Supporting information for the article entitled

SYNTHESIS AND OPTICAL PROPERTIES OF 2,2′-BIIMIDAZOLE AND BENZO[*d*]IMIDAZOLE DERIVATIVES: CHANGING π-CONJUGATION BY PHOTOEXCITATION

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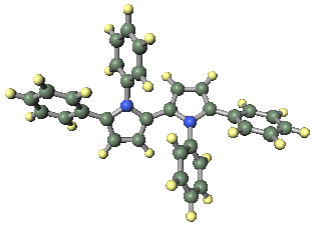
Cartesian Coordinates of the Results of DFT and TDDFT Calculation

Calculation was performed on Gaussian09 program with DFT and TDDFT/B3LYP/6-31+G** level. When the optimization with TDDFT calculation was executed, keyword “nstate=5” was used.

1,1',5,5'-Tetraphenyl-2,2'-bipyrrole (1) [ground state]

Theory: DFT/B3LYP

Total energy: -1343.43860731 A.U.



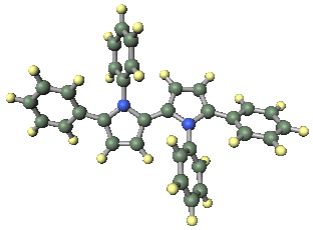
Cartesian coordinates:

C	1	2.788300	1.000500	-0.578100	C	30	-5.159799	-1.506400	-1.103500
C	2	2.105999	2.077300	-1.124000	C	31	-6.518800	-1.520400	-0.788600
C	3	0.742300	1.724899	-1.240799	C	32	-6.971800	-0.947400	0.403200
C	4	0.590499	0.429900	-0.768300	C	33	-6.048400	-0.369500	1.278900
N	5	1.852600	-0.011000	-0.352200	C	34	-4.687300	-0.364700	0.971400
C	6	-0.590599	-0.429900	-0.768300	H	35	2.550900	3.032300	-1.366500
C	7	-0.742600	-1.724799	-1.240999	H	36	-2.551300	-3.032100	-1.366700
C	8	-2.106300	-2.077200	-1.124199	H	37	0.924900	-1.144599	1.874100
C	9	-2.788500	-1.000400	-0.577900	H	38	1.432800	-3.437200	2.688000
N	10	-1.852700	0.011000	-0.351899	H	39	2.965699	-4.906799	1.389400
C	11	2.151399	-1.330200	0.117200	H	40	3.972800	-4.074400	-0.728500
C	12	1.587799	-1.792799	1.310700	H	41	3.436999	-1.787299	-1.545300
C	13	1.877500	-3.080900	1.763499	H	42	-3.436899	1.787599	-1.544800
C	14	2.737899	-3.906400	1.033499	H	43	-3.972499	4.074600	-0.727899
C	15	3.303500	-3.438999	-0.156000	H	44	-2.965300	4.906700	1.390200
C	16	3.007200	-2.155400	-0.619400	H	45	-1.432600	3.436799	2.688600
C	17	-2.151399	1.330100	0.117599	H	46	-0.924900	1.144300	1.874600
C	18	-3.007099	2.155500	-0.618899	H	47	3.985100	-0.069600	1.673600
C	19	-3.303200	3.439099	-0.155399	H	48	6.387000	-0.072600	2.210999
C	20	-2.737600	3.906300	1.034200	H	49	8.030499	0.951000	0.645000
C	21	-1.877300	3.080700	1.764100	H	50	7.225100	1.969700	-1.482200
C	22	-1.587799	1.792600	1.311199	H	51	4.817399	1.933099	-2.042299
C	23	4.216900	0.930300	-0.229899	H	52	-4.817900	-1.932700	-2.041900
C	24	4.687499	0.364400	0.970600	H	53	-7.225500	-1.969300	-1.481200
C	25	6.048699	0.369199	1.277799	H	54	-8.030300	-0.951000	0.646400
C	26	6.971900	0.947400	0.402000	H	55	-6.386499	0.072099	2.212300
C	27	6.518599	1.520699	-0.789499	H	56	-3.984700	0.069099	1.674300
C	28	5.159499	1.506699	-1.104100	H	57	-0.053699	2.338299	-1.636900
C	29	-4.217000	-0.930200	-0.229400	H	58	0.053200	-2.338299	-1.637299

1,1',5,5'-Tetraphenyl-2,2'-bipyrrole (1) [excited state]

Theory: TDDFT/B3LYP

Total energy: -1343.42583000 A.U.



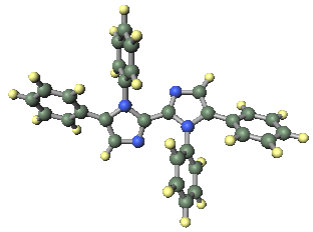
Cartesian coordinates:

C	1	2.761100	1.015099	-0.388699	C	30	-4.954299	-1.905299	-1.080999
C	2	1.972400	2.156200	-0.673500	C	31	-6.338700	-1.994899	-0.977100
C	3	0.639700	1.823300	-0.527899	C	32	-7.032699	-1.186799	-0.068600
C	4	0.564500	0.429200	-0.228200	C	33	-6.318100	-0.286400	0.730099
N	5	1.895800	-0.035399	-0.122600	C	34	-4.933500	-0.182700	0.625500
C	6	-0.564799	-0.429599	-0.228300	H	35	2.366700	3.138599	-0.888400
C	7	-0.640100	-1.823600	-0.528400	H	36	-2.367399	-3.138599	-0.888899
C	8	-1.973000	-2.156300	-0.673799	H	37	1.264400	-1.407500	2.094800
C	9	-2.761500	-1.015199	-0.388599	H	38	1.941799	-3.725500	2.627300
N	10	-1.896000	0.035200	-0.122600	H	39	3.361600	-5.023399	1.034000
C	11	2.285100	-1.375100	0.185100	H	40	4.087700	-3.958200	-1.109299
C	12	1.875500	-1.971099	1.397200	H	41	3.400700	-1.644600	-1.647999
C	13	2.261200	-3.276200	1.691000	H	42	-3.400300	1.644799	-1.647999
C	14	3.062700	-4.007199	0.798500	H	43	-4.086700	3.958699	-1.109199
C	15	3.472200	-3.404399	-0.405999	H	44	-3.360099	5.023599	1.033900
C	16	3.088999	-2.103300	-0.715100	H	45	-1.940699	3.725299	2.627200
C	17	-2.284900	1.374999	0.185200	H	46	-1.264100	1.407000	2.094700
C	18	-3.088500	2.103400	-0.715100	H	47	4.406400	-0.514600	1.263800
C	19	-3.471299	3.404700	-0.405999	H	48	6.843200	-0.341800	1.443400
C	20	-3.061600	4.007299	0.798500	H	49	8.112899	1.255600	0.013000
C	21	-2.260300	3.276100	1.691000	H	50	6.878500	2.693000	-1.610600
C	22	-1.874999	1.970899	1.397100	H	51	4.433000	2.525600	-1.803699
C	23	4.214800	0.998200	-0.281699	H	52	-4.433599	-2.524900	-1.804200
C	24	4.933200	0.182399	0.624900	H	53	-6.879099	-2.692100	-1.611100
C	25	6.317900	0.286199	0.729600	H	54	-8.113300	-1.255200	0.013200
C	26	7.032300	1.187100	-0.068700	H	55	-6.843300	0.341299	1.444300
C	27	6.338199	1.995500	-0.976900	H	56	-4.406599	0.513899	1.264699
C	28	4.953800	1.905800	-1.080700	H	57	-0.201899	2.482999	-0.652900
C	29	-4.215200	-0.998100	-0.281599	H	58	0.201300	-2.483400	-0.653600

1,1',5,5'-Tetraphenyl-2,2'-biimidazole (2) [ground state]

Theory: DFT/B3LYP

Total energy: -1375.53742096 A.U.



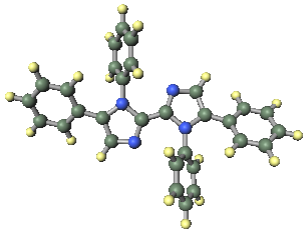
Cartesian coordinates:

C	1	2.745300	1.011899	-0.448400	C	29	-4.202200	-0.992100	-0.248900
C	2	1.937200	2.064500	-0.836500	C	30	-5.021499	-1.679000	-1.165199
N	3	0.624299	1.694300	-0.879800	C	31	-6.403200	-1.744000	-0.982200
C	4	0.597299	0.419100	-0.524100	C	32	-6.998500	-1.112800	0.113399
N	5	1.868000	-0.053799	-0.237000	C	33	-6.196900	-0.422800	1.027099
C	6	-0.597299	-0.419100	-0.524100	C	34	-4.813700	-0.365300	0.852999
N	7	-0.624299	-1.694300	-0.879800	H	35	2.247599	3.076400	-1.057199
C	8	-1.937200	-2.064500	-0.836500	H	36	-2.247499	-3.076400	-1.057199
C	9	-2.745300	-1.011899	-0.448400	H	37	1.273900	-1.217500	2.081900
N	10	-1.868000	0.053799	-0.237000	H	38	1.900400	-3.521600	2.782000
C	11	2.226400	-1.386000	0.160400	H	39	3.223400	-4.967600	1.249699
C	12	1.846000	-1.858500	1.418500	H	40	3.902199	-4.107800	-0.983600
C	13	2.201500	-3.151300	1.806500	H	41	3.244900	-1.812099	-1.683899
C	14	2.945100	-3.962999	0.945300	H	42	-3.244900	1.812099	-1.683899
C	15	3.327899	-3.479800	-0.309100	H	43	-3.902199	4.107800	-0.983600
C	16	2.965999	-2.191900	-0.706700	H	44	-3.223400	4.967600	1.249699
C	17	-2.226400	1.386000	0.160400	H	45	-1.900400	3.521600	2.782000
C	18	-2.965999	2.191900	-0.706700	H	46	-1.273900	1.217500	2.081900
C	19	-3.327899	3.479800	-0.309100	H	47	4.206200	-0.159100	1.582199
C	20	-2.945100	3.962999	0.945300	H	48	6.647899	-0.067300	1.885300
C	21	-2.201500	3.151300	1.806500	H	49	8.074700	1.156699	0.253000
C	22	-1.846000	1.858500	1.418500	H	50	7.015299	2.278600	-1.703099
C	23	4.202200	0.992100	-0.248900	H	51	4.567500	2.150600	-2.031599
C	24	4.813700	0.365300	0.852999	H	52	-4.567500	-2.150600	-2.031599
C	25	6.196900	0.422800	1.027099	H	53	-7.015299	-2.278600	-1.703099
C	26	6.998500	1.112800	0.113399	H	54	-8.074700	-1.156699	0.253000
C	27	6.403200	1.744000	-0.982200	H	55	-6.647899	0.067300	1.885300
C	28	5.021499	1.678900	-1.165199	H	56	-4.206200	0.159100	1.582199

1,1',5,5'-Tetraphenyl-2,2'-biimidazole (2) [excited state]

Theory: TDDFT/B3LYP

Total energy: -1375.52399859 A.U.



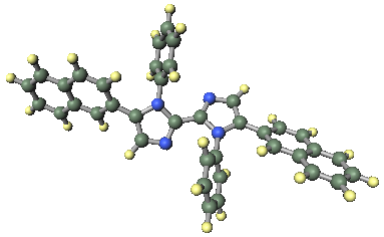
Cartesian coordinates:

C	1	2.743399	0.986500	-0.234600	C	29	-4.189400	-1.038100	-0.193600
C	2	1.864700	2.091899	-0.366400	C	30	-4.842099	-2.105600	-0.869900
N	3	0.589699	1.746200	-0.212200	C	31	-6.221599	-2.255600	-0.817100
C	4	0.583400	0.397700	-0.035100	C	32	-7.006499	-1.349400	-0.088900
N	5	1.908299	-0.104599	-0.007399	C	33	-6.381900	-0.290800	0.582899
C	6	-0.583600	-0.397700	-0.035200	C	34	-5.001300	-0.126099	0.532299
N	7	-0.589900	-1.746100	-0.212599	H	35	2.156300	3.124200	-0.506800
C	8	-1.864900	-2.091800	-0.366899	H	36	-2.156400	-3.124100	-0.507499
C	9	-2.743600	-0.986400	-0.234800	H	37	1.401300	-1.704800	2.072599
N	10	-1.908399	0.104599	-0.007499	H	38	2.156600	-4.051499	2.335400
C	11	2.318600	-1.465000	0.135400	H	39	3.507800	-5.138999	0.546199
C	12	1.988900	-2.181300	1.295200	H	40	4.089099	-3.856099	-1.509799
C	13	2.416099	-3.499599	1.436499	H	41	3.324399	-1.510799	-1.771099
C	14	3.176399	-4.111400	0.431600	H	42	-3.324100	1.511200	-1.771399
C	15	3.505500	-3.389000	-0.721800	H	43	-4.088400	3.856600	-1.509999
C	16	3.079399	-2.070399	-0.874400	H	44	-3.507199	5.139299	0.546199
C	17	-2.318600	1.465100	0.135400	H	45	-2.156400	4.051399	2.335500
C	18	-3.079100	2.070700	-0.874500	H	46	-1.401400	1.704700	2.072699
C	19	-3.504999	3.389399	-0.721900	H	47	4.546800	-0.692800	1.074800
C	20	-3.175900	4.111700	0.431600	H	48	6.977399	-0.414399	1.155800
C	21	-2.415899	3.499700	1.436499	H	49	8.085400	1.464100	-0.050000
C	22	-1.988900	2.181400	1.295200	H	50	6.691299	3.075899	-1.351999
C	23	4.189300	1.038100	-0.193500	H	51	4.254200	2.802400	-1.458700
C	24	5.000999	0.125800	0.532000	H	52	-4.254200	-2.802200	-1.459099
C	25	6.381700	0.290299	0.582500	H	53	-6.691199	-3.075999	-1.352199
C	26	7.006400	1.348899	-0.089100	H	54	-8.085500	-1.464800	-0.049700
C	27	6.221499	2.255400	-0.817000	H	55	-6.977599	0.413700	1.156400
C	28	4.841999	2.105600	-0.869700	H	56	-4.547099	0.692500	1.075300

5,5'-Di(naphthalen-2-yl)-1,1'-diphenyl-2,2'-biimidazole (3) [ground state]

Theory: DFT/B3LYP

Total energy: -1682.83983826 A.U.



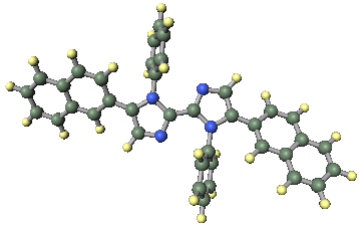
Cartesian coordinates:

C	1	-2.809099	-0.647300	-0.194299	H	35	-2.503300	-2.775000	-0.702700
C	2	-2.105300	-1.779999	-0.559299	H	36	2.414400	3.025700	-1.250400
N	3	-0.773299	-1.516299	-0.690600	H	37	-1.058700	1.599399	2.133500
C	4	-0.629699	-0.229300	-0.411000	H	38	-1.491399	3.977100	2.725899
N	5	-1.843900	0.356099	-0.086900	H	39	-2.780199	5.429100	1.170000
C	6	0.622099	0.510799	-0.525600	H	40	-3.620200	4.499799	-0.979100
N	7	0.715700	1.778000	-0.900499	H	41	-3.157400	2.127900	-1.572800
C	8	2.050400	2.042900	-0.984899	H	42	2.915800	-1.944199	-1.911200
C	9	2.808700	0.932800	-0.656599	H	43	3.444600	-4.284699	-1.248299
N	10	1.873500	-0.058900	-0.349599	H	44	2.953899	-5.061600	1.063000
C	11	-2.086900	1.731000	0.248399	H	45	1.948900	-3.490600	2.709500
C	12	-1.616300	2.242600	1.459800	H	46	1.451599	-1.144400	2.042499
C	13	-1.862600	3.576800	1.787100	H	47	-4.055899	0.707100	1.866800
C	14	-2.586799	4.392000	0.912499	H	48	-6.464200	0.835300	2.307899
C	15	-3.059999	3.869999	-0.294499	C	49	-8.443900	-0.307400	0.827199
C	16	-2.807900	2.539399	-0.631799	C	50	-7.486399	-1.732600	-1.395499
C	17	2.158300	-1.414799	0.028999	H	51	-4.790099	-1.661800	-1.651800
C	18	2.719000	-2.290300	-0.902000	H	52	4.521199	2.097399	-2.331500
C	19	3.008899	-3.602199	-0.524799	H	53	6.978699	2.063700	-2.288499
C	20	2.732100	-4.038599	0.774000	C	54	8.540399	0.695100	-0.523100
C	21	2.167900	-3.156400	1.699700	C	55	7.060400	-0.744099	1.380800
C	22	1.885500	-1.840000	1.331000	H	56	4.393699	-0.474999	1.120300
C	23	-4.248600	-0.497899	0.064000	C	57	-9.324000	-0.946800	-0.020299
C	24	-4.750600	0.219800	1.192199	H	58	-8.812499	0.244700	1.688199
C	25	-6.101200	0.287600	1.441899	H	59	-10.392600	-0.901699	0.168900
C	26	-7.043200	-0.357199	0.593600	C	60	-8.839699	-1.665900	-1.142599
C	27	-6.552300	-1.085399	-0.538799	H	61	-7.114300	-2.283399	-2.255700
C	28	-5.153700	-1.128800	-0.777399	H	62	-9.541799	-2.165399	-1.804000
C	29	4.271200	0.809700	-0.599000	C	63	8.438300	-0.777699	1.400799
C	30	5.040600	1.534100	-1.562599	H	64	6.485800	-1.302200	2.115500
C	31	6.414699	1.509000	-1.542800	H	65	8.957000	-1.362999	2.154599
C	32	7.121500	0.751499	-0.568600	C	66	9.186599	-0.051699	0.439499
C	33	6.363500	0.016400	0.400000	H	67	9.111200	1.252599	-1.261700
C	34	4.945200	0.071600	0.363000	H	68	10.271899	-0.086199	0.464900

5,5'-Di(naphthalen-2-yl)-1,1'-diphenyl-2,2'-biimidazole (3) [excited state]

Theory: TDDFT/B3LYP

Total energy: -1682.83019917 A.U.



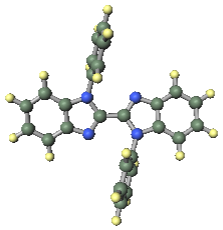
Cartesian coordinates:

C	1	-2.826800	-0.473899	0.053699	H	35	-2.456300	-2.674099	-0.092000
C	2	-2.064200	-1.667499	-0.052599	H	36	2.449699	3.174600	-0.383199
N	3	-0.754200	-1.427200	-0.034900	H	37	-1.474400	2.234400	2.137700
C	4	-0.611299	-0.086700	0.047399	H	38	-1.991399	4.667700	2.142500
N	5	-1.878099	0.538400	0.114500	H	39	-2.974800	5.733500	0.121300
C	6	0.630599	0.592300	-0.015899	H	40	-3.434400	4.359700	-1.902899
N	7	0.763200	1.932500	-0.148500	H	41	-2.910000	1.927999	-1.898699
C	8	2.067400	2.168200	-0.282400	H	42	2.671200	-1.560699	-2.057700
C	9	2.836199	0.979900	-0.215600	H	43	3.192200	-3.992900	-1.957600
N	10	1.895000	-0.028700	-0.028500	H	44	2.966799	-5.223299	0.191999
C	11	-2.160900	1.946500	0.118000	H	45	2.223500	-4.017100	2.237699
C	12	-1.903800	2.708500	1.261200	H	46	1.712400	-1.584600	2.127900
C	13	-2.195000	4.072899	1.256900	H	47	-4.387100	1.503199	1.252799
C	14	-2.747000	4.671800	0.120500	H	48	-6.816900	1.520400	1.418300
C	15	-3.006700	3.900000	-1.017000	C	49	-8.531500	-0.347699	0.421999
C	16	-2.713700	2.535700	-1.021200	C	50	-7.243800	-2.466899	-0.899000
C	17	2.165399	-1.439100	0.029800	H	51	-4.556600	-2.221699	-0.950900
C	18	2.579600	-2.106600	-1.124299	H	52	4.463899	2.779900	-1.302000
C	19	2.869300	-3.471199	-1.061699	H	53	6.902200	2.775400	-1.384900
C	20	2.742299	-4.161900	0.146300	C	54	8.551299	0.833100	-0.413599
C	21	2.325199	-3.484100	1.297099	C	55	7.177199	-1.309200	0.777200
C	22	2.038700	-2.120199	1.242300	H	56	4.510100	-1.030600	0.750700
C	23	-4.265500	-0.365899	0.135899	C	57	-9.276900	-1.382900	-0.135600
C	24	-4.950199	0.699400	0.796200	H	58	-9.031400	0.471999	0.932400
C	25	-6.321100	0.706800	0.895299	H	59	-10.360399	-1.374899	-0.062399
C	26	-7.123199	-0.338600	0.337200	C	60	-8.623100	-2.443900	-0.798800
C	27	-6.450399	-1.421199	-0.334300	H	61	-6.743800	-3.285800	-1.410100
C	28	-5.044199	-1.412100	-0.415900	H	62	-9.209700	-3.248500	-1.233900
C	29	4.277099	0.870600	-0.262399	C	63	8.556900	-1.310800	0.725699
C	30	5.007600	1.952300	-0.859100	H	64	6.642200	-2.137200	1.234800
C	31	6.377200	1.948100	-0.914699	H	65	9.113899	-2.142999	1.146700
C	32	7.139399	0.866400	-0.374900	C	66	9.252900	-0.235199	0.126600
C	33	6.426400	-0.225800	0.229500	H	67	9.084100	1.661500	-0.873900
C	34	5.015100	-0.202500	0.270799	H	68	10.338300	-0.247099	0.091100

1,1'-Diphenyl-2,2'-bibenzo[*d*]imidazole (4) [ground state]

Theory: DFT/B3LYP

Total energy: -1220.71366108 A.U.



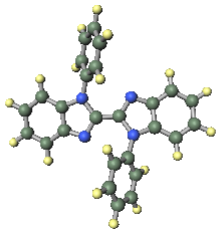
Cartesian coordinates:

C	1	0.822500	-2.359400	1.516000	C	25	-1.561100	3.553900	-1.800499
C	2	-0.576400	-2.249200	1.698999	C	26	-3.477300	1.278200	0.255000
N	3	-1.043600	-1.099000	1.098100	C	27	-4.786999	0.799299	0.193400
C	4	0.015899	-0.521599	0.565899	C	28	-5.143800	-0.148300	-0.770300
N	5	1.192299	-1.238100	0.783400	C	29	-4.189300	-0.612000	-1.679900
C	6	-0.015600	0.758199	-0.132400	C	30	-2.879900	-0.130499	-1.628400
N	7	1.044100	1.517700	-0.330800	H	31	2.127300	-1.702199	-1.667100
C	8	0.576800	2.645600	-0.972600	H	32	4.459899	-1.319000	-2.452600
C	9	-0.822200	2.551999	-1.162999	H	33	6.160999	-0.403899	-0.886499
N	10	-1.192199	1.329499	-0.616100	H	34	5.527300	0.127000	1.459199
C	11	-2.527800	0.804699	-0.652800	H	35	3.184400	-0.236800	2.225400
C	12	2.527600	-0.985899	0.320799	H	36	2.632700	-3.514499	1.860999
C	13	2.878000	-1.300100	-0.994000	H	37	1.385499	-5.264000	3.121900
C	14	4.187100	-1.083700	-1.428100	H	38	-1.054199	-5.093200	3.468600
C	15	5.143000	-0.570500	-0.546900	H	39	-2.344899	-3.156600	2.555000
C	16	4.787800	-0.272999	0.771900	H	40	2.345699	3.855500	-1.274100
C	17	3.478400	-0.479499	1.209300	H	41	1.054800	5.672400	-2.407200
C	18	1.561200	-3.437999	2.013000	H	42	-1.385200	5.474400	-2.736400
C	19	0.851899	-4.409800	2.715800	H	43	-2.632700	3.468099	-1.946099
C	20	-0.544000	-4.311699	2.913400	H	44	-3.182100	2.001000	1.008699
C	21	-1.272399	-3.238500	2.410599	H	45	-5.525600	1.161099	0.902600
C	22	1.273000	3.779000	-1.420199	H	46	-6.162099	-0.523499	-0.812900
C	23	0.544600	4.782900	-2.049999	H	47	-4.463300	-1.345799	-2.432000
C	24	-0.851600	4.670499	-2.238200	H	48	-2.130200	-0.479200	-2.331699

1,1'-Diphenyl-2,2'-bibenzo[*d*]imidazole (4) [excited state]

Theory: TDDFT/B3LYP

Total energy: -1220.70179464 A.U.



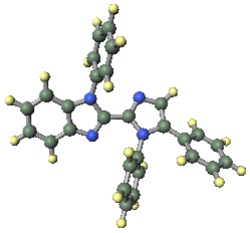
Cartesian coordinates:

C	1	-2.618398	-1.249317	-0.301430	C	25	3.990630	1.518445	-0.338009
C	2	-1.631661	-2.294671	-0.418506	C	26	3.468667	-1.721840	-0.613362
N	3	-0.381260	-1.802501	-0.285093	C	27	4.074690	-2.932200	-0.277928
C	4	-0.528361	-0.463675	-0.114862	C	28	3.709828	-3.603674	0.894686
N	5	-1.910410	-0.082199	-0.100946	C	29	2.732235	-3.053290	1.730100
C	6	0.528395	0.463541	-0.115016	C	30	2.123058	-1.842798	1.405571
N	7	0.381214	1.802391	-0.285514	H	31	-1.365441	1.415191	2.052852
C	8	1.631590	2.294628	-0.418685	H	32	-2.441587	3.568637	2.641051
C	9	2.618345	1.249346	-0.301328	H	33	-4.179439	4.548178	1.152116
N	10	1.910347	0.082162	-0.101022	H	34	-4.822920	3.357480	-0.940264
C	11	2.491274	-1.173448	0.228578	H	35	-3.726291	1.214279	-1.537296
C	12	-2.491241	1.173415	0.228617	H	36	-4.728555	-0.733405	-0.218804
C	13	-2.122588	1.843029	1.405356	H	37	-5.427725	-3.095975	-0.561264
C	14	-2.731721	3.053533	1.729905	H	38	-3.762352	-4.902850	-0.831455
C	15	-3.709644	3.603730	0.894756	H	39	-1.310950	-4.418635	-0.725779
C	16	-4.074919	2.932022	-0.277612	H	40	1.310816	4.418564	-0.726271
C	17	-3.469001	1.721622	-0.613045	H	41	3.762223	4.902894	-0.831573
C	18	-3.990724	-1.518378	-0.338281	H	42	5.427601	3.096099	-0.560952
C	19	-4.371321	-2.847241	-0.528854	H	43	4.728477	0.733508	-0.218386
C	20	-3.411642	-3.886498	-0.678182	H	44	3.725648	-1.214643	-1.537782
C	21	-2.050365	-3.631495	-0.623699	H	45	4.822448	-3.357791	-0.940770
C	22	2.050262	3.631480	-0.623971	H	46	4.179682	-4.548094	1.152045
C	23	3.411524	3.886547	-0.678243	H	47	2.442416	-3.568223	2.641444
C	24	4.371199	2.847339	-0.528657	H	48	1.366143	-1.414819	2.053255

2-(1,5-Diphenylimidazol-2-yl)-1-phenylbenzo[*d*]imidazole (5) [ground state]

Theory: DFT/B3LYP

Total energy: -1298.12577787 A.U.



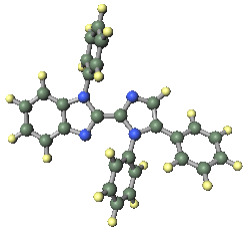
Cartesian coordinates:

C	1	3.327799	0.844399	-0.268699	C	27	-5.677300	-0.543600	0.927499
C	2	2.525900	1.974700	-0.554200	C	28	-4.288600	-0.483699	0.806300
N	3	1.196000	1.609399	-0.624600	C	29	4.716100	0.926599	-0.126800
C	4	1.172799	0.312800	-0.388000	C	30	5.289299	2.186400	-0.294900
N	5	2.441099	-0.222100	-0.162799	C	31	4.504700	3.322900	-0.590100
C	6	-0.027200	-0.514999	-0.429599	C	32	3.121900	3.233599	-0.721100
N	7	-0.041500	-1.788200	-0.795100	H	33	-1.656500	-3.167500	-1.042400
C	8	-1.353099	-2.158099	-0.801700	H	34	1.976200	-1.375899	2.192800
C	9	-2.174099	-1.107400	-0.430899	H	35	2.657700	-3.672700	2.869300
N	10	-1.306899	-0.043900	-0.182700	H	36	3.901000	-5.118800	1.273000
C	11	2.812399	-1.552400	0.218999	H	37	4.449400	-4.268100	-0.999099
C	12	2.512000	-2.018499	1.501299	H	38	3.729599	-1.981699	-1.676900
C	13	2.898500	-3.306500	1.875700	H	39	-2.606900	1.738799	-1.669500
C	14	3.598600	-4.118199	0.978700	H	40	-3.296200	4.025300	-0.967499
C	15	3.908799	-3.639799	-0.297500	H	41	-2.730600	4.848300	1.310500
C	16	3.514100	-2.357000	-0.681700	H	42	-1.488900	3.376199	2.885300
C	17	-1.684200	1.283500	0.217700	H	43	-0.829199	1.082400	2.181599
C	18	-2.377900	2.103100	-0.673600	H	44	-3.935400	-2.214400	-2.100900
C	19	-2.757700	3.385600	-0.274800	H	45	-6.394199	-2.344899	-1.867299
C	20	-2.438699	3.847900	1.004900	H	46	-7.524800	-1.260399	0.069600
C	21	-1.741300	3.021300	1.890500	H	47	-6.160100	-0.070199	1.777699
C	22	-1.367900	1.734300	1.501000	H	48	-3.708400	0.025899	1.567500
C	23	-3.637599	-1.089799	-0.284100	H	49	5.319700	0.054600	0.102100
C	24	-4.421400	-1.758600	-1.243500	H	50	6.365300	2.295600	-0.196200
C	25	-5.809100	-1.825199	-1.113900	H	51	4.994199	4.284300	-0.714699
C	26	-6.444200	-1.214700	-0.029099	H	52	2.510999	4.102700	-0.943400

2-(1,5-Diphenylimidazol-2-yl)-1-phenylbenzo[*d*]imidazole (5) [excited state]

Theory: TDDFT/B3LYP

Total energy: -1298.11301160A.U.



Cartesian coordinates:

C	1	3.309700	0.874599	-0.228699	C	27	-5.802299	-0.483300	0.604499
C	2	2.464000	2.032699	-0.278000	C	28	-4.430499	-0.275299	0.520499
N	3	1.161899	1.685799	-0.163300	C	29	4.701699	0.966900	-0.282000
C	4	1.145200	0.334400	-0.066400	C	30	5.244200	2.248100	-0.413000
N	5	2.458600	-0.205700	-0.088600	C	31	4.424300	3.404200	-0.485799
C	6	-0.016899	-0.464900	-0.083200	C	32	3.042200	3.317300	-0.417799
N	7	-0.000200	-1.808899	-0.316900	H	33	-1.540300	-3.197300	-0.668000
C	8	-1.264799	-2.167499	-0.483500	H	34	2.068600	-1.626700	2.142400
C	9	-2.169000	-1.078400	-0.294900	H	35	2.900899	-3.926600	2.578900
N	10	-1.350800	0.018199	-0.028700	H	36	4.211399	-5.129299	0.838800
C	11	2.900600	-1.542399	0.158200	H	37	4.680700	-4.020600	-1.340199
C	12	2.640799	-2.156899	1.388200	H	38	3.821700	-1.728099	-1.777699
C	13	3.109399	-3.448500	1.626200	H	39	-2.892100	1.413400	-1.697799
C	14	3.847600	-4.123899	0.648899	H	40	-3.677699	3.740100	-1.373000
C	15	4.113400	-3.500399	-0.573900	H	41	-3.002499	5.019099	0.658799
C	16	3.640200	-2.210899	-0.822600	H	42	-1.529500	3.941600	2.356900
C	17	-1.774100	1.367000	0.148500	H	43	-0.750200	1.614200	2.033699
C	18	-2.604999	1.968300	-0.810700	H	44	-3.652799	-2.945399	-1.477499
C	19	-3.043200	3.277500	-0.622400	H	45	-6.074800	-3.286400	-1.313600
C	20	-2.660099	3.998800	0.516400	H	46	-7.485500	-1.709599	0.014999
C	21	-1.831599	3.392100	1.469999	H	47	-6.405700	0.205800	1.188700
C	22	-1.388899	2.083800	1.293899	H	48	-3.989500	0.559199	1.049000
C	23	-3.604700	-1.169900	-0.220099	H	49	5.334499	0.088199	-0.224700
C	24	-4.245200	-2.262300	-0.877400	H	50	6.323099	2.362600	-0.458699
C	25	-5.616499	-2.450599	-0.792599	H	51	4.897500	4.375700	-0.592899
C	26	-6.411599	-1.563300	-0.049000	H	52	2.405399	4.194400	-0.465199