Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2022

Supporting Information

Planar in Brooker's Mode and Twisted in Reichardt's Mode: Defying the Steric Forces in Biphenyl Types of Zwitterionic Systems Through Metameric Resonance Stabilizations.

Sanyasi Sitha*

Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park, Johannesburg, South Africa 2006.

Optimized geometric parameters (in Cartesian coordinates) of all the molecules considered in this work [Method: ωB97xD/6-31G(d,p)].

Note 1: Energies reported are in atomic units (Hartrees) and the Cartesian coordinates are in the units of Å.
Note 2: Optimized geometries of the molecules 1 and 2, in other methods can be directly obtained from the author, through an email request.

Molecule 1

	X	Y	Z
C	3.15957700	-1.14321500	-0.33283600
C	1.78299300	-1.11860500	-0.35440800
C	1.78300400	1.11861400	0.35440900
C	3.15958500	1.14320700	0.33284900
C	3.88071700	-0.00000800	0.00000400
H	3.65955300	-2.06117700	-0.61808600
H	1.19014400	-1.95559300	-0.69184900
H	1.19015900	1.95559800	0.69186300
H	3.65957300	2.06115600	0.61811700
H	4.96372000	-0.00001300	0.00001200
C	-0.32222600	0.00001100	-0.00000800
C	-1.04223300	1.17922400	-0.32442700
C	-1.04221500	-1.17920700	0.32441400
C	-2.40391200	1.18413600	-0.33380000
H	-0.50479400	2.07055000	-0.64021400
C	-2.40389500	-1.18414300	0.33379500
H	-0.50476100	-2.07052800	0.64019000
C	-3.19506200	-0.00001200	-0.00001100
H	-2.95234900	2.07364200	-0.62508400
H	-2.95231000	-2.07365700	0.62509200
N	1.07888900	0.00001100	-0.00001900
O	-4.42989300	-0.00000800	0.00002600

E(ωB97xD)=-554.3233823
Sum of electronic and zero-point Energies= -554.147675
Sum of electronic and thermal Energies= -554.137979
Sum of electronic and thermal Enthalpies= -554.137035
Sum of electronic and thermal Free Energies= -554.183283

Molecule 2

	X	Y	Z
C	3.18075500	-1.18213000	0.00003900
C	1.82898900	-1.21035600	-0.00002000
C	1.82899500	1.21035900	0.00001000
C	3.18076100	1.18212600	-0.00004300
H	3.78093400	-2.08347800	0.00016800
H	1.35581100	-2.18197800	0.00009400
H	1.35582300	2.18198300	-0.00011500
H	3.78094400	2.08347100	-0.00016800
H	4.87505000	-0.00000600	0.00001500
C	-0.36209600	0.00000400	0.00000200
C	-1.13197800	1.22381200	0.00008600
C	-1.13197400	-1.22380900	-0.00007600
C	-2.48309800	1.23584300	0.00005100
H	-0.61609000	2.17876300	-0.00009300
C	-2.48309200	-1.23584200	-0.00003700
H	-0.61608300	-2.17875800	0.00010900
C	-3.27401700	-0.00000100	-0.00000100
H	-3.03771100	2.16864600	0.00003800
H	-3.03770500	-2.16864600	-0.00001600
O	-4.50386600	-0.00000500	-0.00001200
C	1.03105200	0.00000400	-0.00000300
N	3.86916800	-0.00000300	0.00000300

E(ωB97xD)=-554.3474746
Sum of electronic and zero-point Energies= -554.170977
Sum of electronic and thermal Energies= -554.160836
Sum of electronic and thermal Enthalpies= -554.159892
Sum of electronic and thermal Free Energies= -554.207475

BIA-1

	X	Y	Z
C	2.84943100	1.12646400	0.42084700
C	1.45894500	1.12556600	0.42168900
C	1.45895000	-1.12556900	-0.42169500
C	2.84940700	-1.12647600	-0.42085400
C	3.55020300	0.00000200	0.00000300
H	3.38652300	2.00732800	0.75843600
H	0.91978200	1.99947100	0.77512700
H	0.91975200	-1.99944600	-0.77515100
H	3.38652900	-2.00732100	-0.75844400
H	4.63557700	-0.00002400	-0.00000600
C	-0.74271700	0.00001000	-0.00000800
C	-1.45895600	-1.12556700	0.42169200
C	-1.45895100	1.12556400	-0.42168000
C	-2.84941800	-1.12648400	0.42085400

H	-0.91978100	-1.99945500	0.77515300
C	-2.84944000	1.12647500	-0.42085000
H	-0.91980700	1.99948000	-0.77512000
C	-3.55016500	0.00000100	-0.00000900
H	-3.38654000	-2.00732800	0.75844300
H	-3.38653000	2.00733800	-0.75844000
H	-4.63558900	-0.00002600	-0.00000100
C	0.74272500	0.00001100	0.00001000

E(ωB97xD)=-463.1591402
Sum of electronic and zero-point Energies= -462.975507
Sum of electronic and thermal Energies= -462.966690
Sum of electronic and thermal Enthalpies= -462.965745
Sum of electronic and thermal Free Energies= -463.010055

BIA-2

	X	**Y**	**Z**
C	2.68172800	-1.13050100	-0.33514400
C	2.68157800	1.13057800	0.33522100
C	3.41581000	0.00007000	0.00006800
H	3.17429000	-2.05910300	-0.61451600
H	3.17404500	2.05922200	0.61463100
H	4.49921700	0.00013600	0.00011300
C	-0.75025900	-0.00009800	-0.00019700
C	-2.68162300	1.13056600	-0.33513600
C	-2.68168600	-1.13052100	0.33521900
C	-3.41580500	0.00004800	0.00008500
H	-3.17412600	2.05920500	-0.61449500
H	-3.17421400	-2.05912400	0.61464700
H	-4.49920400	0.00010800	0.00016000
C	0.75025700	-0.00006800	-0.00002100
N	1.34971400	1.14466200	0.33506800
N	1.34985200	-1.14471400	-0.33509000
N	-1.34975800	1.14464900	-0.33515000
N	-1.34981100	-1.14472500	0.33501500

E(ωB97xD)=-527.2780001
Sum of electronic and zero-point Energies= -527.142384
Sum of electronic and thermal Energies= -527.133888
Sum of electronic and thermal Enthalpies= -527.132944
Sum of electronic and thermal Free Energies= -527.177438

BIA-3

	X	**Y**	**Z**
C	2.88670400	1.12862600	0.24405300
C	1.50042800	1.18816100	0.26237900
C	2.69247200	-1.19143000	-0.25385800
C	3.50526900	-0.08632400	-0.02480600
H	3.47451300	2.01816600	0.44781500
H	0.99737000	2.11813000	0.50096000
H	3.13447100	-2.16489000	-0.45458500
H	4.58496700	-0.18203400	-0.04897900
C	-0.72496500	0.02573200	-0.00591500

C	-1.41230100	-1.16974000	0.22687300
C	-1.46232800	1.18967100	-0.24394000
C	-2.80105400	-1.19577300	0.23997500
H	-0.83781900	-2.07392600	0.39307400
C	-2.85275000	1.16260800	-0.23352000
H	-0.95421800	2.12312800	-0.46509900
C	-3.52686100	-0.02926800	0.01271500
H	-3.31882400	-2.13115200	0.42759100
H	-3.40877700	2.07458400	-0.42655200
H	-4.61209000	-0.05046800	0.02170000
C	0.76337700	0.02760700	-0.00243100
N	1.36178100	-1.14725000	-0.24643900

E(ωB97xD)=-479.1907733
Sum of electronic and zero-point Energies= -479.018819
Sum of electronic and thermal Energies= -479.010119
Sum of electronic and thermal Enthalpies= -479.009175
Sum of electronic and thermal Free Energies= -479.053500

BIA-4

	X	**Y**	**Z**
C	2.84687200	1.09630800	0.39210000
C	1.45838600	1.13448500	0.40589300
C	2.68066500	-1.14476800	-0.40624600
C	3.47775700	-0.06833100	-0.02528400
H	3.42396500	1.95887600	0.71006100
H	0.93174700	2.01859900	0.74900000
H	3.13846200	-2.07355400	-0.73957000
H	4.55876900	-0.14887500	-0.05364200
C	-0.74670700	0.00155500	-0.00072700
C	-1.45838800	1.13448300	-0.40589800
C	-2.68066400	-1.14477200	0.40625100
C	-2.84687700	1.09630900	-0.39209600
H	-0.93175000	2.01860000	-0.74900300
C	-3.47775200	-0.06833100	0.02529400
H	-3.13846000	-2.07355500	0.73958000
H	-3.42397100	1.95887800	-0.71004800
H	-4.55875200	-0.14887400	0.05366100
C	0.74670600	0.00155700	0.00071700
N	1.34945900	-1.12436100	-0.39741700
N	-1.34945900	-1.12436400	0.39740800

E(ωB97xD)=-495.2151971
Sum of electronic and zero-point Energies= -495.055634
Sum of electronic and thermal Energies= -495.046993
Sum of electronic and thermal Enthalpies= -495.046049
Sum of electronic and thermal Free Energies= -495.090318

BIA-5

	X	**Y**	**Z**
C	2.83584100	1.17292700	0.00008600
C	1.44891800	1.21188600	-0.00004300
C	2.68693900	-1.20811300	0.00020100

C	3.47536000	-0.06190800	0.00011600
H	3.40971300	2.09439000	0.00017300
H	0.89608300	2.14305900	-0.00008100
H	3.14900900	-2.19266100	-0.00003800
H	4.55686600	-0.14084200	0.00015400
C	-0.74579500	-0.00480200	-0.00008300
C	-2.83586200	-1.17291400	0.00008200
C	-2.68691400	1.20811500	0.00015800
C	-3.47536800	0.06190900	0.00011500
H	-3.40970500	-2.09439400	0.00015400
H	-3.14899700	2.19265800	-0.00003500
H	-4.55686000	0.14087800	0.00016400
C	0.74580300	0.00478100	-0.00018700
N	1.35515900	-1.18719900	-0.00021700
C	-1.44892100	-1.21187600	-0.00003200
H	-0.89615700	-2.14308200	-0.00011800
N	-1.35515400	1.18719400	-0.00018900

E(ωB97xD)=-495.2259786
Sum of electronic and zero-point Energies= -495.065924
Sum of electronic and thermal Energies= -495.057373
Sum of electronic and thermal Enthalpies= -495.056429
Sum of electronic and thermal Free Energies= -495.100455

BIA-6

	X	**Y**	**Z**
C	2.72713300	-1.17717700	0.00013300
C	2.72712900	1.17717700	-0.00013200
C	3.46424500	-0.00000100	0.00000700
H	3.21887900	-2.14753500	0.00016600
H	3.21888000	2.14753400	-0.00014300
H	4.54730800	0.00000300	0.00001800
C	-0.70586900	-0.00000100	-0.00000300
C	-2.80024700	1.20493300	0.00008600
C	-2.80024900	-1.20493200	-0.00008100
C	-3.49823700	0.00000000	0.00000400
H	-3.33972200	2.14675600	0.00015500
H	-3.33972200	-2.14675600	-0.00014700
H	-4.58393400	0.00000100	0.00000700
C	0.77970400	-0.00000200	-0.00001000
N	1.39694700	1.18977200	-0.00005700
C	-1.41083000	1.20697100	0.00006800
H	-0.85531800	2.13776800	0.00012400
C	-1.41083000	-1.20697100	-0.00007100
H	-0.85531900	-2.13776800	-0.00013000
N	1.39694800	-1.18977100	0.00004800

E(ωB97xD)= -495.2270865
Sum of electronic and zero-point Energies= -495.067234
Sum of electronic and thermal Energies= -495.058615
Sum of electronic and thermal Enthalpies= -495.057671
Sum of electronic and thermal Free Energies= -495.101904

Molecule 1 (triplet state)

	X	Y	Z
C	3.15258400	1.14227900	0.39233200
C	1.79371800	1.14590600	0.38286500
C	1.79375500	-1.14591700	-0.38287100
C	3.15262200	-1.14225400	-0.39230900
C	3.89151500	0.00002100	0.00002000
H	3.65960900	2.04308500	0.72022500
H	1.20153500	1.98362100	0.72287600
H	1.20160300	-1.98364500	-0.72290200
H	3.65967700	-2.04304600	-0.72019600
H	4.97317800	0.00003600	0.00003000
C	-0.33161600	-0.00002300	-0.00003300
C	-1.04232500	-1.15927600	0.38682500
C	-1.04231200	1.15926400	-0.38681000
C	-2.41411200	-1.16929500	0.38066400
H	-0.49250400	-2.03240500	0.72114500
C	-2.41409900	1.16929000	-0.38067300
H	-0.49247800	2.03243300	-0.72100400
C	-3.17752700	-0.00006900	-0.00022200
H	-2.97185300	-2.04902200	0.68323000
H	-2.97182800	2.04907700	-0.68308500
N	1.07053600	-0.00001500	-0.00000800
O	-4.42923900	0.00005200	0.00012600

E(ωB97xD)=-554.2915797
Sum of electronic and zero-point Energies= -554.119804
Sum of electronic and thermal Energies= -554.109518
Sum of electronic and thermal Enthalpies= -554.108573
Sum of electronic and thermal Free Energies= -554.157489

Molecule 2 (triplet state)

	X	Y	Z
C	3.20326300	1.19932400	-0.00015400
C	1.84434300	1.20525700	-0.00015200
C	1.84433500	-1.20525300	0.00015400
C	3.20325500	-1.19932900	0.00015600
H	3.80032800	2.10129800	-0.00027600
H	1.36270000	2.17479300	-0.00029900
H	1.36268400	-2.17478500	0.00030100
H	3.80031400	-2.10130700	0.00028000
H	4.90311900	-0.00000800	-0.00000200
C	-0.39995300	0.00000500	0.00000000
C	-1.13850600	-1.20871800	-0.00009200
C	-1.13851200	1.20872500	0.00009100
C	-2.51371900	-1.22080500	-0.00009100
H	-0.61983700	-2.16015400	-0.00018800
C	-2.51372600	1.22080400	0.00008900
H	-0.61985100	2.16016500	0.00018800
C	-3.27795300	-0.00000200	-0.00000300
H	-3.06649000	-2.15464600	-0.00016700
H	-3.06650200	2.15464200	0.00016500
O	-4.53749100	-0.00000500	-0.00000100
C	1.07926000	0.00000400	0.00000100

N	3.89870600	-0.00000500	0.00000200

E(ωB97xD)=-554.297171
Sum of electronic and zero-point Energies= -554.125151
Sum of electronic and thermal Energies= -554.115290
Sum of electronic and thermal Enthalpies= -554.114346
Sum of electronic and thermal Free Energies= -554.161702

MS-1_S (Molecule 2 in 90.0° conformation - Singlet)

	X	Y	Z
C	0.00000000	1.18357100	-3.19050100
C	0.00000000	1.20215500	-1.81738500
C	0.00000000	-1.20215500	-1.81738500
C	0.00000000	-1.18357100	-3.19050100
H	0.00000000	2.07424300	-3.80621800
H	0.00000000	2.14671600	-1.28754500
H	0.00000000	-2.14671600	-1.28754500
H	0.00000000	-2.07424300	-3.80621800
H	0.00000000	0.00000000	-4.85370700
C	0.00000000	0.00000000	0.38745700
C	1.21279000	0.00000000	1.11011300
C	-1.21279000	0.00000000	1.11011300
C	1.21903200	0.00000000	2.48358200
H	2.15812300	0.00000000	0.56658100
C	-1.21903200	0.00000000	2.48358200
H	-2.15812300	0.00000000	0.56658100
C	0.00000000	0.00000000	3.27814700
H	2.16037800	0.00000000	3.02569400
H	-2.16037800	0.00000000	3.02569400
O	0.00000000	0.00000000	4.52245000
C	0.00000000	0.00000000	-1.07479000
N	0.00000000	0.00000000	-3.84250100

E(ωB97xD)=-554.2937104
Sum of electronic and zero-point Energies= -554.118541
Sum of electronic and thermal Energies= -554.109122
Sum of electronic and thermal Enthalpies= -554.108178
Sum of electronic and thermal Free Energies= -554.153664

MS-1_T (Molecule 2 in 90.0° conformation - Triplet)

	X	Y	Z
C	0.00000000	1.20684400	-3.18355600
C	0.00000000	1.21377100	-1.82429500
C	0.00000000	-1.21377100	-1.82429500
C	0.00000000	-1.20684400	-3.18355600
H	0.00000000	2.10596500	-3.78512800
H	0.00000000	2.16843500	-1.30919800
H	0.00000000	-2.16843500	-1.30919800
H	0.00000000	-2.10596500	-3.78512800
H	0.00000000	0.00000000	-4.88141800
C	0.00000000	0.00000000	0.40519500
C	1.21882100	0.00000000	1.12538700
C	-1.21882100	0.00000000	1.12538700

C	1.23511500	0.00000000	2.49729700
H	2.14875000	0.00000000	0.56468800
C	-1.23511500	0.00000000	2.49729700
H	-2.14875000	0.00000000	0.56468800
C	0.00000000	0.00000000	3.25957000
H	2.16301500	0.00000000	3.05976400
H	-2.16301500	0.00000000	3.05976400
O	0.00000000	0.00000000	4.50811700
C	0.00000000	0.00000000	-1.07774200
N	0.00000000	0.00000000	-3.87770300

E(ωB97xD)=-554.2972064

Sum of electronic and zero-point Energies=	-554.126216
Sum of electronic and thermal Energies=	-554.116761
Sum of electronic and thermal Enthalpies=	-554.115817
Sum of electronic and thermal Free Energies=	-554.162205