99115
O -4.69938 8.63637 -4.48503
O -4.89204 -7.88159 6.23205
C -3.85897 7.82939 -5.19692
O -3.78977 8.11630 -6.39114
C -3.13942 6.72922 -4.51946
C -6.44929 3.49187 -2.23757
C -2.09679 -4.73997 3.30669
C -1.72694 4.62276 -3.30278
C -8.95120 2.51921 -1.44206
C -4.94944 -7.50963 4.92075
C -6.78915 -3.09965 2.28702
C -3.96142 -6.54920 4.38412
C -9.17360 -1.84646 1.53060
H -5.47466 3.88736 -2.55933
H -9.93650 2.13371 -1.13756
H -5.86191 -3.60554 2.59441
H -10.10685 -1.34667 1.22887
H -1.32876 -4.06310 2.90221
H -1.15699 3.80865 -2.83283
O -5.86216 -8.04167 4.28979
C -2.86006 5.56878 -5.25085
C -2.15818 4.52641 -4.63147
C -7.13166 2.55845 -3.02105
C -2.58491 -5.80967 2.54614
C -3.51615 -6.71598 3.06802
C -8.38862 2.05596 -2.63640
C -7.42103 -3.43793 1.08837
C -8.62682 -2.82542 0.69459
H -4.31425 3.16617 -4.53195
H -10.79715 -4.49847 1.05459
H -3.16728 5.48748 -6.30777
H -5.58791 0.72471 -2.90836
H -11.13474 -2.20866 -0.24423
H -4.58254 -5.03199 1.26778
O -6.51622 2.13707 -4.19784
C -3.78920 2.23588 -4.79695
O -1.74539 3.44661 -5.41485
H -5.75324 -2.75001 -0.50279
H -3.89549 -7.54908 2.45247
O -6.81457 -4.41031 0.29358
O -2.02488 -6.03634 1.28609
C -11.35149 -4.32960 0.09436
C -5.76857 0.93179 -4.00352
C -9.03943 1.00497 -3.49031
H -10.98556 0.79186 -2.51190
C -9.22327 -3.20166 -0.63163

C -4.05686 -5.05515 0.30100
H -10.82578 2.20735 -3.62151
C -10.74384 -3.16827 -0.67012
C -9.15628 -1.15487 -2.13999
O -10.38401 -6.52080 -0.56587
H -10.11066 -0.82825 -1.69835
C -10.55666 1.12381 -3.49278
H -12.41886 -4.08866 0.34901
C -5.98396 -3.83326 -0.71983
C -2.46654 2.26603 -5.25491
C -4.43993 1.00575 -4.69370
C -8.51981 -0.34545 -3.08688
C -2.75920 -5.56879 0.19825
C -8.59962 -2.36262 -1.70856
C -4.68942 -4.57911 -0.84938
H -8.69527 1.18135 -4.56264
C -11.35691 -5.58036 -0.73750
H -8.91599 -4.27839 -0.84044
C -7.30444 -0.79902 -3.63794
C -7.38333 -2.78146 -2.27902
O -6.61500 -0.05594 -4.59568
H -11.07966 -3.21450 -1.74208
C -6.74083 -2.02000 -3.25739
C -2.08553 -5.63285 -1.03076
C -3.80212 -0.17703 -5.07557
C -1.78306 1.09811 -5.61882
O -6.78136 -3.98033 -1.89745
C -4.06066 -4.64967 -2.09345
C -11.18883 0.30781 -4.60271
C -2.47936 -0.11749 -5.52695
C -2.76522 -5.17476 -2.16870
H -1.06218 -6.03444 -1.10171
H -4.34221 -1.13441 -5.02959
H -5.80311 -2.36935 -3.71396
H -0.74057 1.13227 -5.97388
O -12.18402 -5.87239 -1.60095
H -12.28792 0.18903 -4.40749
H -1.43202 -2.73807 -3.73122
O -11.70224 2.09240 -6.23893
H -4.58158 -4.30224 -2.99842
H -10.73034 -0.71764 -4.63354
C -11.00625 0.95112 -5.94643
C -2.03903 -3.19007 -4.52843
O -2.06364 -5.30771 -3.36297
O -1.73500 -1.23459 -5.89437
C -2.49722 -4.50942 -4.42441
C -2.33828 -2.47874 -5.69685
O -10.28813 0.56020 -6.86324
C -3.25085 -5.10651 -5.44224
C -3.08487 -3.05264 -6.73358
C -3.54408 -4.36765 -6.59309
H -3.29059 -2.48713 -7.65876
H -3.56901 -6.15616 -5.33720
C -4.30564 -4.96630 -7.71084
O -4.16818 -4.70453 -8.90488
O -5.26961 -5.89987 -7.45930
H -4.50500 6.37073 6.07616
H -11.75055 6.14473 2.05867
H -12.15238 0.27419 5.95503
H -4.77559 8.32677 -3.57180
H -4.12124 -7.48478 6.66243
H -9.75225 -6.23482 0.10934
H -12.25183 2.34482 -5.48524
H -5.38856 -6.01750 -6.50673
O 4.42502 -6.40234 7.00868
C 3.61371 -5.38420 7.41978

O 3.53261 -5.27741 8.64268
C 2.93510 -4.52952 6.42175
H 2.65220 -6.11598 4.94658
C 2.50432 -5.05378 5.19894
C 2.69707 -3.18890 6.74815
H 3.00716 -2.79004 7.72928
C 1.83769 -4.21541 4.29742
C 2.03540 -2.37147 5.82324
O 1.24493 -4.75989 3.15658
C 1.60402 -2.86514 4.58605
O 1.66672 -1.08151 6.21217
C 2.05696 -4.88775 2.03358
H 3.92012 -4.17795 2.91398
H 1.06797 -2.22040 3.87499
C 2.46921 -0.04932 5.73073
C 3.41134 -4.53993 2.00830
C 1.39584 -5.36991 0.89385
H 4.21371 -1.25506 5.22694
H 0.86301 1.36707 6.16483
H 5.44096 -2.64791 3.73620
H 0.32957 -5.64611 0.92733
C 6.42166 -2.41056 3.29870
C 1.88591 1.22548 5.78170
C 3.76535 -0.25026 5.24303
O 11.13419 -6.84888 1.75926
O 6.24180 -4.34672 1.92333
C 6.98513 -3.23669 2.32285
C 7.11982 -1.26898 3.69962
O 6.51992 -0.45567 4.65918
H 10.83013 -0.78477 4.12781
H 10.60570 -4.13108 1.85518
O 11.63971 0.25159 6.54793
C 4.11897 -4.66291 0.81001
C 2.14284 -5.49627 -0.28569
C 10.48967 -6.48742 0.60815
H 8.72237 0.54280 4.64888
C 8.38542 -0.95901 3.16678
C 4.49331 0.85013 4.78606
C 8.25388 -2.96506 1.77629
H 8.37048 -4.90462 0.89238
C 2.65891 2.30933 5.34174
C 10.57358 0.18481 3.62076
C 8.94090 -1.83284 2.22670
C 5.50506 -4.09701 0.72245
C 10.31335 -3.99758 0.77838
C 3.49964 -5.15423 -0.33997
C 9.05809 0.31769 3.58327
H 12.33193 1.33757 4.15279
C 11.02142 1.24799 5.84359
C 8.79888 -3.86512 0.70468
C 5.79383 0.62833 4.07314
O 1.43311 -5.99836 -1.37223
O 2.04640 3.55690 5.44725
H 11.93366 -5.09930 -0.15254
C 10.81964 -5.17204 -0.03501
C 3.95812 2.13743 4.84933
O 6.28226 -4.77855 -0.26565
C 11.22842 1.33447 4.35953
O 9.68576 -7.32581 0.20685
H 9.93497 -1.60908 1.80864
O 10.34875 2.00369 6.54080
O 6.67755 1.73674 4.26234
H 2.89205 -7.76814 -2.65993
H 10.81455 -3.06408 0.41274
H 10.99662 0.13678 2.58378
H 5.42452 -2.99224 0.50457
H 3.87797 5.29098 6.21646

H 5.57882 0.44542 2.98047
H 4.07452 -5.27336 -1.27094
C 2.71219 -6.84135 -3.22778
H 4.55770 3.00158 4.52405
C 2.00545 -5.79080 -2.63049
C 8.27868 -3.41872 -0.63153
C 2.58623 4.55910 4.63600
C 7.01757 -3.88836 -1.04877
C 8.54983 1.43966 2.72325
H 10.36012 -5.15296 -1.06016
C 3.51229 5.45139 5.18939
C 7.35000 2.07993 3.09048
H 10.80492 2.31058 3.99881
O 4.69844 -8.61200 -4.53095
O 4.89526 7.85083 6.27044
C 3.85722 -7.80124 -5.23755
O 3.78737 -8.08117 -6.43339
C 3.13758 -6.70539 -4.55321
C 6.44799 -3.48036 -2.25643
C 2.09836 4.72194 3.33308
C 1.72483 -4.60673 -3.32343
C 8.95037 -2.51154 -1.45774
C 4.95155 7.48503 4.95736
C 6.79014 3.08789 2.30144
C 3.96335 6.52679 4.41718
C 9.17424 1.83886 1.53707
H 5.47316 -3.87429 -2.57951
H 9.93584 -2.12750 -1.15197
H 5.86304 3.59209 2.61202
H 10.10735 1.34071 1.23219
H 1.33015 4.04675 2.92611
H 1.15477 -3.79565 -2.84840
O 5.86350 8.02034 4.32804
C 2.85700 -5.54093 -5.27774
C 2.15501 -4.50254 -4.65188
C 7.12969 -2.54284 -3.03560
C 2.58548 5.79529 2.57703
C 3.51689 6.69949 3.10224
C 8.38689 -2.04222 -2.64928
C 7.42122 3.43239 1.10414
C 8.62682 2.82204 0.70644
H 4.31062 -3.14278 -4.54647
H 10.79724 4.49358 1.07356
H 3.16339 -5.45342 -6.33441
H 5.58595 -0.70973 -2.91248
H 11.13424 2.21043 -0.23703
H 4.58217 5.02427 1.29354
O 6.51333 -2.11553 -4.20976
C 3.78559 -2.21118 -4.80683
O 1.74082 -3.41846 -5.42859
H 5.75258 2.75241 -0.48953
H 3.89547 7.53552 2.49020
O 6.81411 4.40876 0.31474
O 2.02410 6.02743 1.31859
C 11.35094 4.32967 0.11211
C 5.76582 -0.91125 -4.00880
C 9.03704 -0.98684 -3.49826
H 10.98381 -0.77855 -2.52009
C 9.22241 3.20514 -0.61821
C 4.05603 5.05261 0.32715
H 10.82339 -2.18839 -3.63677
C 10.74295 3.17212 -0.65782
C 9.15466 1.16609 -2.13700
O 10.38289 6.52419 -0.53614
H 10.10937 0.83730 -1.69767
C 10.55428 -1.10555 -3.50236
H 12.41853 4.08761 0.36480

C 5.98299 3.83680 -0.70112
C 2.46262 -2.23893 -5.26403
C 4.43668 -0.98168 -4.69839
C 8.51763 0.36147 -3.08760
C 2.75818 5.56642 0.22781
C 8.59817 2.37157 -1.69904
C 4.68823 4.58305 -0.82610
H 8.69217 -1.15778 -4.57124
C 11.35561 5.58462 -0.71342
H 8.91487 4.28289 -0.82129
C 7.30186 0.81775 -3.63554
C 7.38150 2.79323 -2.26657
O 6.61183 0.07947 -4.59656
H 11.07809 3.22380 -1.72975
C 6.73841 2.03673 -3.24840
C 2.08396 5.63705 -1.00055
C 3.79888 0.20299 -5.07435
C 1.77919 -1.06918 -5.62218
O 6.77966 3.99006 -1.87845
C 4.05891 4.66025 -2.06948
C 11.18563 -0.28386 -4.60855
C 2.47581 0.14582 -5.52512
C 2.76328 5.18538 -2.14126
H 1.06044 6.03871 -1.06895
H 4.33921 1.16003 -5.02432
H 5.80037 2.38834 -3.70257
H 0.73649 -1.10149 -5.97682
O 12.18195 5.88101 -1.57613
H 12.28485 -0.16596 -4.41347
H 1.42976 2.75685 -3.71569
O 11.69798 -2.06014 -6.25413
H 4.57949 4.31792 -2.97658
H 10.72703 0.74169 -4.63386
C 11.00221 -0.92034 -5.95541
C 2.03617 3.21310 -4.51093
O 2.06123 5.32473 -3.33454
O 1.73147 1.26476 -5.88698
C 2.49424 4.53194 -4.40034
C 2.33477 2.50791 -5.68325
O 10.28348 -0.52478 -6.86975
C 3.24716 5.13443 -5.41552
C 3.08065 3.08729 -6.71742
C 3.53979 4.40161 -6.57038
H 3.28587 2.52664 -7.64567
H 3.56520 6.18357 -5.30522
C 4.30060 5.00614 -7.68546
O 4.16248 4.75052 -8.88076
O 5.26458 5.93854 -7.42968
H 4.51120 -6.40062 6.04518
H 11.75320 -6.15469 2.02209
H 12.15564 -0.30411 5.94870
H 4.77513 -8.30772 -3.61598
H 4.12498 7.45178 6.69968
H 9.75170 6.23477 0.13814
H 12.24808 -2.31637 -5.50208
H 5.38413 6.05121 -6.47658

Table S11. XYZ coordinates of the optimized geometry of C1 at B3LYP/6-31G(d) level.

C 1.44389 0.83991 -0.04184
C 0.98681 -0.49148 -0.12128
C 3.70481 0.00382 0.13406
H 4.77728 0.13011 0.23202
C 3.23896 -1.35926 0.05341
C 3.39261 2.48138 0.18026
H 2.97394 3.00583 1.04746
H 3.11911 3.06241 -0.70848
H 4.48150 2.48337 0.27041
C 2.86014 1.07660 0.09131
O 1.86597 -1.54338 -0.07320
O 3.92562 -2.36761 0.08472
C -0.35459 -0.82443 -0.24628
C -1.34248 0.18649 -0.31282
C -0.89094 1.53849 -0.21758
N -2.67343 -0.11744 -0.47940
C -3.69603 0.93451 -0.51342
H -4.56152 0.52120 -1.03881
C 0.44996 1.84051 -0.09306
H 0.74245 2.88380 -0.02853
C -3.12666 -1.51104 -0.54414
H -4.09331 -1.51049 -1.05540
H -0.60393 -1.87591 -0.28759
H -1.60006 2.35518 -0.23951
C -3.26842 -2.20633 0.81655
H -4.02118 -1.70917 1.43643
H -3.58029 -3.24690 0.67097
H -2.32245 -2.20919 1.36726
C -4.13230 1.45256 0.86315
H -4.58146 0.65349 1.46145
H -3.28620 1.86234 1.42418
H -4.87739 2.24728 0.74230
H -2.44429 -2.07658 -1.18830
H -3.33543 1.76294 -1.13232

Table S12. XYZ coordinates of the optimized geometry of C153 at B3LYP/6-31G(d) level.

C 1.90759 -0.14506 -0.06529
C 1.17429 -1.37862 -0.06964
C 1.20013 1.08736 -0.04660
C -0.93852 -0.14808 -0.02381
C -0.19043 1.05022 -0.03397
C -2.97533 1.19172 0.00850
H -4.05099 1.29994 0.02702
C -2.20294 2.41318 -0.00742
C -3.22734 -1.27178 0.01641
C -2.36736 -0.02725 0.00009
O -0.82531 2.27007 -0.03107
O -2.64666 3.54777 -0.00332
N 3.28251 -0.15532 -0.05954
C 1.91223 -2.70069 -0.12684
H 1.33858 -3.46913 0.40311
H 1.98761 -3.03581 -1.17177
C 3.31986 -2.57009 0.45464
H 3.89480 -3.48770 0.29309
H 3.26942 -2.39688 1.53664
C 4.03665 -1.40113 -0.21196
H 4.20366 -1.61907 -1.27945
H 5.02079 -1.24613 0.24192
C -0.20374 -1.35473 -0.03703
H -0.73177 -2.30174 -0.03174
C 4.03330 1.08336 -0.26896
H 5.04588 0.92439 0.11418
H 4.12350 1.29797 -1.34632
C 3.36781 2.25264 0.44825
H 3.94066 3.16776 0.26617
H 3.38227 2.06456 1.52872
C 1.92733 2.41616 -0.03863
H 1.92561 2.84579 -1.05083
H 1.38891 3.13037 0.59199
F -4.54378 -0.99001 0.04520
F -2.95938 -2.04101 1.09700
F -3.00594 -2.03710 -1.07745

Table S13. XYZ coordinates of the optimized geometry of C480 at B3LYP/6-31G(d) level.

C -1.36033 -0.00150 -0.04954
C -1.06798 1.40070 -0.04923
C -0.29333 -0.93760 -0.03432
C 1.33309 0.92007 -0.00938
C 1.01373 -0.45269 -0.02217
C 3.67995 0.33197 0.01120
H 4.73644 0.57562 0.02553
C 3.35902 -1.07266 -0.00594
C 3.10747 2.76141 0.02858
H 2.69386 3.26677 0.90939
H 2.71653 3.28330 -0.85295
H 4.19373 2.87866 0.04367
C 2.72173 1.30631 0.00997
O 2.00863 -1.40095 -0.02395
O 4.14949 -2.00359 -0.00712
N -2.67028 -0.44009 -0.03841
C -2.19173 2.41707 -0.10322
H -1.90514 3.31764 0.45180
H -2.35224 2.73497 -1.14405
C -3.49564 1.83285 0.44171
H -4.33285 2.51565 0.26280
H -3.41993 1.67903 1.52534
C -3.77545 0.49651 -0.23795
H -3.96269 0.65303 -1.31387
H -4.67646 0.03523 0.17996
C 0.24815 1.82007 -0.01815
H 0.44773 2.88778 -0.01071
C -2.97093 -1.84910 -0.28630
H -3.98669 -2.03880 0.07497
H -2.96633 -2.06171 -1.36875
C -1.97141 -2.75078 0.43018
H -2.21376 -3.80001 0.23115
H -2.06029 -2.59195 1.51193
C -0.54923 -2.43108 -0.03380
H -0.39106 -2.83444 -1.04467
H 0.18352 -2.93307 0.60606