Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Induced Polarization Restricts Conformational Distribution of a Light-Harvesting Molecular Triad in the Ground State

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Supplementary text

Partial atomic charges

a. Fitting of partial charges for the THF

We used two twisted conformations and one envelope conformation of the THF to fit the partial charges. Many independent experimental and theoretical studies showed that the ground state THF could be characterized by C2 symmetry. Twisted conformation is the lowest energy conformer identified in the single crystal [1] by X ray structure analysis. C2 symmetry was also identified for THF by Gallinella E., et al. [2] The equilibrium THF conformation in clathrate hydrate also belonged to C2 symmetry. [3] However, recent studies showed that the equilibrium geometry could belong to "envelope" conformation, i.e. CS point group. [4] Ultraviolet absorption spectra showed wagging of an oxygen atom in the vapor phase [5] Studies of THF by electron diffraction showed nearly free pseudorotation indicating no energy difference between twist (C2) and envelope (CS) conformational states in the gas phase. Reasonable agreement between experiment and theory was obtained by including six conformations into the fitting of intensity functions. [6] Therefore, we decided to consider both twist (C2) and envelope (CS) conformational states for the fitting of partial charges.

THF molecule exhibits low conformational barriers and can adopt many conformational states. It is rather puckered than planar, according to the pseudorotational model introduced by Kilpatrick et al. [7] Experiment (crystal and gas phases) and *ab initio* calculations [8] showed that twisted THF conformation could be identified as the lowest energy conformer. *Ab initio* calculations showed that C2 and CS conformational energy difference varies within ~1 kcal/mol. The energy variation depends on the basis set used in calculations. Addition of polarizable functions, d-type functions on non-hydrogen atoms, leads to significant reduction in energy difference, to about 0.3 kcal/mol. In contrast, the relative energy for the planar conformation is about 3.0 kcal/mol, indicating low population state. Based on these results, we do not include planar conformation into the fitting of partial charges. In principal, it is legitimate to fit the lowest energy conformer that would correspond to the ground state and ignore other states.

Almenningen, A. et al. [6] determined that THF conformations have nearly the same energies including C2 and CS. The energy difference varied from -0.73 to 1.25 kcal/mol. Theoretical radial distributions g(r) in the gas phase were calculated using various THF models. Overall quality of the fit was significantly improved by giving the same weights to C2 and CS conformers despite the fact that CS should be weighted less in accordance to the conformational energies calculated using Westheimer-Hendrickson Method. [6, 9] In addition to experimental results, quantum mechanical calculations showed energy difference within 1 kcal/mol between C2 and CS states. The energy variation depends on the basis set used in calculations. Addition of polarizable functions, d-type functions on non-hydrogen atoms, leads to significant reduction of about 0.3 kcal/mol in energy difference. The calculations were performed using split 6-31G* basis set. The results of the calculations are published by Cremer et al. [8] We obtain similar results, the difference in energies for envelope and twist conformations is about 0.3 kcal/mol. Since the energies for the two conformers are very close as obtained from experiment and *ab initio* calculations, we decided to give equal weights to both conformations while fitting partial charges.

Hydrogen atoms have been separated into two groups. We have fitted partial charges independently for each single conformer and calculated a dipole moment. Partial atomic charges on hydrogen atoms varied within 0.02 e. The error of the dipole moment was estimated for twist (C2) and envelope (CS) conformations. The error for the twist conformation was estimated to be +1.2% in comparison with QM calculations. The error was much higher for the envelope conformation, +7.5%, mostly due to the relative position of oxygen atom. Based on these calculations we make an assumption of partial charge equality.

b. Fitting of partial charges for the molecular triad

Fitting partial atomic charges for the polarizable force fields is computationally challenging for such a big molecule. Therefore, we divided the triad molecule into three constituents: carotenoid-polyene (C), diaryl-porphyrin (P), and C_{60}-pyrolle closely following its synthesis approach. [10] Breaking the triad molecule into these constituents facilitates finding the ground state optimized geometries for each constituent. It is known that finding equilibrium geometry for large molecules is not a trivial task. [11, 12] It was shown earlier that the absorption spectrum of the triad is very close to a linear combination of spectra for three constituents. The density of states calculated using DFT showed negligible hybridization of molecular orbitals from three constituents. These results indicate minor effects on electronic structure from covalent bonding of three constituents. [13] In turn, we obtain very small perturbations for combining three constituents into the triad as discussed in the Section II.1 Development of partial charges. The molecular dipole moments of both individual constituents and linear equilibrium triad is achieved as compared to QM calculations, see Table 3. The error for the linear triad using non-polarizable force field is +0.8% and polarizable force field is -14.4%.

We start fitting by breaking down the triad into three independent compounds. A methyl group has been added to the terminal atoms on each compound to account for covalent bonding as discussed in the methodology of partial charge fitting section in the main text. The three components fullerene-pyrrole, porphyrin-diaryl, and carotene-amide are shown in Fig. 1(b-d). Atomic dipole polarizabilities are given in Table S1 and resulting charges are given in Table S2 for tetrahydrofuran and in Table S4 for the triad.

c. The AM1-BCC method

The AM1-BCC (Austin Model 1 – Bond Charge Correction) is a fast and efficient method for generating partial charges for organic molecules. This model was designed to reproduce partial atomic charges obtained with the RESP method and HF/6-31G* theory level. This model combines AM1 population analysis [14] and further additive bond correction. The additive bond correction approach was parameterized considering a large set of training molecules. A combination of two steps (AM1-BCC methodology) gives accurate partial atomic charges for molecular dynamics simulations of organic molecules. The method validation was performed for a number of compounds by calculation of free energy of solvation. [15]

Important to note: The fitting of partial charges for the THF molecule in an additive model was performed for the twist conformation that would belong to C2 point group. Both methods give reasonable value of the dipole moment. We employ RESP methodology to fit partial charges to electrostatic potential surface obtained at B3LYP/cc-pvTZ//HF/6-31G* level of theory. The resulting dipole moment of THF using RESP methodology gives 1.64 D while AM1-BCC method gives dipole moment of 1.85 D. Taking into account all three conformations we obtain 1% of an improvement. Therefore, electrostatic potential dictates the quality of the fit.

Supplementary figures

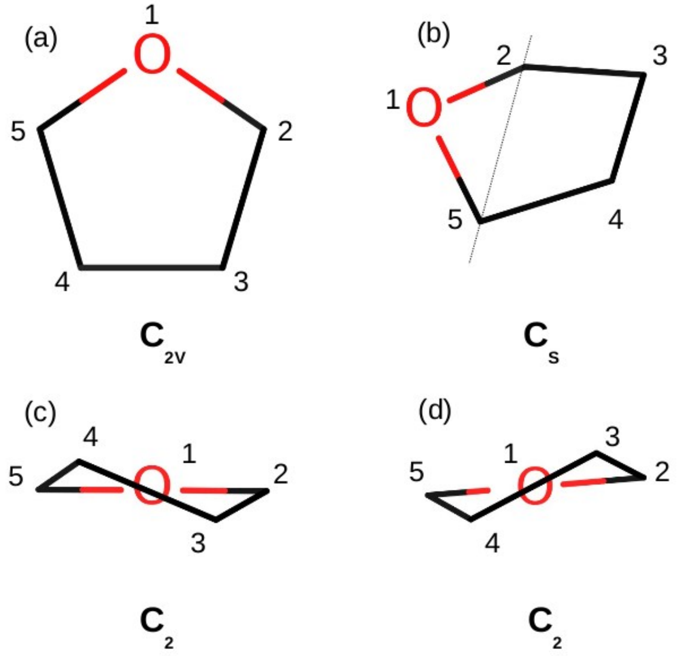


Fig. S1. Four conformations of tetrahydrofuran ordered by its conformational energy from the highest to the lowest. a) a planar conformation; b) an envelope conformation (${}^{1}E$); c) and d) twist conformations (${}^{4}T_{3}$ and ${}^{3}T_{4}$) identified in both crystal and the gas phase. Dotted line indicates bending in the envelope conformation. Crystallographic symmetry associated with the molecular conformation is given below each conformer. Only the envelope (${}^{1}E$) and twisted conformations (${}^{4}T_{3}$ and ${}^{3}T_{4}$) were used to fit the partial atomic charges for the non-polarizable and polarizable force fields. Hydrogen atoms are omitted for clarity.

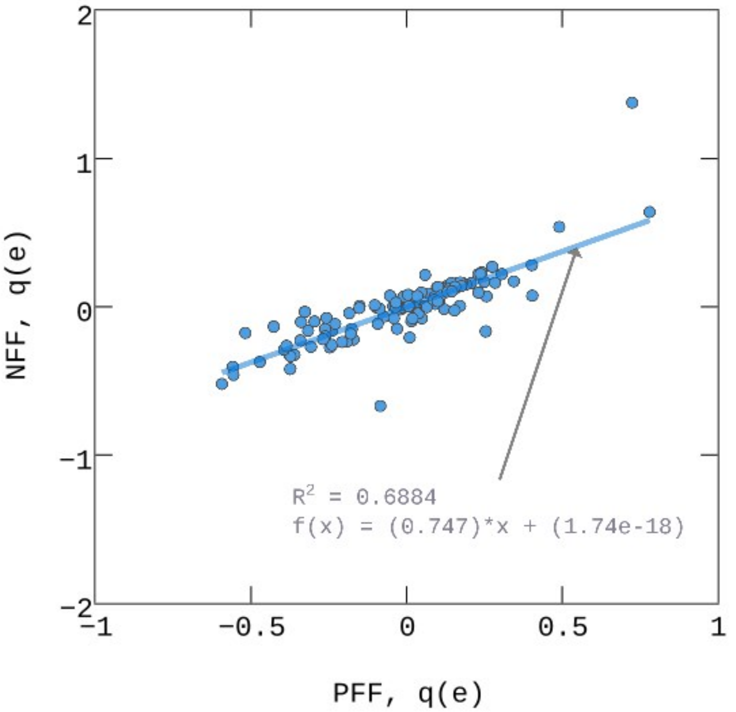


Fig. S2. Correlation of fitted charges for non-polarizable (NFF) and polarizable force fields (PFF). The linear regression equation and the correlation coefficient are provided in the figure.

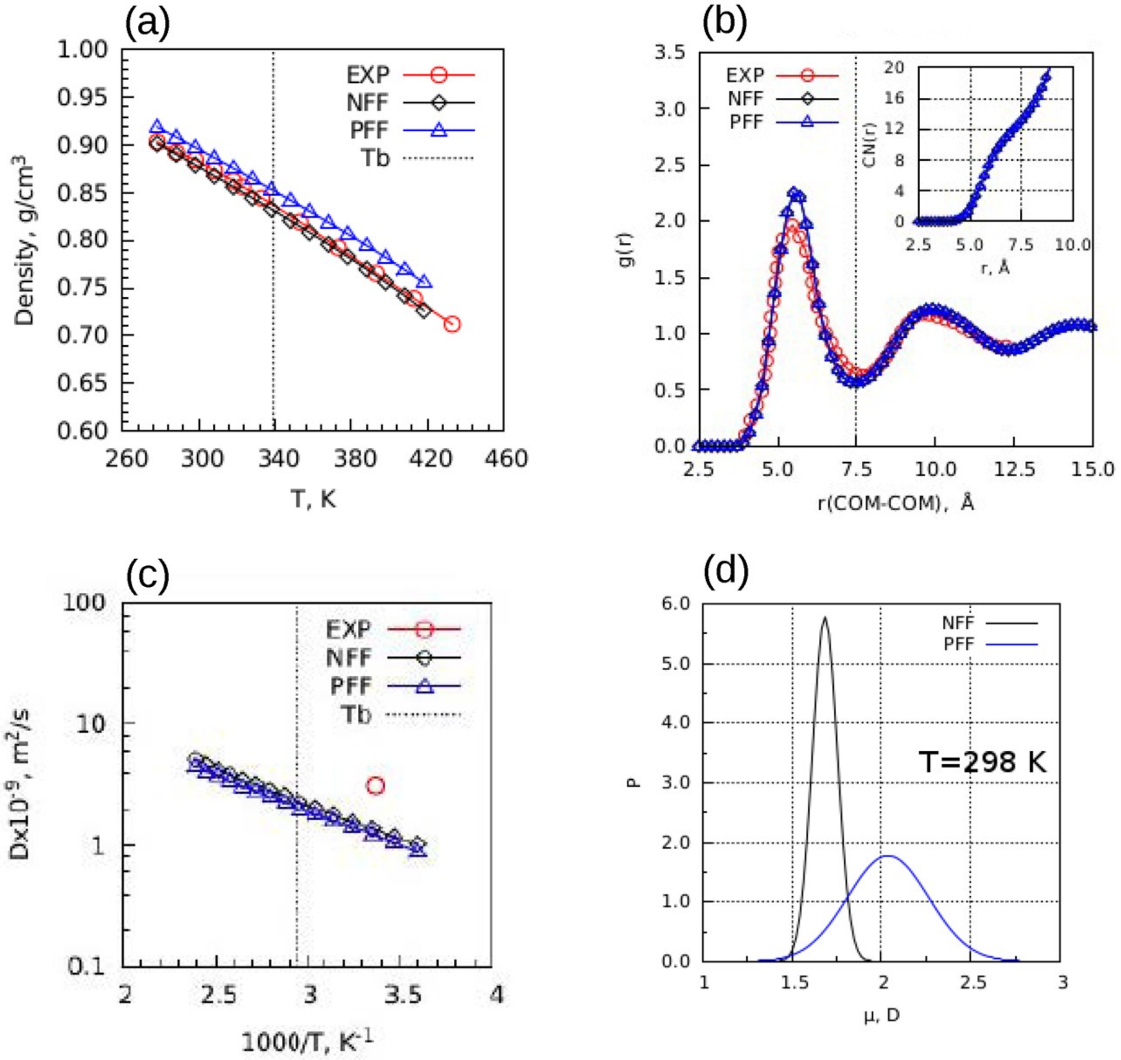
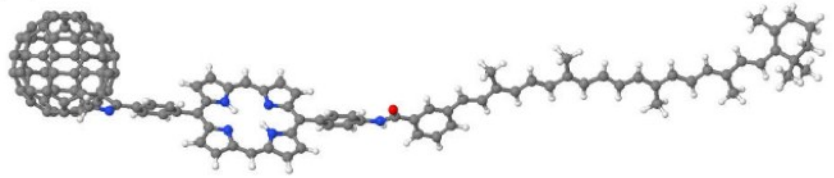
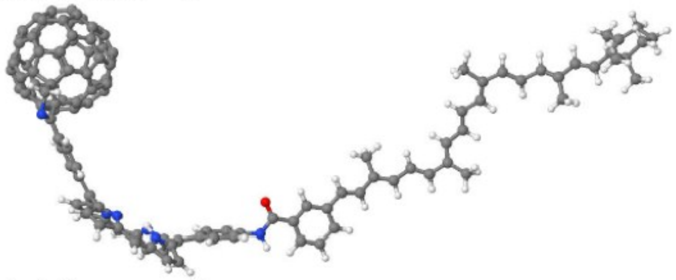


Fig. S3. Thermodynamic properties of tetrahydrofuran (THF). (a) liquid density ρ; (b) liquid structure g(r); (c) self-diffusion coefficient D; and (d) distributions of dipole moments P(μ). Red open circles indicate experimental data obtained from Ref.[16]. The figures were obtained using matplotlib[17].

(a) linear



(b) bent _1



(c) bent _2

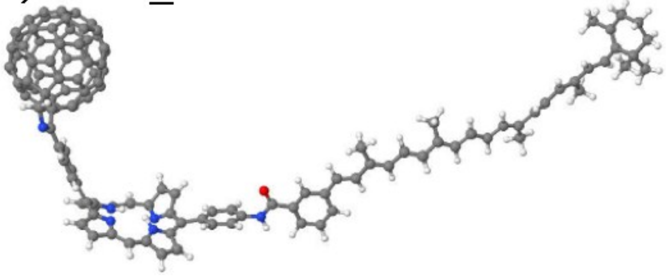


Fig. S4. Illustration of linear and bent conformations of the triad that was used to calculate the permanent dipole moments for the force fields. Atomic coordinates for these conformations are taken from the previous computational studies.[18]

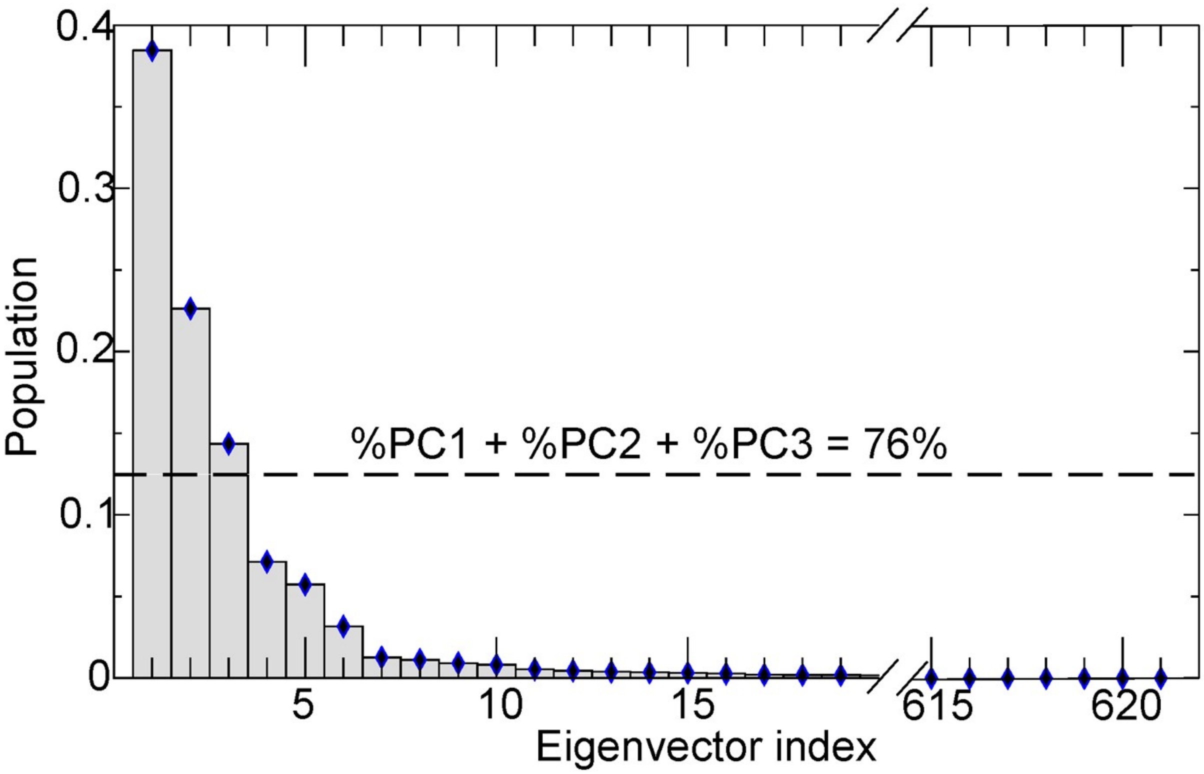


Fig. S5. Population of the variance that each principal component (PC) contributes. The leading three PCs comprise ~ 76% of the total variance.

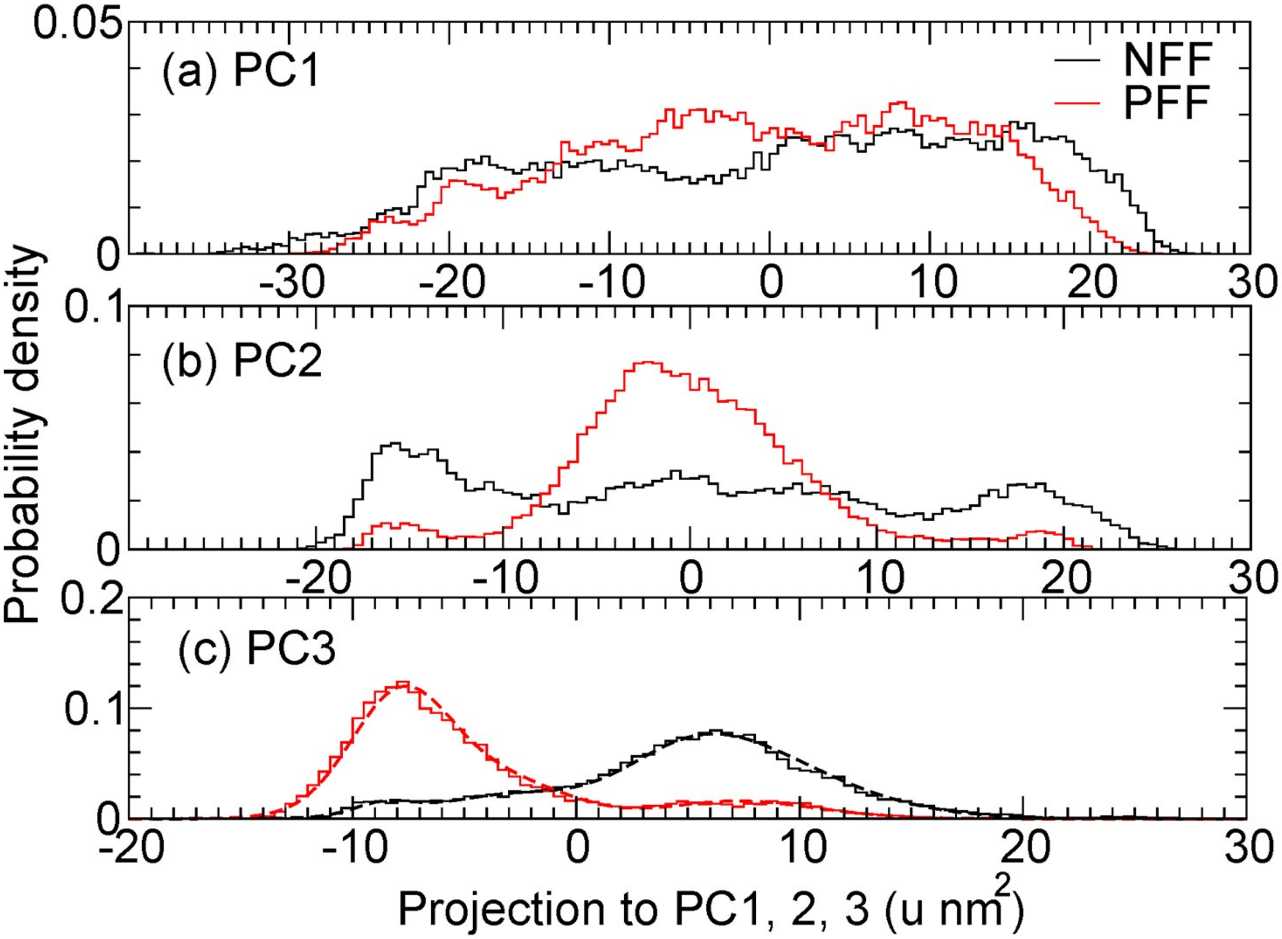


Fig. S6. Distribution of the projection to the three leading principal components (PCs) of the triad conformations. Non-polarizable (NFF) and polarizable force fields (PFF) are in black and red, respectively.

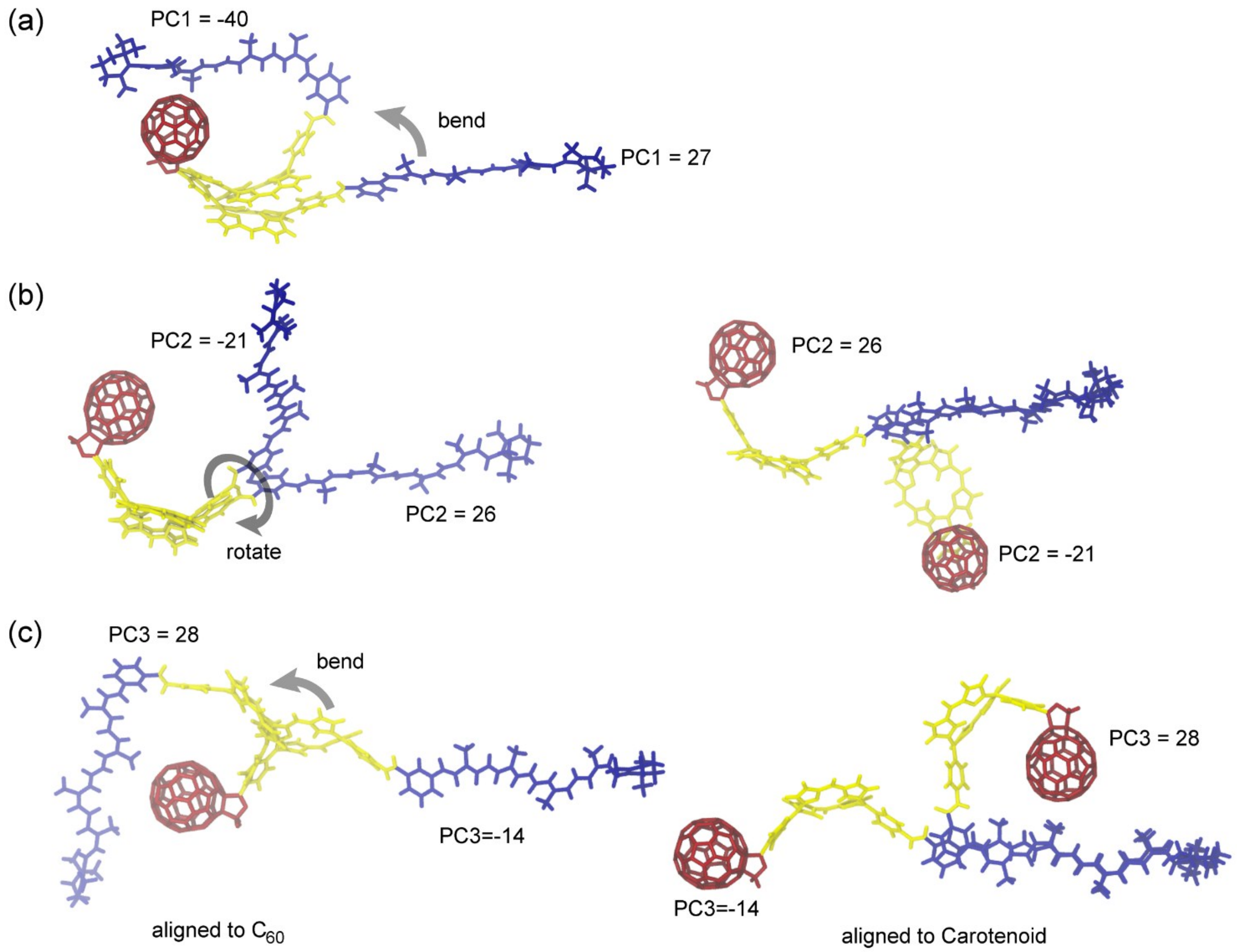


Fig. S7. Illustration of the motion represented by the leading three principal components (PCs). Structures that correspond to the extreme values of each PC are overlapped onto the fullerene (C_{60}) or carotenoid for guidance. C_{60}, porphyrin, and carotenoid are colored in red, yellow and blue, respectively. PC1 mainly represents a bending in the between the carotenoid and the porphyrin; PC2 represents a rotation about the "porphyrin-carotenoid" amide linkage; PC3 mainly represents a bending within porphyrin (between porphyrin and the benzene ring).

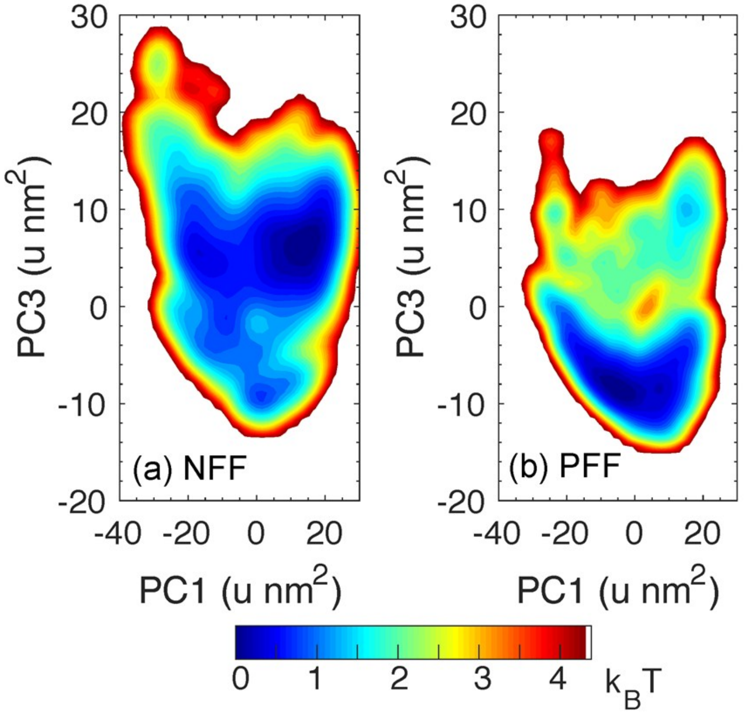


Fig. S8. Free energy surface of triad from principal component (PC) analysis on ensemble of triad employing non-polarizable (NFF) and polarizable force fields (PFF) projected onto PC1 and PC3. The ensemble of structures was obtained at the temperature of 298 K.

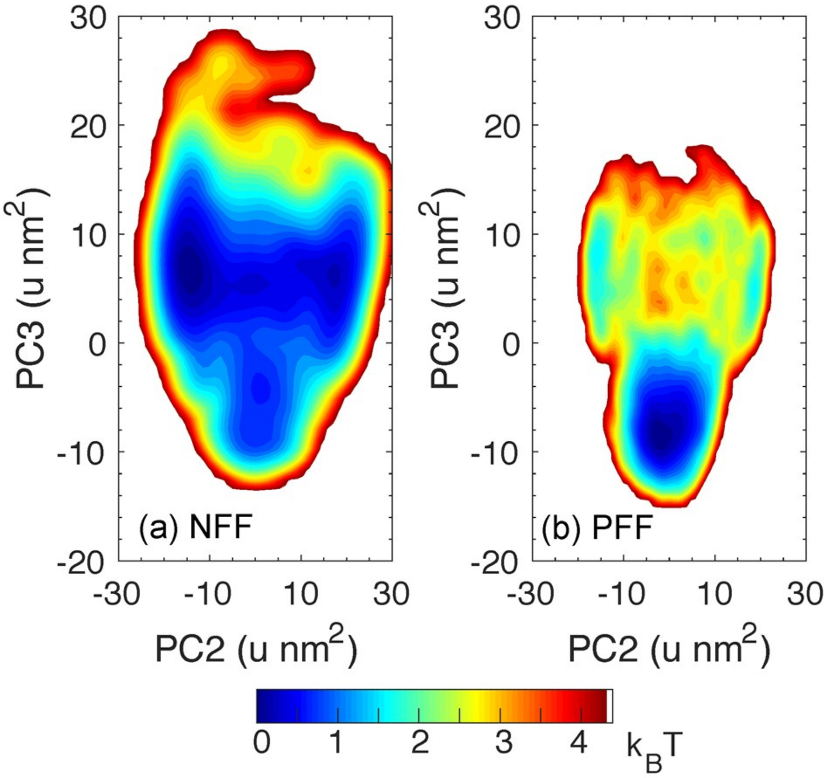


Fig. S9. Free energy surface of triad from principal component (PC) analysis on ensemble of triad employing non-polarizable (NFF) and polarizable force fields (PFF) projected onto PC2 and PC3. The ensemble of structures was obtained at the temperature of 298 K.

Supplementary tables

Table S1. Atomic dipole polarizability values. The values are taken from AMBER force field ff12polL. Two units are provided: Å and atomic unit (a. u.).

#	AMBER/FF12polL	Å^3	a.u.
1	C2 (sp2)	1.295	8.74220
2	C3 (sp3)	0.940	6.34290
3	N	0.960	6.48040
4	O2	0.605	4.08190
5	O3	0.615	4.14910
6	H	0.425	2.87130

Table S2. Partial atomic charges for THF fitted using AM1-BCC, DFT, RESP, and i-RESP methods for non-polarizable (NFF) and polarizable (PFF) force fields. The charges from DFT is taken from study by Balamurugan et al.[19] The unit is the elementary charge.

Charge (e)	AM1-BCC	DFT	RESP (NFF)	i-RESP (PFF)
C1	0.127400	0.254900	0.215638	0.184363
C2	-0.106400	-0.009200	-0.015749	0.003987
O	-0.427600	-0.494600	-0.407191	-0.381812
H1	0.044700	-0.002400	-0.005102	-0.008515
H2	0.051700	0.003200	0.006956	0.009793

Table S3. Partial charges on methyl (-CH3) groups of the triad constituents in electrons. All charges are listed in units of elementary charges.

Force Field	C_m	H_m	Residual
Carotene-amide (C)			
NFF	-0.211844	0.091065	0.061351
PFF	-0.130541	0.063672	0.060476
Diaryl-porphyrin (P), 2 methyl groups			
NFF	-0.359905	0.099518	-0.061351
PFF	-0.421871	0.120465	-0.060476
Fullerene-pyrrole (C_{60})			
NFF	0.418843	-0.119164	0.061351
PFF	0.074687	-0.004737	0.060476

Table S4. Partial atomic charges for the triad fitted using AM1-BCC, DFT, RESP, and i-RESP methods for non-polarizable (NFF) and polarizable force fields (PFF). The unit is the elementary charge. The AM1-BCC charges are taken from study by Su et al.[20] The DFT charges are taken from study by Balamurugan et al.[19]

#	Atom	AM1-BCC	DFT	RESP (NFF)	i-RESP (PFF)
1	ca	-0.016713	-	0.006498	0.171352
2	ca	0.000160	0.002800	-0.003747	-0.009193
3	ca	-0.047148	0.003500	-0.066576	-0.073155
4	ca	0.031439	0.002300	0.005281	-0.150484
5	ca	-0.000742	0.032300	0.004110	-0.043110
6	ca	-0.006275	0.021200	-0.003747	-0.009193
7	ca	-0.007091	0.003400	-0.007042	0.028492
8	ca	-0.005807	-	-0.005136	-0.096100
9	ca	0.002396	0.012000	-0.017880	-0.019211
10	ca	-0.001827	-	-0.007042	0.028492
11	ca	-0.022158	-	-0.075188	-0.257366
12	ca	-0.014486	-	-0.015983	0.120785
13	ca	0.002826	-	0.018263	0.092096
14	ca	-0.005181	0.023400	0.037656	0.102108
15	ca	-0.002743	0.002000	0.000302	0.010899
16	ca	0.001264	0.006500	-0.017880	-0.019211
17	ca	0.000297	-	0.002605	0.055627
18	ca	-0.000618	0.022400	-0.002399	-0.035153
19	ca	-0.000149	-	0.002605	0.055627
20	ca	0.002206	-	-0.005629	-0.010959
21	c3	-0.264693	0.239100	1.377631	0.724851
22	ca	0.201616	-	-0.034292	-0.327017
23	ca	0.232951	-	-0.034292	-0.327017
24	ca	-0.020650	0.172100	-0.078267	0.048904
25	ca	-0.012057	-	0.006498	0.171352
26	ca	-0.077860	0.011200	-0.165641	0.254321
27	ca	-0.020705	0.045600	0.070285	0.256820
28	ca	0.038635	0.012400	0.005281	-0.150484
29	ca	-0.026466	0.042100	-0.066576	-0.073155
30	ca	-0.024536	-	-0.075188	-0.257366
31	ca	-0.112163	0.006500	-0.165641	0.254321
32	ca	0.001826	0.024800	0.006716	-0.001925
33	ca	0.000863	-	-0.005629	-0.010959

34	ca	-0.001375	0.022300	0.006716	-0.001925
35	ca	-0.004771	-	0.004486	0.006836
36	c3	0.035737	0.076900	0.037374	-0.039213
37	ca	0.129666	0.012800	0.075072	0.403911
38	ca	0.122994	0.039000	0.075072	0.403911
39	ca	-0.027222	0.041000	-0.043121	-0.184461
40	ca	-0.003751	0.016000	0.000302	0.010899
41	ca	0.062639	0.183500	-0.078267	0.048904
42	ca	-0.071392	-	-0.134165	-0.427121
43	ca	-0.025553	0.035500	-0.043121	-0.184461
44	ca	-0.020042	0.016900	0.073656	0.013888
45	ca	0.003041	0.010000	0.009724	-0.029570
46	ca	-0.071361	-	-0.134165	-0.427121
47	ca	-0.022085	0.004900	0.073656	0.013888
48	ca	-0.060502	-	0.010630	-0.008490
49	ca	-0.034168	-	0.010630	-0.008490
50	ca	-0.007041	0.045800	0.004486	0.006836
51	ca	-0.016488	0.049400	0.070285	0.256820
52	ca	0.007937	-	0.009724	-0.029570
53	ca	0.007688	0.013100	0.004110	-0.043110
54	ca	0.009676	0.016100	0.018263	0.092096
55	ca	-0.009344	0.010300	-0.015983	0.120785
56	ca	-0.004367	0.019700	0.037656	0.102108
57	ca	-0.001233	0.022900	-0.005136	-0.096100
58	ca	0.000750	-	-0.011963	-0.087133
59	ca	0.000326	-	-0.011963	-0.087133
60	ca	-0.000808	0.037600	-0.002399	-0.035153
61	c2	-0.026536	0.189800	-0.669370	-0.084319
62	n2	0.081411	-	-0.103429	-0.339175
63	c3	-0.673646	0.808800	0.068293	-0.010237
64	h1	0.308087	-	-0.044180	0.038218
65	h1	0.309103	-	-0.044180	0.038218
66	ca	0.266250	0.119800	0.171474	0.344519
67	ca	-0.475571	-	-0.160555	-0.239166
68	ha	0.313334	-	0.121163	0.142920
69	ca	-0.368377	-	-0.257156	-0.239849
70	ha	0.289897	-	0.143249	0.151874

71	ca	0.357672	0.012600	0.270152	0.275181
72	ca	-0.435015	-	-0.160555	-0.239166
73	ha	0.310791	-	0.121163	0.142920
74	ca	-0.420295	0.150400	-0.257156	-0.239849
75	ha	0.298006	-	0.143249	0.151874
76	ce	0.137777	-	0.010946	-0.102404
77	cc	0.127101	0.193800	-0.076898	-0.040652
78	cd	-0.355038	-	-0.149189	-0.176626
79	ha	0.311506	-	0.140558	0.152530
80	cd	-0.418760	0.027100	-0.221273	-0.170854
81	ha	0.293892	-	0.158170	0.160436
82	cc	0.367502	0.185000	0.088643	0.071435
83	na	-0.432148	-	0.160607	0.207288
84	hn	0.423154	0.152600	-0.008032	-0.151634
85	ce	-0.531677	-	-0.274713	-0.246874
86	ha	0.272243	-	0.150645	0.191496
87	cd	0.196320	0.390600	0.215111	0.059375
88	cd	-0.422129	-	-0.233509	-0.191447
89	ha	0.287796	-	0.145647	0.145928
90	cc	-0.353829	-	-0.181649	-0.180020
91	ha	0.308578	-	0.134874	0.124355
92	cc	-0.019165	0.432100	0.074246	-0.053098
93	nd	-0.166705	-	-0.207861	0.009983
94	ce	0.127977	-	0.010946	-0.102404
95	cd	0.130630	0.281600	-0.076898	-0.040652
96	cd	-0.357237	-	-0.149189	-0.176626
97	ha	0.314710	-	0.140558	0.152530
98	cc	-0.418613	0.018600	-0.221273	-0.170854
99	ha	0.293539	-	0.158170	0.160436
100	cc	0.368522	0.264200	0.088643	0.071435
101	na	-0.430625	-	0.160607	0.207288
102	hn	0.422970	0.159300	-0.008032	-0.151634
103	cf	-0.532470	-	-0.274713	-0.246874
104	ha	0.272871	-	0.150645	0.191496
105	cd	0.196944	0.377700	0.215111	0.059375
106	cd	-0.421352	-	-0.233509	-0.191447
107	ha	0.288621	-	0.145647	0.145928

108	cc	-0.354778	0.006600	-0.181649	-0.180020
109	ha	0.309869	-	0.134874	0.124355
110	cd	-0.026173	0.421500	0.074246	-0.053098
111	nc	-0.167784	-	-0.207861	0.009983
112	ca	0.444651	0.359100	0.270152	0.275181
113	ca	-0.368446	-	-0.257156	-0.239849
114	ha	0.335352	-	0.143249	0.151874
115	ca	-0.430704	0.044600	-0.160555	-0.239166
116	ha	0.304457	-	0.121163	0.142920
117	ca	0.272135	0.079800	0.171474	0.344519
118	ca	-0.487757	-	-0.257156	-0.239849
119	ha	0.259166	-	0.143249	0.151874
120	ca	-0.419754	0.035800	-0.160555	-0.239166
121	ha	0.306114	-	0.121163	0.142920
122	n	-0.449120	-	-0.419810	-0.373955
123	hn	0.323013	0.173500	0.281096	0.402870
124	c	0.023666	0.811600	0.639350	0.781086
125	o	-0.218336	-	-0.521022	-0.593622
126	ca	0.241385	-	-0.176289	-0.518125
127	ca	-0.560048	0.106000	-0.097954	0.015667
128	ha	0.305363	-	0.095981	0.047561
129	ca	0.494315	0.088400	0.166869	0.250249
130	ca	-0.426518	0.044000	-0.150097	-0.262109
131	ha	0.264580	-	0.126580	0.158130
132	ca	-0.267811	0.105300	-0.148990	-0.030517
133	ha	0.264702	-	0.126088	0.102448
134	ca	-0.406077	0.070500	-0.079172	0.018652
135	ha	0.257076	-	0.080945	0.004236
136	ce	-0.387748	-	-0.199281	-0.261521
137	ha	0.275647	0.039300	0.145241	0.133682
138	cf	-0.350941	0.090400	-0.237527	-0.207410
139	ha	0.247944	-	0.125712	0.132320
140	cf	0.385837	-	0.232519	0.240991
141	c3	-0.892965	0.775100	-0.098827	-0.295969
142	hc	0.256388	-	0.042821	0.104681
143	hc	0.269083	-	0.042821	0.104681
144	hc	0.267937	-	0.042821	0.104681

145	ce	-0.405087	0.092500	-0.327862	-0.375896
146	ha	0.249376	-	0.151812	0.162133
147	ce	-0.272814	-	0.003221	0.060065
148	ha	0.264414	0.073000	0.132706	0.098015
149	cf	-0.371848	0.126100	-0.324298	-0.360431
150	ha	0.257101	-	0.162018	0.178068
151	cf	0.390079	-	0.218140	0.229956
152	c3	-0.895183	0.827400	-0.218167	-0.268217
153	hc	0.265561	-	0.066786	0.089461
154	hc	0.268155	-	0.066786	0.089461
155	hc	0.257415	-	0.066786	0.089461
156	ce	-0.401838	0.063400	-0.269906	-0.307344
157	ha	0.251906	-	0.121560	0.136876
158	ce	-0.262607	-	-0.114854	-0.092670
159	ha	0.249826	0.022700	0.160218	0.144016
160	cf	-0.270031	0.001000	-0.114854	-0.092670
161	ha	0.253537	0.022300	0.160218	0.144016
162	cf	-0.398769	0.047400	-0.269906	-0.307344
163	ha	0.248796	-	0.121560	0.136876
164	ce	0.388277	-	0.220913	0.237574
165	c3	-0.894545	0.843100	-0.218167	-0.268217
166	hc	0.256805	-	0.066786	0.089461
167	hc	0.267123	-	0.066786	0.089461
168	hc	0.266989	-	0.066786	0.089461
169	ce	-0.369570	0.111400	-0.333341	-0.373352
170	ha	0.254182	-	0.164104	0.172493
171	cf	-0.280385	-	-0.001038	0.065332
172	ha	0.265336	0.067100	0.132708	0.100649
173	cf	-0.406936	0.050900	-0.289004	-0.394176
174	ha	0.248415	-	0.139915	0.175418
175	ce	0.375886	-	0.162823	0.284562
176	c3	-0.897414	0.783600	-0.227340	-0.341643
177	hc	0.256169	-	0.073319	0.109058
178	hc	0.268464	-	0.073319	0.109058
179	hc	0.262840	-	0.073319	0.109058
180	ce	-0.373239	0.068900	-0.263831	-0.385960
181	ha	0.276660	-	0.133858	0.155133

182	cf	-0.400745	0.143500	0.095541	0.230992
183	ha	0.251899	-	0.071958	0.034130
184	cf	0.218456	-	-0.404857	-0.558344
185	c2	0.167888	-	0.220639	0.306175
186	c3	-0.905687	0.980300	-0.372028	-0.471765
187	hc	0.292921	-	0.100096	0.131615
188	hc	0.256999	-	0.100096	0.131615
189	hc	0.244371	-	0.100096	0.131615
190	c3	-0.552933	0.687600	-0.116183	-0.229536
191	hc	0.249435	-	0.047017	0.087528
192	hc	0.242174	-	0.047017	0.087528
193	c3	-0.507182	0.301900	-0.025102	0.154097
194	hc	0.239162	-	0.027690	-0.034086
195	hc	0.242736	-	0.027690	-0.034086
196	c3	-0.507741	0.521200	-0.161590	-0.316596
197	hc	0.233384	-	0.036943	0.099561
198	hc	0.232511	-	0.036943	0.099561
199	c3	0.185277	-	0.538791	0.490670
200	c3	-0.825084	0.722900	-0.458483	-0.556553
201	hc	0.259261	-	0.105184	0.146008
202	hc	0.242851	-	0.105184	0.146008
203	hc	0.238169	-	0.105184	0.146008
204	c3	-0.818034	0.693000	-0.458483	-0.556553
205	hc	0.238206	-	0.105184	0.146008
206	hc	0.255434	-	0.105184	0.146008
207	hc	0.246127	-	0.105184	0.146008
	Total:	**0.000000**	**0.000000**	**0.000000**	**0.000000**

Table S5. Atom indices for the molecular triad. Each atom is labelled in the format of element and numerical index. Carbon atoms C20 and C193 (in orange) are used to define then end-to-end distance. Atoms C61, C76, C94 and N122 (in red) are used to define the pseudo dihedral angle.

Atom	Sub-Unit	Atom	Sub-Unit	Atom	Sub-Unit
C1	Fullerene	C71		C141	
C2		C72		H142	
C3		H73		H143	
C4		C74		H144	
C5		H75		C145	
C6		C76	Porphyrin	H146	
C7		C77		C147	
C8		C78		H148	
C9		H79		C149	
C10		C80		H150	
C11		H81		C151	
C12		C82		C152	
C13		N83		H153	
C14		H84		H154	
C15		C85		H155	
C16		H86		C156	
C17		C87		H157	
C18		C88		C158	
C19		H89		H159	
C20		C90		C160	
C21		H91		H161	
C22		C92		C162	
C23		N93		H163	
C24		C94		C164	
C25		C95		C165	
C26		C96		H166	
C27		H97		H167	
C28		C98		H168	
C29		H99		C169	
C30		C100		H170	
C31		N101		C171	
C32		H102		H172	
C33		C103		C173	
C34		H104		H174	
C35		C105		C175	
C36		C106		C176	
C37		H107		H177	
C38		C108		H178	
C39		H109		H179	
C40		C110		C180	

C41		N111		H181	
C42		C112	Phenyl	C182	
C43		C113		H183	
C44		H114		C184	
C45		C115		C185	
C46		H116		C186	
C47		C117		H187	
C48		C118		H188	
C49		H119		H189	
C50		C120		C190	
C51		H121		H191	
C52		N122	Carotene	H192	
C53		H123		C193	
C54		C124		H194	
C55		O125		H195	
C56		C126		C196	
C57		C127		H197	
C58		H128		H198	
C59		C129		C199	
C60		C130		C200	
C61	Pyrrole	H131		H201	
N62		C132		H202	
C63		H133		H203	
H64		C134		C204	
H65		H135		H205	
C66	Phenyl	C136		H206	
C67		H137		H207	
H68		C138			
C69		H139			
H70		C140			

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