Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

The Second-Order NLO and TADF Properties of Donor−Acceptor Dihydropyrene – Cyclophanediene System: the Impact of Molecular Architectures and Polarizable Environment

Yao Yao[a], Hong-Liang Xu[a,*], and Zhong-Min Su [b]

a. Institute of Functional Material Chemistry, National & Local United Engineering Laboratory for Power Batteries, Department of Chemistry, Northeast Normal University, Changchun, 130024, People's Republic of China.

b. School of Chemistry & Environmental Engineering, Changchun University of Science and Technology, Changchun, 130012, People's Republic of China.

Email: hlxu@nenu.edu.cn

Table S1 The isotropic component of the molecular polarizability α (Bohr^3), the volume occupied by a single molecule V (Bohr^3) and the static dielectric constant ε were calculated at the ωB97XD/6-31G (d, p) level.

Table S2 The relative free energies differences (ΔG kcal/mol) between DHP forms and CPD forms and single point energy (a.u.).

Table S3 The energy of the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and energy gap (E_{gap}) in the gas phase and acetonitrile solution.

Table S4 The diagonal tensorial and off-diagonal components (a.u.) of all investigated compounds calculated at ωB97XD/6-31 + G (d, p) level in acetonitrile solution.

Table S5 The calculated static/dynamic β_{HRS} values, depolarization (DR) and anisotropy (ρ) ratios at ωB97XD/6-31 + G (d, p) level in benzene, acetone and acetonitrile.

Table S6 The optimal ω values of LC-BLYP and LC-ωPBE for all the studied compounds in the gas and solid phases.

Fig. S1 The optimized structures of compounds **1C**, **2C** and **2O** in acetonitrile solvent incorporation with important dihedral angles.

Fig. S2 Isosurfaces (isovalue = 4) of the static β density of all the studied compounds calculated at the ωB97XD/6-31+ G (d, p) level in acetonitrile solution (pure color and blue color parts represent the positive and negative contribution to β).

Fig.S3 The dynamic β_{HRS} values at different wavelengths calculated at ωB97XD/6-31 + G (d, p) level in acetonitrile.

Fig. S4 The UV-Vis absorption spectrum of compound **1C** calculated by five different functionals in acetonitrile solvent at ωB97XD/6-31 + G (d) level (left). The absorption spectrum of compound **1C** determined in the experiment (right).

Fig. S5 Convergent behaviors of β_{tot} values for compounds and its dependent on the first 100 states.

Computational Details

The static dielectric constant ε was evaluated via Clausius–Mossotti equation [1], which reads:

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi\alpha}{3\ V} \tag{1}$$

where α is the isotropic component of the molecular polarizability, V is volume occupied by a single molecule and ε is the static dielectric constant.

The β_{yyy} can be calculated in the following formula:

$$\beta_{yyy} = -\frac{1}{2}\int -\rho_{yy}^{2}(r)\, y dr \tag{2}$$

The β densities, ρ_{yy}, is defined according to

$$\rho_{yy}^{(2)}(\mathrm{r}) = \frac{\partial^2 \rho(\mathrm{r})}{\partial F_{\mathrm{y}}^2}|_{F=0} \tag{3}$$

The $\rho_{yy}^{(2)}(\vec{r})$ can be calculated at each spatial point in the discretized space by using the following second-order numerical differentiation formulas:

$$\rho_{yy}^{(2)}(\vec{r}) = \frac{\rho(\vec{r},F^y) - 2\rho(\vec{r},0) + \rho(\vec{r},-F^y)}{(F^y)^2} \tag{4}$$

Where $\rho(\vec{r},F^y)$ represent the electron density at spatial point $\vec{r}$ in the presence of electric field F^y. The applied electric field along y-axis is 0.003 a.u.

Table S1 The isotropic component of the molecular polarizability α ($Bohr^3$), the volume occupied by a single molecule V ($Bohr^3$) and the static dielectric constant ε were calculated at ωB97XD/6-31G (d, p) level.

Compound	α	V	ε
1C	431	3231	4.8
1O	325	3248	3.2
2C	469	4421	3.4
2O	408	4437	2.9

Table S2 The relative free energies differences (ΔG kcal/mol) between close-ring forms and open-ring forms, as well as single point energy (a.u.) calculated at M06-2X/6-311++G (d, p) level at room temperature in acetonitrile solvents.

	1C	**1O**	**2C**	**2O**
E(SP)	-1205.510	-1205.481	-1519.945	-1519.921
G	-1205.154	-1205.127	-1519.375	-1519.350
ΔG	–		-15.865	

Table S3 The energy of the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and energy gap (E_{gap}) in the gas phase and acetonitrile solution.

Gas phase			
Compound	HOMO (eV)	LUMO (eV)	E_{gap} (eV)
1C	-6.69	-1.63	5.06
1O	-7.28	-1.10	6.18
2C	-6.65	-1.32	5.33
2O	-7.13	-0.97	6.16
Solvent = acetonitrile			
1C	-6.55	-1.65	4.90
1O	-7.20	-1.04	6.16
2C	-6.56	-1.43	5.13
2O	-7.04	-0.98	6.06

Table S4 The diagonal tensorial and off-diagonal components (a.u.) of all investigated compounds calculated at ωB97XD/6-31 + G (d, p) level in acetonitrile solution.

	2-C	**2-O**
β_{XXX}	-444.71	-1225.27
β_{XXY}	-1049.88	-2604.22
β_{XYY}	-14188.10	-4443.18
β_{YYY}	-37737.00	-7581.60
β_{XXZ}	-234.67	102.25
β_{XYZ}	715.63	209.69
β_{YYZ}	2093.75	601.26
β_{XZZ}	80.91	96.66
β_{YZZ}	372.40	-39.81
β_{ZZZ}	39.27	161.11

As shown in Table 2, the β_y total component of compound **2C** is the largest tensor compared to β_x and β_z values. From Table S4, the diagonal tensorial component β_{yyy} and off-diagonal tensorial components β_{xxy} and β_{zzy} are -37737 a.u., -1049.88 a.u. and 372.40 a.u., respectively, which clearly shows that the large β_y total component can be attributed to the large β_{yyy}. In addition, the β_x total component is the second largest one, which can be attributed the large off-diagonal tensorial component β_{xyy}. The same results can be found in compound **2O**. Notably, the β_{yyy} value of compound **2C** is 5.0 times larger than that of compound **2O**, leading inevitably to the large difference in β_{tot}.

Table S5 The calculated static/dynamic β_{HRS} values, depolarization (DR) and anisotropy (ρ) ratios at ωB97XD/6-31 + G (d, p) level in benzene, acetone and acetonitrile.

	Static (λ=∞)			Dynamic (λ = 1907 nm)		
Compound	β_{HRS}	DR	ρ	β_{HRS}	DR	ρ
benzene						
1C	21666	4.69	0.89	39524	4.85	0.86
1O	4119	4.76	0.87	5210	4.82	0.82
2C	9195	4.79	0.86	16423	4.97	0.84
2O	2922	4.81	0.86	3686	4.90	0.86
acetone						
1C	48372	4.62	0.90	36932	4.82	0.86
1O	6302	4.72	0.88	5081	4.81	0.86
2C	17194	4.25	1.00	12958	4.71	0.88
2O	4730	4.87	0.84	3453	4.94	0.83
acetonitrile						
1C	51111	4.62	0.91	36310	4.81	0.86
1O	6454	4.72	0.88	5032	4.82	0.86
2C	17998	4.23	1.01	12705	4.70	0.88
2O	4870	4.88	0.84	3409	4.95	0.83

Table S6 The optimal ω values of LC-BLYP and LC-ωPBE for all the studied compounds in the gas and solid phases.

	Gas phase	
Compound	LC-BLYP	LC-ωPBE
1C	0.1826	0.1778
1O	0.2053	0.2012
2C	0.1679	0.1646
2O	0.1837	0.1806
	Solid phase	
1C	0.0385	0.0379
1O	0.0607	0.0600
2C	0.0486	0.0480
2O	0.0648	0.0641

As shown in Table S5, compared with the default ω of the LC-BLYP (0.33 $Bohr^{-1}$) and LC-ωPBE functional (0.40 $Bohr^{-1}$), the optimal ω values of molecules significantly are reduce respectively to 0.1679 – 0.2053 and 0.1646 – 0.2012 $Bohr^{-1}$ in vacuum. Significantly, the ω values decrease further to 0.0385 – 0.0648 and 0.0379 – 0.0641 $Bohr^{-1}$ for LC-BLYP and LC-ωPBE functional, when considered a dielectric constant ε of solid film. The smaller ω values obtained in the simulated solid-state environment can be attributed to a fact that the electron density in the crystal is more spatially delocalized than that of in the gas-phase isolated molecule [2].

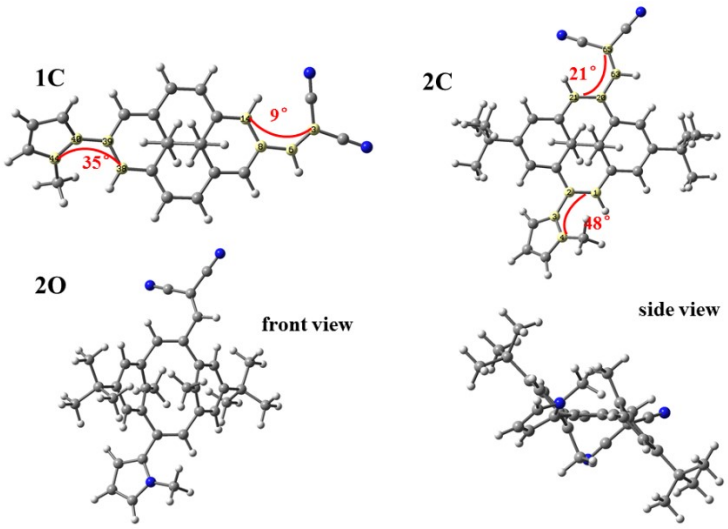

Fig.S1 The optimized structures of compounds **1C**, **2C** and **2O** in acetonitrile solvent incorporation with important dihedral angles.

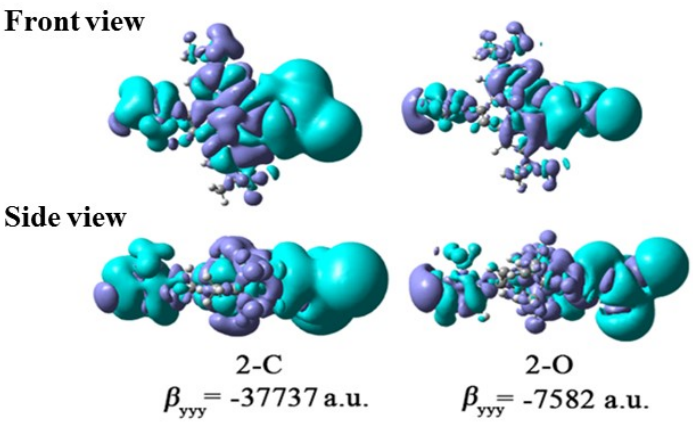

Fig. S2 Isosurfaces (isovalue = 4) of the static β density of all the studied compounds calculated at ωB97XD/6-31+ G (d, p) level in acetonitrile solution (pure color and blue color parts represent the positive and negative contribution to β).

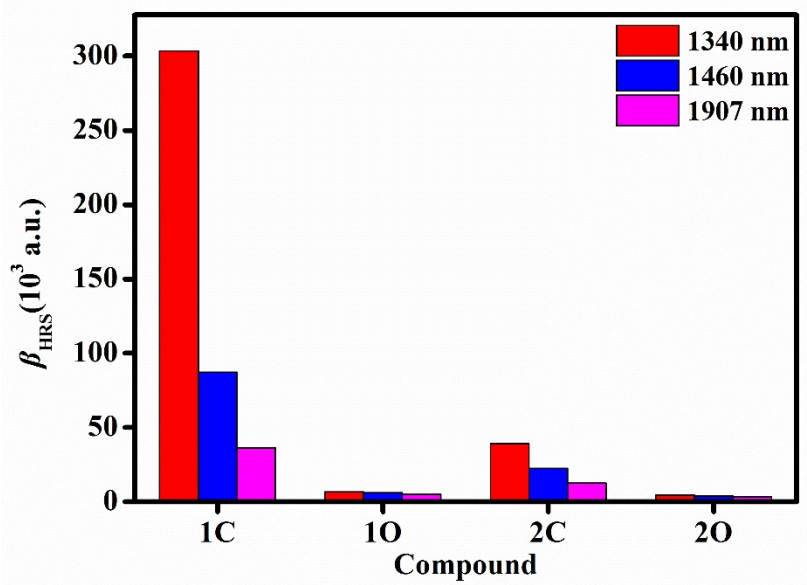

Fig.S3 The dynamic β_{HRS} values at different wavelengths calculated at ωB97XD/6-31 + G (d, p) level in acetonitrile.

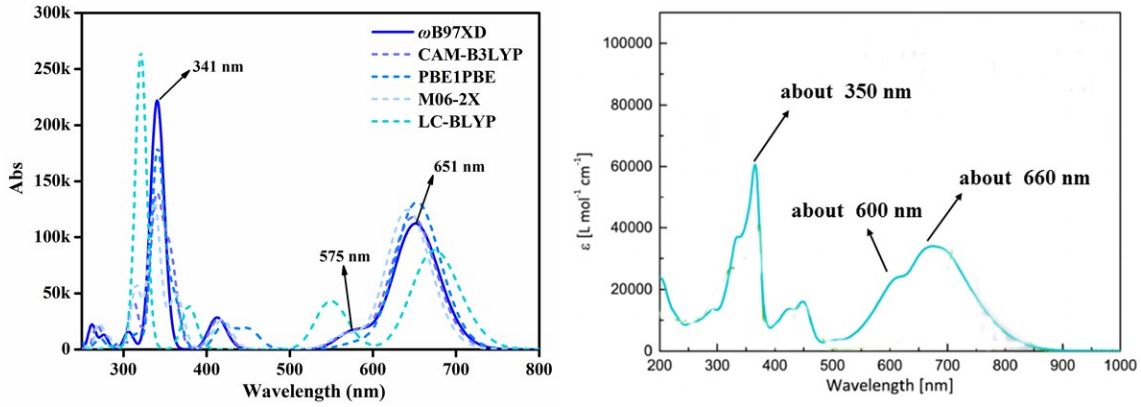

Fig. S4 The UV-Vis absorption spectrum of compound **1C** calculated by five different functionals in acetonitrile solvent at ωB97XD/6-31 + G (d) level (left). The absorption spectrum of compound **1C** determined in the experiment (righ)[3].

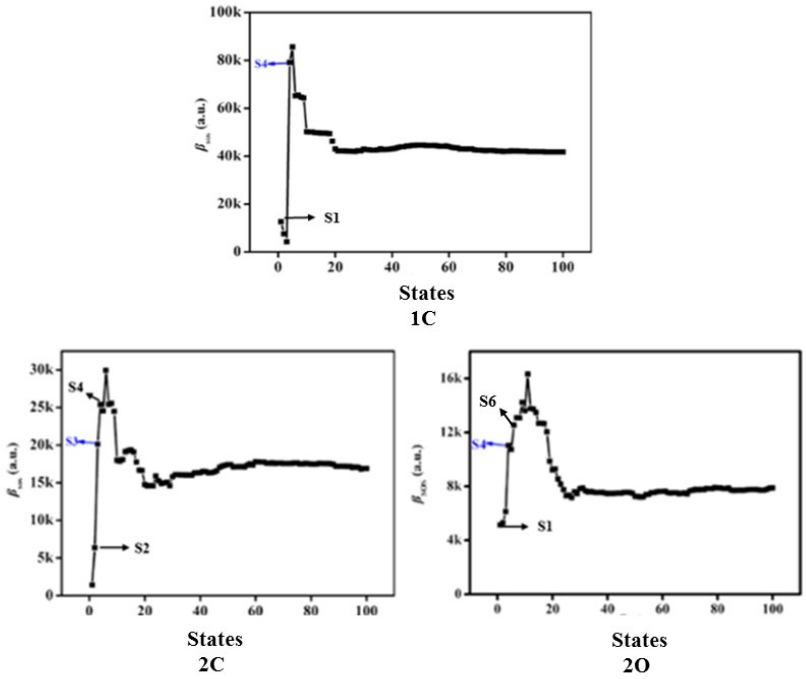

Fig. S5 Convergent behaviors of β_{tot} values for compounds and its dependent on the first 100 states.

Optimized structure (gas phase)

Compound 1C

8.43190600	-0.94876900	-0.12655300
7.36873300	-0.48533100	-0.10552100
6.04558400	0.06709600	-0.07881700
5.97077400	1.49592900	-0.11858600
5.92781800	2.65503500	-0.15098000
4.97828900	-0.78004200	-0.00546500
5.25200100	-1.83160800	0.04416600
3.56003100	-0.52662200	0.03705000
2.73430200	-1.64312500	0.21326000
3.18489300	-2.63297000	0.25005900
1.34685700	-1.53733500	0.29307600
0.72858700	-0.15856300	0.43412100
1.62252700	0.95362800	-0.08037400
2.97198300	0.76324800	-0.16503900
3.59965700	1.60231700	-0.44111500
-0.61666300	-0.12271900	-0.30478300
-0.45129800	-0.35606200	-1.84189700
0.17014000	0.42153500	-2.29013900
-0.00009100	-1.33063400	-2.03870000
-1.43726700	-0.32575700	-2.31181100
0.55913700	0.08923700	1.96379300
-0.07610800	-0.67462800	2.41788800
0.12548200	1.07220100	2.16047100
1.54296600	0.04768300	2.43707000
1.00014200	2.21157300	-0.32575400
1.63840400	3.07298700	-0.50317000
-0.36180100	2.36565200	-0.30445600
-0.79741400	3.35417200	-0.41837300
0.49649800	-2.63255700	0.38360100
0.92694500	-3.62856200	0.45241300
-0.89876100	-2.48471100	0.41687200
-1.52507400	-3.35255200	0.60212100
-1.50055200	-1.25504200	0.17537700
-1.23907800	1.25123900	-0.17298200
-3.06277400	2.34469000	-0.12659200
-3.52322500	-1.87991100	0.49437100
-2.59966100	1.36316200	-0.08676000
-2.88377900	-1.04282500	0.23191000
-3.44164200	0.22248500	0.07077800
-4.88252600	0.44569100	0.15415600
-5.54956500	1.51078600	0.73788600
-6.93522600	1.27675100	0.61445300

-7.07999100	0.08450200	-0.05550800
-5.84180100	-0.42587400	-0.32956400
-5.62998300	-1.61878300	-1.12747000
-5.54673800	-2.51408100	-0.50384100
-4.72006100	-1.51638000	-1.71993800
-6.47489500	-1.74295800	-1.80674000
-7.96895000	-0.43873600	-0.37607600
-7.73728700	1.90466600	0.97234700
-5.07358000	2.34221700	1.23773600

Compound 1O

-2.57208800	-1.64080500	-0.14730600
-1.21718800	-1.55171800	-0.45562900
-0.71376800	-0.33355500	-0.95831900
-1.45117300	0.83918700	-0.67409600
-2.80702800	0.73379900	-0.37965400
-3.41555900	-0.52164600	-0.21408700
-0.32036300	-2.64601000	0.01214300
0.76229900	-2.46198000	0.79420100
0.54383700	-0.29238600	-1.77961700
-0.79737700	2.15115500	-0.40278800
0.26438000	2.32888000	0.40875500
1.16566500	1.23913300	0.87900600
0.66881800	0.00912000	1.35763000
1.41175300	-1.14405200	1.04522300
2.75849700	-1.02265800	0.68801200
3.35458900	0.22760400	0.50745700
2.51195900	1.34497100	0.52669900
-0.59292600	-0.06507700	2.17617700
4.78330700	0.40124600	0.21611500
-4.82959000	-0.73451900	0.02008200
2.90175900	2.30008500	0.18666800
3.33849100	-1.92730600	0.53079800
-0.65372500	-3.66717900	-0.16055000
0.58344500	3.35203800	0.59635900
-2.97553500	-2.59553500	0.18142100
-3.37159100	1.64458800	-0.21743000
1.18622200	0.55579900	-1.54637600
1.11648500	-1.21460000	-1.68332800
0.24002600	-0.19511400	-2.82841300
-1.34981800	0.65442100	1.86501200
-1.02784800	-1.06421100	2.17366500
-0.32714700	0.17287600	3.21238600
1.28752100	-3.34993400	1.14071200

-1.32357000	3.03813400	-0.74865800
5.48478200	-0.34933700	-0.70623900
6.78648400	0.07859900	-0.72864300
6.93181800	1.10075600	0.17667600
5.66334700	1.30968300	0.76956900
5.40926400	2.02249000	1.54103300
7.84630900	1.63493600	0.38784300
7.50008700	-0.37793200	-1.39879300
4.94914500	-1.35809200	-1.59668900
5.53400800	-1.36584600	-2.51807900
4.98581100	-2.35725600	-1.15049400
3.91282200	-1.12200200	-1.84485000
-5.88296600	0.11242500	-0.11907800
-5.09500300	-1.73966700	0.33999900
-7.20618000	-0.35591200	0.18093600
-5.78575200	1.46955900	-0.56857500
-5.71642400	2.56925400	-0.93020200
-8.26859300	-0.74920700	0.42728100

Compound 2C

-0.99420600	-2.38000100	-0.28369400
-2.09595300	-1.46847400	-0.23913300
-3.46011600	-2.01105200	-0.32500400
-3.92124000	-2.99879700	0.52149400
-5.20248800	-3.32793200	0.16885700
-5.57362800	-2.56226200	-0.90995100
-4.47391700	-1.72729500	-1.22073400
-4.40172600	-1.00917500	-2.02510000
-6.52709400	-2.59927600	-1.41563800
-5.74865300	-4.07566800	0.72500100
-3.20796100	-3.56917400	1.64630600
-2.57621700	-4.40938500	1.34282200
-2.57631700	-2.80992600	2.11033500
-3.93127700	-3.92032400	2.38405400
0.30306700	-1.98934900	-0.07685500
1.40251000	-2.88263600	-0.15560600
2.70055300	-2.44318100	-0.10951300
2.96195200	-1.03235700	-0.02083700
1.98358300	-0.10091000	0.14606600
2.21582100	1.32610200	0.24152300
1.14263600	2.20318800	0.26626900
-0.19197300	1.78749400	0.07396100
-1.25119800	2.65067400	0.17850700

-2.60468900	2.22231300	0.06610100
-2.86720100	0.87391300	-0.06816500
-1.85260300	-0.10366500	-0.18066200
-0.42114200	0.36534200	-0.37999300
-0.17670300	0.36221800	-1.92008300
0.55347200	-0.56300600	0.36149600
0.32590900	-0.54346000	1.90441000
-0.69888600	-0.83601400	2.14521400
0.51403700	0.44740900	2.32302300
1.01278100	-1.25392500	2.37077500
0.83427600	0.70002800	-2.16091100
-0.88780800	1.04697800	-2.38831400
-0.32697800	-0.63554900	-2.33760100
-3.71646400	3.27031100	0.17555800
-3.53269200	4.31065400	-0.94680300
-3.59521100	3.83518500	-1.93048700
-4.31500400	5.07438900	-0.88550000
-2.56649300	4.81908100	-0.88051900
-3.63442200	3.97052100	1.54611600
-3.75187500	3.24712700	2.35878400
-4.42981600	4.71780000	1.63518400
-2.68073400	4.48676200	1.68866200
-5.11406600	2.65288000	0.03401100
-5.23408500	2.13658900	-0.92366500
-5.86876800	3.44350600	0.08271400
-5.32970200	1.94152800	0.83733800
3.90076600	-3.38832000	-0.21161800
4.70558500	-3.06217000	-1.48542400
4.08359700	-3.18041700	-2.37775400
5.09494200	-2.04031600	-1.47926500
5.56127600	-3.73978100	-1.57141900
3.47901700	-4.86200800	-0.27563400
2.88422100	-5.07617900	-1.16908900
2.90020500	-5.15534400	0.60590700
4.36985900	-5.49581300	-0.31442200
4.79626200	-3.19794900	1.02868900
5.17346700	-2.17451300	1.10941300
5.66169600	-3.86640200	0.97488000
4.24378900	-3.42654400	1.94535800
3.57262100	1.80053700	0.41723300
4.27180600	1.10426700	0.87295500
4.10572600	3.00960100	0.09175800
3.39897900	4.05202500	-0.59255900
2.84155800	4.90408600	-1.14809200

5.47736200	3.28368500	0.41159900
6.58821700	3.48645200	0.67537500
1.18190600	-3.93331600	-0.31138900
-1.20186200	-3.42533200	-0.49749500
-3.88982300	0.51946600	-0.04517300
-1.04141000	3.69412000	0.40020600
1.31501000	3.25649900	0.46132300
3.99073000	-0.70727300	-0.13878700

Compound 2O

-1.10582300	-2.77954800	-0.44389500
-0.18590000	-1.81511400	-0.86465500
-0.64809000	-0.53443300	-1.22470300
-1.90215700	-0.15776100	-0.71672400
-2.80257400	-1.13724600	-0.28077800
-2.45386300	-2.48582500	-0.22850700
1.24910700	-2.11366900	-0.62434300
2.11282300	-1.34220900	0.08837800
1.77669700	0.06750700	0.49046100
0.52414900	0.41183400	1.02786700
0.04681800	1.70396400	0.73024300
0.95072300	2.70796700	0.35011900
2.29061100	2.42887800	0.09193100
2.64661400	1.07873900	0.07647500
-0.25042600	-0.52961100	1.90749300
-1.37113000	2.00910300	0.44679000
-2.20839100	1.25840400	-0.32570800
-3.51266900	1.76411600	-0.72982600
-4.35460100	2.59386100	-0.06016900
-4.10633200	3.09776000	1.25940200
-3.92208600	3.51003600	2.32745400
3.31940900	3.49966400	-0.28183200
3.79981800	3.26861100	-1.72710900
0.16813500	0.37861700	-2.10044100
-3.43016400	-3.58772100	0.19376600
-2.98487300	-4.17516700	1.54661800
3.46927100	-1.78947000	0.41736800
2.73711800	4.91594300	-0.18505200
4.51708800	3.39903900	0.68136200
-4.86341800	-3.05963500	0.34359700
-3.43202300	-4.69670400	-0.87443300
-5.59405100	2.99054200	-0.66631200
-6.59235700	3.29991500	-1.16785600
0.56092100	3.70893300	0.19567100

3.62736300	0.78062700	-0.28174700
1.56169800	-3.12924000	-0.85280800
-1.68724800	3.02248600	0.68242400
-0.73000900	-3.77451700	-0.21822400
-3.77509100	-0.81355000	0.07649000
0.20466300	1.40910000	-1.74681000
1.18971200	0.01506500	-2.21259400
-0.29127600	0.38960400	-3.09532300
-1.32505000	-0.50154000	1.72694000
0.09838600	-1.55743900	1.81324800
-0.08712800	-0.21665900	2.94484200
4.52475400	4.03772500	-2.01412500
2.95926400	3.31176800	-2.42703900
4.28493900	2.29504000	-1.84238600
4.98925800	2.41324600	0.63791700
5.27514400	4.14670000	0.42470100
4.20007900	3.57361000	1.71410500
1.92781700	5.07416000	-0.90531200
2.35348000	5.12640000	0.81833100
3.51774400	5.65044900	-0.40469200
-2.95481600	-3.39704600	2.31572100
-3.68404300	-4.95262900	1.87251100
-1.99004200	-4.62596400	1.48575300
-3.75398900	-4.30318900	-1.84348500
-2.43840500	-5.13566700	-1.00349700
-4.11764300	-5.50056500	-0.58625000
-5.53698000	-3.88754700	0.58432100
-4.94623900	-2.32696500	1.15263700
-5.22100500	-2.59565500	-0.58116400
-3.87832800	1.39574900	-1.68579200
4.18253300	-1.50871500	1.56988700
5.42376800	-2.17678400	1.48938100
5.44561500	-2.83201400	0.28133100
4.26458100	-2.60234900	-0.37146300
4.01020700	-3.04168100	-1.72922400
6.21561100	-3.43281400	-0.18033200
6.21458500	-2.17636300	2.22469700
3.81956700	-0.89307900	2.38034300
4.96353800	-3.13775200	-2.25193400
3.49689100	-4.00796400	-1.75663600
3.39680100	-2.30515700	-2.25000200

Optimized structure (solvent=acetonitrile)

Compound 1C

8.43055400	-0.94513900	-0.13747200
7.36090000	-0.49359000	-0.10863200
6.04348300	0.06095400	-0.07348700
5.98751100	1.48713700	-0.08822600
5.97780300	2.64873500	-0.09531800
4.96382100	-0.78693500	-0.00715000
5.23407800	-1.83944200	0.03647700
3.55973600	-0.52892800	0.03374900
2.72252900	-1.65048100	0.20144600
3.16886000	-2.64204800	0.22558200
1.34459800	-1.53469100	0.28755200
0.72649900	-0.15572000	0.43309600
1.62296000	0.95534200	-0.08222900
2.97218500	0.76276900	-0.16482400
3.59908900	1.60094500	-0.44684900
-0.61712800	-0.11881500	-0.30988200
-0.44811000	-0.35485200	-1.84770400
0.17460100	0.42327800	-2.29331000
0.00523700	-1.32915100	-2.04050700
-1.43189900	-0.32753500	-2.32188700
0.54852400	0.09138100	1.96094800
-0.08846600	-0.67250300	2.41305100
0.11261300	1.07378200	2.15705300
1.52958500	0.04957400	2.44027300
1.00110000	2.21282000	-0.33567500
1.63854400	3.07394400	-0.51779400
-0.36103400	2.36939800	-0.31966000
-0.79577400	3.35728400	-0.43934000
0.48669800	-2.63489900	0.37506900
0.91765500	-3.63032400	0.44452700
-0.90133600	-2.48854600	0.40134300
-1.53107100	-3.35607800	0.57289300
-1.50276600	-1.24964200	0.16362300
-1.23786400	1.25447200	-0.18575700
-3.05838500	2.35164600	-0.14562500
-3.51800200	-1.87949900	0.48232500
-2.59984400	1.36852200	-0.10125100
-2.88145300	-1.04082000	0.22214700
-3.44059800	0.22886200	0.05819800
-4.87919100	0.45321400	0.14028200
-5.53868900	1.54736100	0.68563900
-6.92496400	1.31043300	0.58768400
-7.07774800	0.08828600	-0.03120700

-5.84597600	-0.43582300	-0.29506100
-5.65005900	-1.66848300	-1.04271600
-5.53385600	-2.52697300	-0.37647900
-4.76686900	-1.58548000	-1.67653400
-6.52055300	-1.83259700	-1.67800200
-7.97050000	-0.44565900	-0.32239000
-7.72347200	1.95430500	0.92591100
-5.05664600	2.40082100	1.14133100

Compound 1O

-2.57015800	-1.63373200	-0.14064200
-1.21755200	-1.53337800	-0.45485700
-0.72249400	-0.30236200	-0.93622500
-1.46028600	0.86421500	-0.61882200
-2.81373000	0.74882500	-0.32303900
-3.41662000	-0.51432400	-0.18480400
-0.31811200	-2.64130500	-0.02484200
0.77184600	-2.48020600	0.75189000
0.52365000	-0.23700000	-1.77159100
-0.80428900	2.16795100	-0.31521600
0.26754900	2.32251600	0.48797600
1.17273700	1.21844300	0.91594600
0.68185100	-0.02246100	1.37295200
1.42283000	-1.16810300	1.02805200
2.76641900	-1.03867600	0.66088300
3.35762500	0.21666300	0.49754400
2.51481100	1.33318600	0.54963600
-0.57279100	-0.11822200	2.20108400
4.78467500	0.40094300	0.19765300
-4.82493100	-0.73542800	0.04497700
2.89688400	2.29749300	0.22714800
3.34170100	-1.94078200	0.47742900
-0.65557100	-3.65595500	-0.22307600
0.58998400	3.33956600	0.70065200
-2.97142900	-2.59584900	0.16621700
-3.37738300	1.65307300	-0.12355800
1.12652900	0.64829800	-1.57434100
1.14051800	-1.12735500	-1.65571600
0.20278700	-0.18865900	-2.81882900
-1.34495500	0.58823100	1.89701500
-0.98984100	-1.12503800	2.19711100
-0.30529600	0.12146400	3.23650100
1.30108600	-3.37650800	1.06811700
-1.33395100	3.06472600	-0.62859100

5.49193400	-0.34329500	-0.72418900
6.78836200	0.09768500	-0.75272900
6.92667200	1.12634600	0.14963700
5.65707300	1.32252100	0.74726500
5.39552900	2.03864300	1.51398700
7.83674800	1.67173500	0.35447900
7.50307300	-0.35423900	-1.42490900
4.96902800	-1.36986100	-1.60864900
5.58291000	-1.40359500	-2.50922000
4.98441100	-2.35602500	-1.13651600
3.94396600	-1.12896200	-1.89413800
-5.88204900	0.10579100	-0.13033400
-5.08596400	-1.73314300	0.38927800
-7.20628800	-0.34859800	0.17687600
-5.79501400	1.44011200	-0.64134400
-5.75481600	2.52100000	-1.06082100
-8.27806400	-0.71575700	0.42576700

Compound 2C

-1.02909500	-2.37496800	-0.23355700
-2.09416900	-1.47903900	-0.21229900
-3.46774900	-1.98550300	-0.31961500
-3.94567000	-3.03880900	0.43450100
-5.23152700	-3.30873300	0.05828700
-5.59231000	-2.44136400	-0.94842600
-4.48060000	-1.60019200	-1.18364800
-4.39856000	-0.81167100	-1.91846600
-6.54786300	-2.41592100	-1.45178700
-5.79160400	-4.08994700	0.55116600
-3.25993200	-3.72182300	1.51916000
-2.68598300	-4.57779300	1.15513000
-2.58285100	-3.03203600	2.02350100
-4.00143300	-4.07347400	2.23707700
0.30711200	-1.98225600	-0.05795800
1.36161000	-2.87610200	-0.14487900
2.69510100	-2.44962700	-0.07640100
2.98418600	-1.07816100	0.01393500
2.00679700	-0.10271600	0.14008200
2.24953100	1.29961100	0.19579700
1.14742100	2.20180100	0.23146900
-0.15283400	1.79985900	0.04340400
-1.24179800	2.68732600	0.13778600
-2.55732400	2.26277200	0.09263800
-2.82113400	0.87018000	0.00822900

-1.83703400	-0.07669200	-0.15174800
-0.40572000	0.37378600	-0.39186600
-0.18819500	0.34120200	-1.93392700
0.57290600	-0.55392500	0.34673600
0.35872400	-0.52001400	1.89721400
-0.66286200	-0.81450100	2.14844300
0.54828800	0.47729000	2.29755700
1.05096400	-1.22334600	2.36547800
0.82967100	0.64615500	-2.19085500
-0.88522500	1.04079100	-2.40184600
-0.37348200	-0.65562300	-2.34059100
-3.69285000	3.28894200	0.21273800
-3.56563800	4.31178300	-0.93292800
-3.63922700	3.81592300	-1.90601400
-4.36774900	5.05419100	-0.86518300
-2.61195200	4.84599800	-0.89649000
-3.58951500	4.01733800	1.56673600
-3.66785100	3.30736300	2.39608500
-4.39957600	4.74783100	1.66382400
-2.64211300	4.55446600	1.66825800
-5.08116900	2.63922600	0.12012200
-5.21288000	2.09340500	-0.81986000
-5.84837200	3.41798000	0.16338200
-5.26700800	1.94948300	0.94951100
3.86411500	-3.43721500	-0.16662700
4.69203000	-3.13524500	-1.43193100
4.07517300	-3.22825200	-2.33101500
5.11922000	-2.12888400	-1.41447700
5.52043300	-3.84657000	-1.50999700
3.39651200	-4.89754300	-0.23544400
2.81049300	-5.09678400	-1.13797100
2.79661000	-5.17322500	0.63751300
4.27043900	-5.55484400	-0.25953400
4.75140600	-3.27430700	1.08394900
5.16540600	-2.26537400	1.16356300
5.58941200	-3.97716400	1.03860400
4.18073700	-3.48042800	1.99484900
3.59646400	1.77055400	0.29470200
4.34087900	1.04790300	0.61461400
4.11231000	3.01997400	0.05373400
3.39065300	4.12869300	-0.48597300
2.84274000	5.04619200	-0.94082300
5.50187000	3.25909600	0.29393400
6.63032700	3.45088200	0.48973200

1.13220600	-3.92042900	-0.32245000
-1.22979000	-3.42920100	-0.40001000
-3.84043600	0.52207500	0.11194800
-1.01786400	3.73857900	0.30267000
1.32918500	3.24817200	0.45042800
4.02286900	-0.78031900	-0.07147300

Compound 2O

-1.10908800	-2.77399300	-0.50046800
-0.18534300	-1.80546200	-0.90529300
-0.64037400	-0.51523300	-1.24033400
-1.88778200	-0.13929800	-0.71524800
-2.78820400	-1.11838800	-0.27811800
-2.45167300	-2.47113600	-0.25946900
1.24515800	-2.10917200	-0.64874700
2.09334600	-1.34441600	0.08827800
1.76154700	0.06804900	0.48757500
0.51305300	0.43034700	1.02435500
0.05579600	1.73006200	0.72941800
0.96962700	2.72503200	0.34684300
2.30457500	2.42640800	0.08632200
2.64177300	1.07020300	0.07264800
-0.28646700	-0.49136200	1.90256000
-1.35779300	2.04010800	0.43777000
-2.19279200	1.27801000	-0.32742200
-3.48771800	1.79189300	-0.74086300
-4.33852200	2.58600900	-0.03673100
-4.11933400	2.99366100	1.31985800
-3.97722300	3.32477100	2.42229100
3.34512500	3.48151000	-0.30010300
3.79966100	3.24410000	-1.75286800
0.17668800	0.40178600	-2.11082500
-3.43319000	-3.57277800	0.15191600
-2.97678200	-4.19237300	1.48673600
3.44003900	-1.80430700	0.44751600
2.78602200	4.90642500	-0.19277900
4.55614900	3.36154200	0.64408300
-4.85957300	-3.03477700	0.32983800
-3.45739000	-4.66024700	-0.93814200
-5.56548100	3.03110000	-0.63073600
-6.55824400	3.38914200	-1.11118200
0.59068500	3.72946400	0.18926700
3.61630100	0.76095400	-0.29347900
1.56115300	-3.12204600	-0.88358600

-1.66840500	3.06111600	0.64766700
-0.73844100	-3.77642800	-0.30112100
-3.75377900	-0.79340000	0.09597700
0.23635200	1.42489600	-1.73961100
1.18934600	0.02119800	-2.24766500
-0.29894500	0.44090100	-3.09724200
-1.34332400	-0.22411700	1.92447000
-0.19059200	-1.54031300	1.62629000
0.09728800	-0.38362800	2.92368300
4.53449000	4.00078600	-2.04749100
2.94920500	3.30625400	-2.43942500
4.26422700	2.26151700	-1.87695700
5.01548400	2.37010800	0.58872000
5.31895600	4.10019400	0.37620600
4.25822200	3.53853700	1.68242900
1.96897600	5.07752700	-0.90098700
2.41941600	5.12040500	0.81638500
3.57603200	5.62769600	-0.42251100
-2.93270400	-3.43036600	2.27153500
-3.67965700	-4.97048900	1.80302400
-1.98675900	-4.65018200	1.40325500
-3.78882000	-4.24452500	-1.89500800
-2.46939000	-5.10581800	-1.08669200
-4.14744200	-5.46252700	-0.65630200
-5.53609000	-3.86243600	0.56335200
-4.92459000	-2.31619100	1.15305200
-5.22369900	-2.54980300	-0.58163300
-3.83438000	1.47070000	-1.72024700
4.11996500	-1.55160600	1.62801400
5.36226600	-2.22288400	1.56695700
5.41575800	-2.85132000	0.34346300
4.25461800	-2.60071000	-0.33565500
4.03052100	-3.01921700	-1.70899200
6.19577400	-3.44384700	-0.11206600
6.13359700	-2.24161300	2.32335600
3.73630100	-0.95189900	2.44163300
4.99613000	-3.11841800	-2.20601200
3.50844700	-3.97856800	-1.75926600
3.43919900	-2.26771600	-2.23323400

References

1 J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999−3094.

2 H. T. Sun, Z. B. Hu, C. Zhong, X. K. Chen, Z. R. Sun and J. L. Brédas, *J. Phys. Chem. Lett.*, 2017, **8**, 2393-2398.

3 K. Klaue, W. J. Han, P. Liesfeld, F. Berger, Y. Garmshausen and S. Hecht, *J. Am. Chem. Soc.*, 2020, **142**, 11857-11864.