Supporting information

First-Principles Study of Nitrogen-doped Nanographene as Efficient Charge transport and Nonlinear Optical Material

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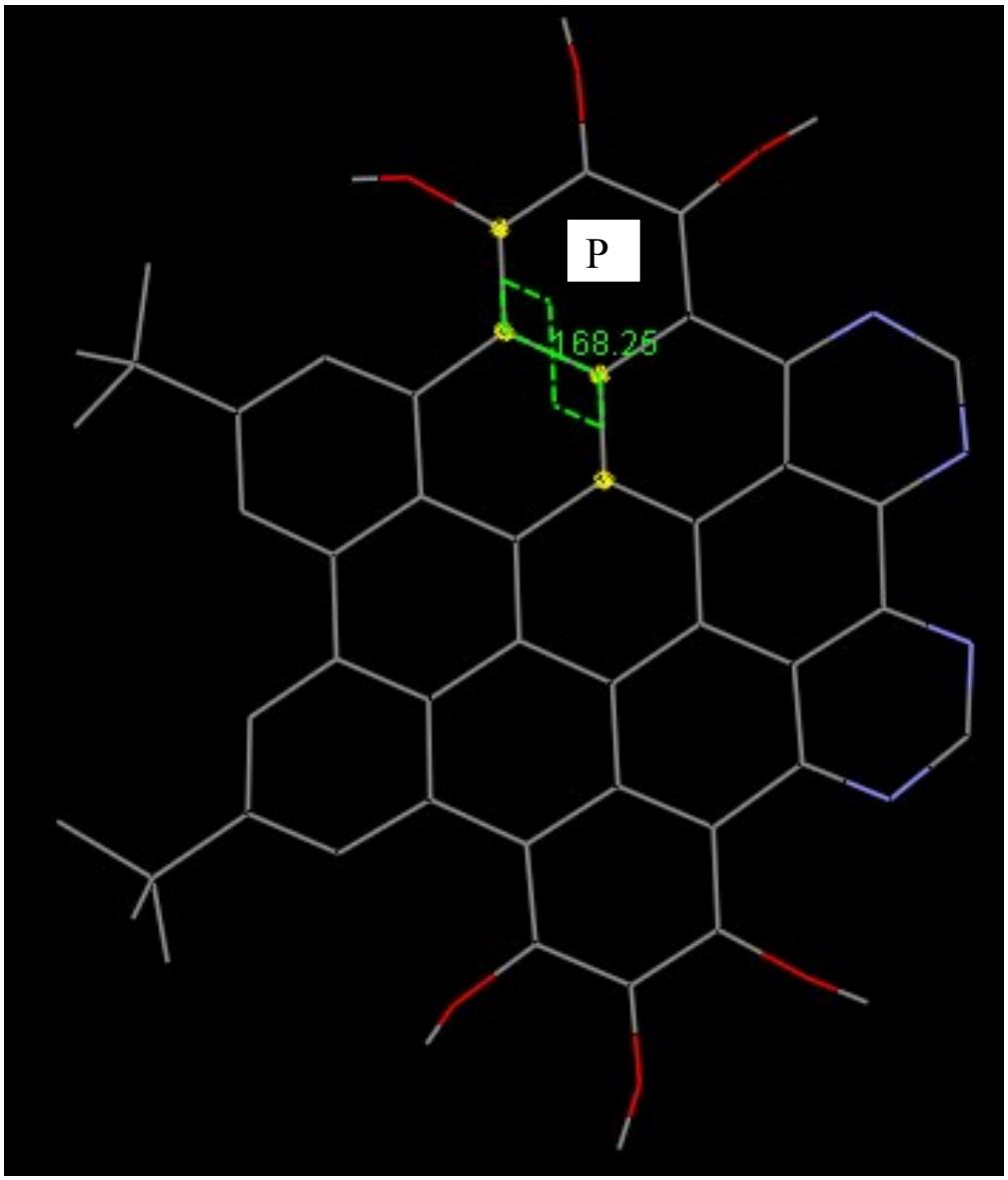


Fig. S1. Experimental Crystallographic structure showing slight distortion of the planar core due to steric congestion

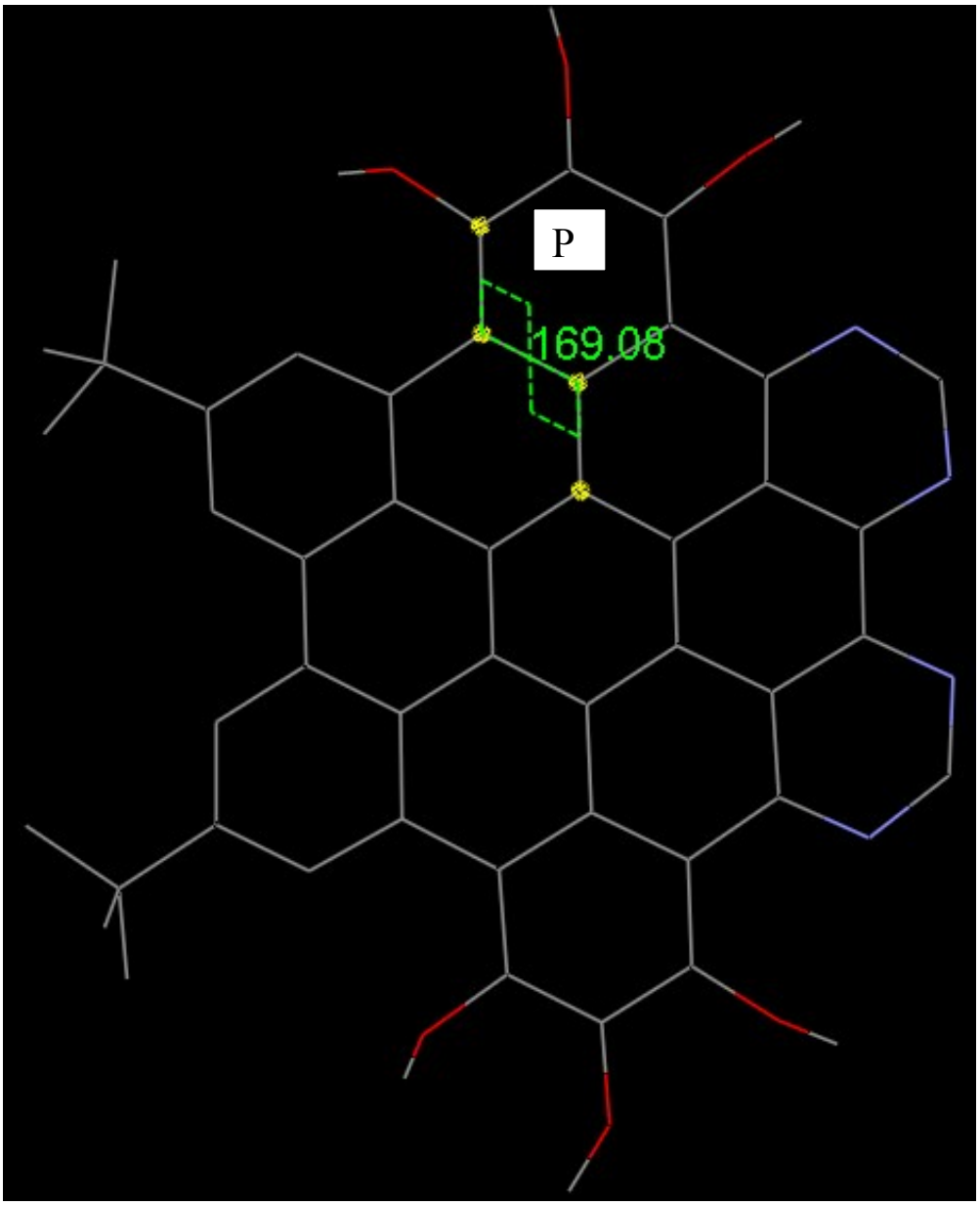


Fig. S2. Computed geometry within PBC showing distortion of the planar core due to steric congestion

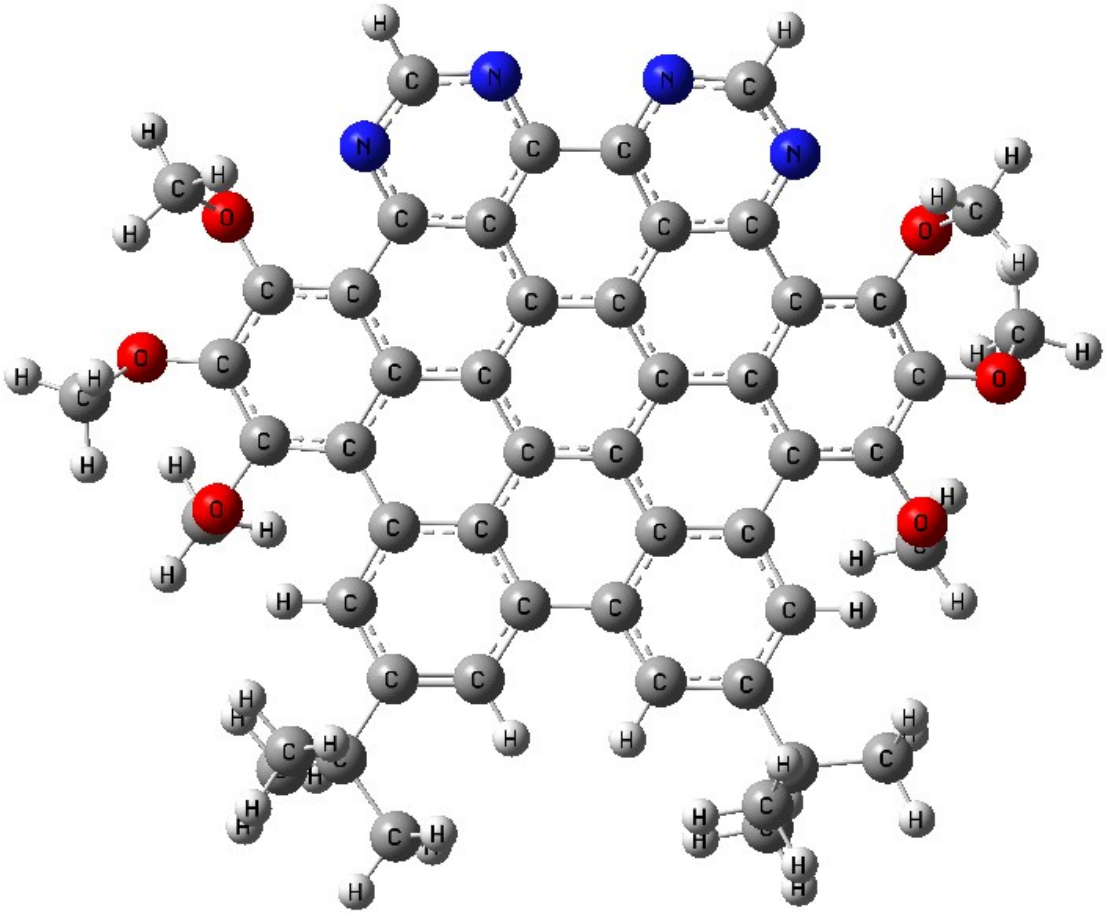
Table S1. The second-order polarizability (β_{tot}), its individual components for NDG compound **1** using four different methods and 6-311G* basis sets

	PBE0	B3LYP	M06	CAM-B3LYP
Components	$\times 10^{-30}$esu	$\times 10^{-30}$esu	$\times 10^{-30}$esu	$\times 10^{-30}$esu
β_{xxx}	-1.29	-1.42	-1.12	-1.03
β_{xxy}	-3.18	-3.15	-2.97	-2.33
β_{xyy}	-0.36	-0.36	-0.36	-0.18
β_{yyy}	0.79	0.76	0.83	-0.63
β_{xxz}	8.23	8.22	7.71	5.79
β_{xyz}	1.14	1.18	1.11	0.81
β_{yyz}	0.38	0.34	0.24	0.35
β_{xzz}	0.40	0.49	0.44	0.33
β_{yzz}	-3.92	-3.85	3.72	-3.21
β_{zzz}	13.43	13.13	12.16	9.77
$\boldsymbol{\beta_{tot}}$	22.96	22.60	20.20	17.09
% Diff. $(\boldsymbol{\beta_{tot}})$ [a]	0	1.5	12.0	25.5

[a] % Difference of $\boldsymbol{\beta_{tot}}$ amplitudes between PBE0 and other methods: [(PBE0-other method)/PBE0]×100

Table S2. The individual CPU times and difference of CPU times between 6-311G* and 6-311+G* basis sets for optimization of NDG compound **1** in three different states with PBE0 functional

	CPU Time		
	Anion	Cation	Neutral
6-311G*	1 Day, 16h	1 Day, 4h	1Day, 1h
6-311+G*	57Days, 15h	45Days, 2h	49Days, 13h
$\Delta_{CPUTime}$	56 Days	44 Days, 2h	48 Days, 12h
Avg. $\Delta_{CPUTime}$	49.34 Days		



Optimized coordinates of **NDG compound 1** at PBE0/6-311G* level of theory

Total energy = -2674.7562515 a. u.

Dipole moment (field-independent basis) = 6.9065 Debye

Optimized Cartesian Coordinates

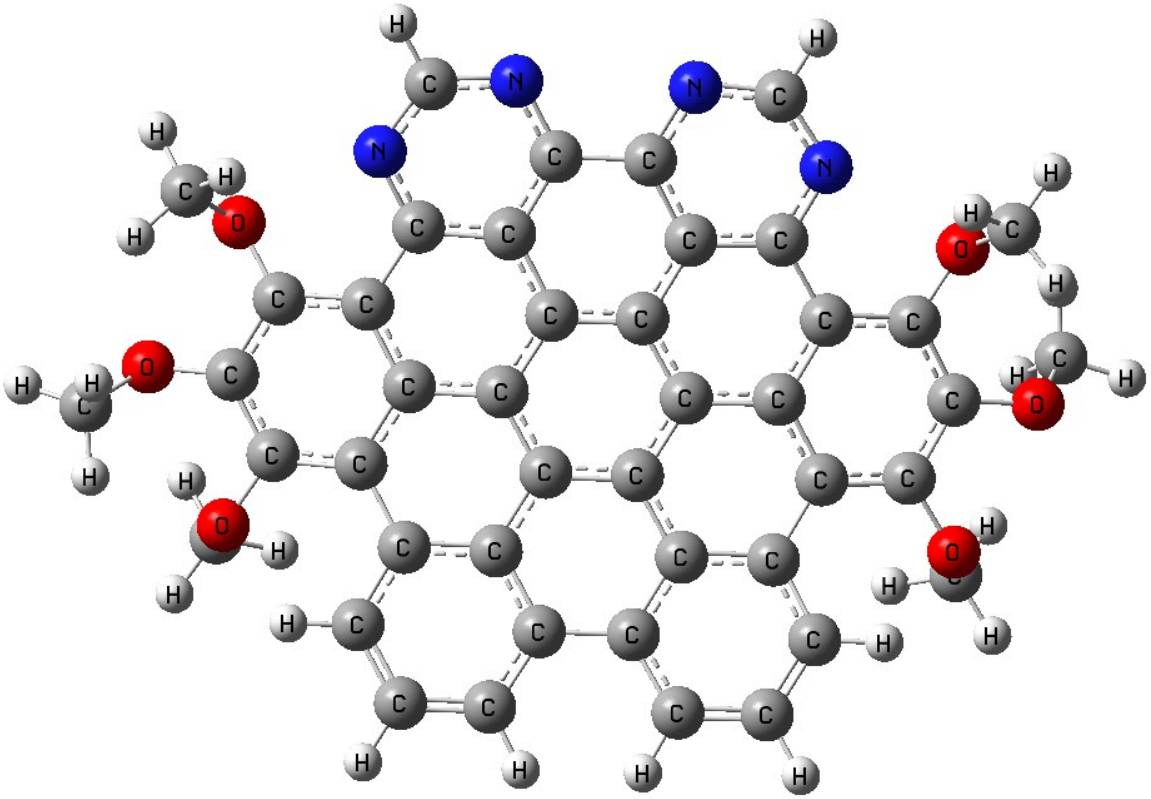
O	5.68831318	0.52345319	3.62690046
O	6.92717632	0.94693796	1.23156563
O	5.67451084	0.62384675	-1.06579530
O	-5.50864119	0.84702523	3.75647647
O	-6.83909451	1.17797823	1.47382663
O	-5.62247303	0.93548290	-0.93369830
N	-3.38750604	-0.23396718	4.96540017
N	-1.31201663	-0.45626354	6.11671802
N	1.45450946	-0.51272487	6.08685664
N	3.51214033	-0.37419445	4.89099179
C	-2.75575024	-0.05449291	3.80280917

C	-1.34916438	-0.14194740	3.73910699
C	-0.66716298	-0.31787280	4.95850586
C	0.79059651	-0.34814320	4.94271234
C	1.45215176	-0.20029840	3.70862231
C	2.86298713	-0.17247627	3.74169062
C	0.74159687	-0.11118857	2.47611563
C	-0.66370401	-0.08264315	2.49060585
C	-1.39619542	-0.02459229	1.29049714
C	-2.83102085	0.11596108	1.32705435
C	-3.50437337	0.20155683	2.57957297
C	-4.86317984	0.55718434	2.60823642
C	1.45003138	-0.07869426	1.26130212
C	2.88797944	0.00656036	1.26673179
C	3.59219396	0.06482689	2.50327007
C	4.96232733	0.37020967	2.49276941
C	6.42951678	-0.62642404	4.01266297
H	7.10268768	-0.94122571	3.20938523
H	5.75128664	-1.43603346	4.29000382
H	7.01167126	-0.33284880	4.88583292
C	7.30691862	2.15797523	1.87542995
H	7.21422148	2.08546155	2.95883750
H	6.69594350	2.99419313	1.51747395
H	8.34643406	2.32768206	1.59607121
C	5.74563138	1.96890152	-1.50844111
H	6.22225383	2.60472002	-0.75725791
H	4.74913737	2.35851977	-1.74253857
H	6.35689436	1.96470278	-2.41080038
C	4.94109362	0.44295501	0.06776242
C	5.61159416	0.61502888	1.28083208
C	3.57789044	0.09401095	0.02990805

C	2.84702354	-0.15725045	-1.21237440
C	3.50291200	-0.42970623	-2.41955530
H	4.57835815	-0.48342303	-2.41345572
C	2.81315592	-0.65288119	-3.60446329
C	1.42541000	-0.57723846	-3.57599569
H	0.88614842	-0.72585496	-4.50275928
C	0.71269536	-0.34961236	-2.40073898
C	1.42970809	-0.17651659	-1.19150483
C	0.72298672	-0.08692494	0.05092597
C	5.04487164	-1.03818403	-4.75658960
H	5.46577215	-0.08731836	-4.41652084
H	5.50691369	-1.27401378	-5.71963681
H	5.34757045	-1.81527864	-4.04899924
C	3.52658786	-0.96949739	-4.91952313
C	3.20451479	0.12317087	-5.94853206
H	3.70639350	-0.08741053	-6.89858773
H	3.54132181	1.10331483	-5.59828865
H	2.13240307	0.19414227	-6.15042996
C	3.04239681	-2.32691829	-5.44829630
H	3.54642425	-2.57155866	-6.38900574
H	1.96614462	-2.33351689	-5.64012409
H	3.25636087	-3.12549805	-4.73229285
C	-0.74610160	-0.29442358	-2.38780108
C	-1.42744287	-0.09878612	-1.16516636
C	-0.69465496	-0.05590818	0.06535566
C	-2.84433240	0.00447355	-1.15852390
C	-3.54082488	0.24493800	0.10586558
C	-5.54866796	0.75531884	1.40615151
C	-4.89318548	0.62753243	0.18225920
C	-3.52916399	-0.18895796	-2.35924488

H	-4.60697865	-0.16865802	-2.34455413
C	-2.87456881	-0.41612910	-3.56789139
C	-1.48947763	-0.43891890	-3.56260488
H	-0.97085700	-0.58768693	-4.49873290
C	-2.82726090	-0.85735096	-6.07049848
H	-3.46223286	-1.00659440	-6.94843636
H	-2.19834213	-1.74715539	-5.96969721
H	-2.18050614	0.00027286	-6.27999879
C	-3.70053377	-0.63003830	-4.83670870
C	-4.57609141	0.60485486	-5.09081457
H	-5.26303305	0.79341743	-4.26166187
H	-5.17760429	0.46688415	-5.99524609
H	-3.96260745	1.50052612	-5.22618212
C	-4.59902076	-1.86106806	-4.65266682
H	-4.00184761	-2.75890683	-4.46904447
H	-5.19962259	-2.03209344	-5.55209186
H	-5.28747636	-1.74255806	-3.81207580
C	-6.35674084	-0.16072083	4.27647570
H	-5.77354211	-1.04071889	4.55753862
H	-7.13926923	-0.42844440	3.55991538
H	-6.81766762	0.26419550	5.16744367
C	-7.81420160	0.32726617	0.88417762
H	-7.71007860	-0.69708334	1.25771597
H	-7.73952080	0.32231345	-0.20415589
H	-8.78145195	0.72486938	1.19051456
C	2.77377149	-0.53936056	5.98263959
H	3.32366642	-0.71351228	6.90507560
C	-2.63341654	-0.43043530	6.04075141
H	-3.16973220	-0.58482967	6.97461687
C	-5.69455307	2.33657487	-1.18295012

H	-4.69619219	2.74515764	-1.36622314
H	-6.16198460	2.85438590	-0.34167528
H	-6.30729833	2.45906040	-2.07599157



Optimized coordinates of **NDG compound 2** at PBE0/6-311G* level of theory

Total energy = -2360.5901685 a. u.

Dipole moment (field-independent basis) = 8.0463 Debye

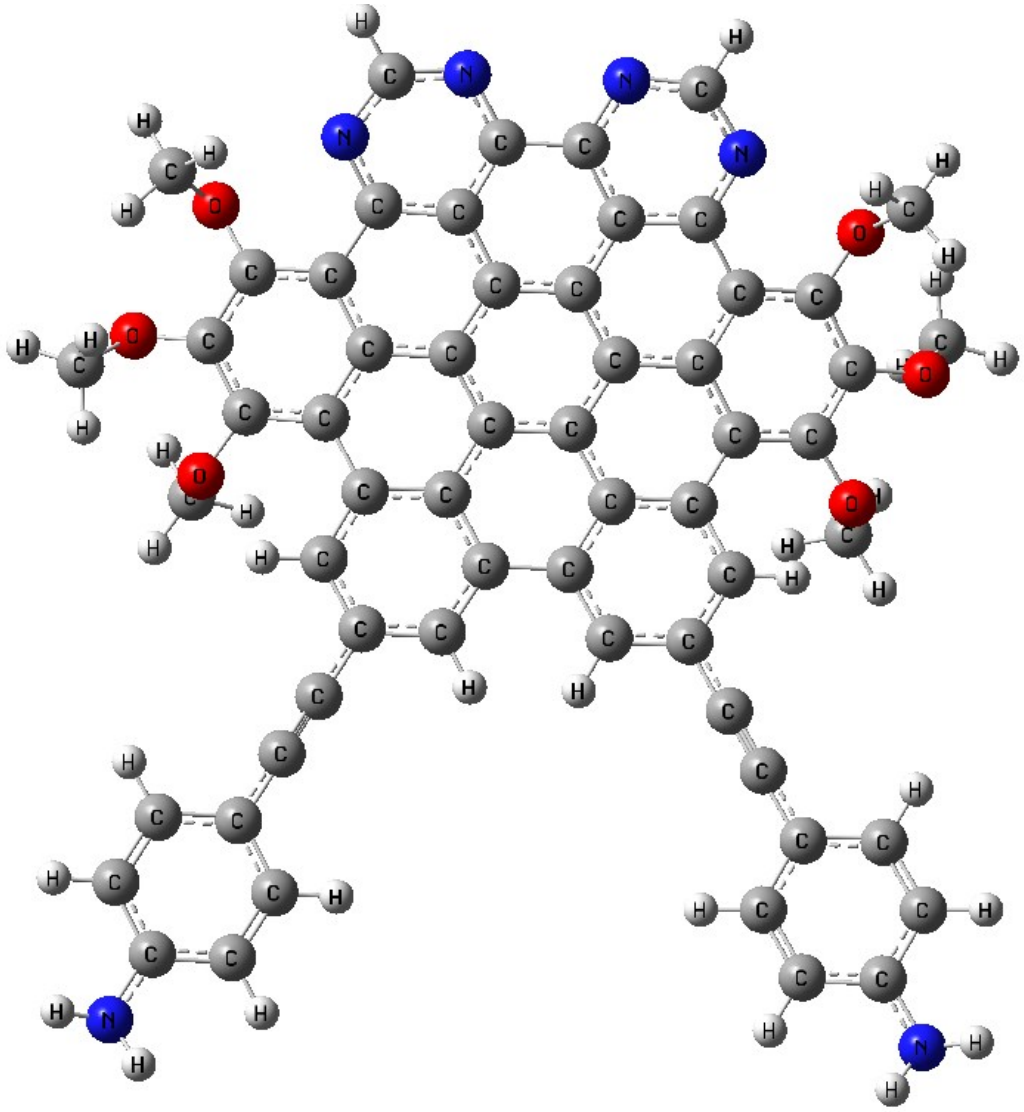
Optimized Cartesian Coordinates

O	5.67158155	-0.20280664	2.59162260
O	6.92997450	-0.20748082	0.16511518
O	5.60538224	-0.54819143	-2.09112888
O	-5.31128098	1.94727132	2.67780451
O	-6.60633407	2.27662562	0.37211005
O	-5.48817536	1.59745501	-1.99799539
N	-3.38364556	0.64349500	3.98414841

N	-1.35559202	0.19291795	5.15236145
N	1.36276076	-0.31417651	5.13099895
N	3.39912440	-0.62136624	3.93095088
C	-2.74837491	0.60647375	2.81024677
C	-1.37660640	0.28267083	2.75538509
C	-0.71471056	0.11384022	3.98657714
C	0.71833142	-0.15408600	3.97527944
C	1.37716473	-0.23244467	2.73353973
C	2.77457166	-0.42743357	2.76680809
C	0.67240367	-0.14727044	1.49675677
C	-0.70913739	0.11065785	1.50710652
C	-1.43981898	0.17475132	0.30597001
C	-2.83106673	0.55357151	0.33048398
C	-3.46250938	0.86757193	1.56834349
C	-4.74278945	1.44565502	1.56264633
C	1.35913288	-0.34430921	0.28482127
C	2.79290449	-0.48977567	0.28759323
C	3.51497123	-0.42623908	1.51310689
C	4.91620798	-0.34423921	1.47558544
C	6.22575418	-1.41469222	3.08677867
H	6.82703822	-1.90902232	2.31766770
H	5.43155397	-2.07473941	3.44160728
H	6.86121346	-1.13609555	3.92705042
C	7.51113267	0.97426208	0.70538073
H	7.44589467	0.99572083	1.79284171
H	7.02172642	1.86624239	0.29883926
H	8.55399578	0.96105744	0.38965570
C	5.90237749	0.72072992	-2.65098395
H	6.51349872	1.31747036	-1.96837315
H	4.98436034	1.26489537	-2.89695917

H	6.46785849	0.53024258	-3.56278270
C	4.87361728	-0.50084254	-0.94426054
C	5.58001576	-0.32069196	0.24708958
C	3.47243003	-0.63146221	-0.94831944
C	2.69757306	-0.88473057	-2.16156372
C	3.28509348	-1.37907332	-3.33139436
H	4.33822569	-1.61106206	-3.34224697
C	2.52842474	-1.59640955	-4.46987608
C	1.17766433	-1.31073309	-4.48257690
H	0.62316459	-1.47502240	-5.39764233
C	0.53314201	-0.84853956	-3.33305234
C	1.29140985	-0.67493133	-2.14891694
C	0.62328339	-0.35057110	-0.92142546
C	-0.89375985	-0.55121144	-3.32944641
C	-1.52371109	-0.12709557	-2.13263724
C	-0.77172153	-0.08799373	-0.91143844
C	-2.90446120	0.21307614	-2.13115605
C	-3.52971220	0.68247781	-0.89629367
C	-5.40609356	1.63924219	0.34708427
C	-4.80053113	1.28707372	-0.85788218
C	-3.63484728	0.02704412	-3.31056753
H	-4.69524869	0.22165234	-3.31885092
C	-3.01845618	-0.41369948	-4.46836747
C	-1.66348941	-0.67751372	-4.48755375
H	-1.21134646	-0.99558475	-5.41819341
C	-6.30707018	1.15084000	3.29393337
H	-5.87400672	0.21693330	3.65953998
H	-7.13482929	0.95012587	2.60714611
H	-6.67596338	1.73107533	4.13891396
C	-7.72048946	1.54520575	-0.12471794

H	-7.80440518	0.57753751	0.38169622
H	-7.64873931	1.38403062	-1.20113568
H	-8.59869195	2.14784380	0.10528022
C	2.65907501	-0.56262015	5.03219619
H	3.18643714	-0.73541318	5.96790248
C	-2.65609566	0.42754775	5.07375299
H	-3.19630727	0.45141768	6.01774328
C	-5.32294549	2.95431491	-2.40032392
H	-4.27351319	3.16146621	-2.63091715
H	-5.67527115	3.63337183	-1.61987321
H	-5.92494002	3.08343370	-3.29952104
H	-3.60826927	-0.55054456	-5.36956353
H	3.00500060	-1.99327364	-5.36098043



Optimized coordinates of **NDG compound 3** at PBE0/6-311G* level of theory

Total energy = -3085.0338107 a. u.

Dipole moment (field-independent basis) = 14.034 Debye

Optimized Cartesian Coordinates

O	5.09579100	5.33168400	0.30349700
O	2.86609800	6.73011500	1.02235600
O	0.45557700	5.65738100	0.92981500
O	4.44525000	-5.83523900	0.40364900
O	2.12419300	-7.01751400	0.96944100
O	-0.20411700	-5.63992500	0.99974700
N	5.66404500	-3.78473500	-0.79451000
N	6.92782600	-1.78990400	-1.11790200

N	7.09365700	0.97103300	-1.11809900
N	6.07803800	3.10311600	-0.79470400
C	4.58004300	-3.07788500	-0.46560100
C	4.60762900	-1.66858000	-0.52120000
C	5.84405100	-1.06969300	-0.82974200
C	5.93133500	0.38554600	-0.83020200
C	4.77530900	1.12796100	-0.52193300
C	4.91618300	2.53118800	-0.46907800
C	3.51240400	0.50424500	-0.30070100
C	3.42769500	-0.89907200	-0.30092100
C	2.19246100	-1.54693800	-0.11502100
C	2.14322700	-2.98396600	-0.00579000
C	3.34533900	-3.74503800	-0.07761100
C	3.31839700	-5.11009200	0.25239200
C	2.36458700	1.29522300	-0.11017000
C	2.48846200	2.72649700	0.00263300
C	3.77219900	3.33856300	-0.06968600
C	3.89956600	4.69618800	0.26485000
C	5.40308800	6.08381300	-0.86299200
H	4.62177200	6.82274600	-1.06506800
H	5.53629200	5.41602400	-1.71664100
H	6.34463900	6.59187400	-0.65606000
C	3.65525800	7.01938900	2.17080900
H	4.71144300	6.81553200	1.99537600
H	3.31267200	6.43493200	3.03199900
H	3.50456800	8.07927500	2.37395300
C	0.14876200	5.71261300	2.31400500
H	0.97495900	6.15181000	2.88018000
H	-0.07976000	4.71604800	2.70592800
H	-0.73007800	6.34956000	2.40912300

C	1.50406400	4.84969800	0.61379800
C	2.77591000	5.42470800	0.66064200
C	1.32730800	3.50199000	0.24791900
C	0.01238800	2.87107900	0.13164200
C	-1.15899800	3.61936100	0.02120900
H	-1.10942400	4.69549800	-0.01562800
C	-2.41105500	3.00629600	-0.06293500
C	-2.49249900	1.61610500	-0.02100200
H	-3.47702100	1.17030700	-0.06555300
C	-1.34920100	0.82608000	0.04527200
C	-0.07830700	1.45244400	0.08352300
C	1.10978500	0.65654100	0.00966000
C	-1.43715200	-0.63109700	0.06868300
C	-0.25079000	-1.40669300	0.10023800
C	1.02436100	-0.76141700	0.01141600
C	-0.33163200	-2.82496000	0.17327100
C	0.89858200	-3.61274200	0.24857700
C	2.10069300	-5.71767600	0.57340600
C	0.91942100	-4.97803500	0.59085000
C	-1.58880200	-3.42575800	0.11339400
H	-1.67472200	-4.49998100	0.10687400
C	-2.75904000	-2.66670000	0.05142500
C	-2.66939600	-1.27652200	0.05473800
H	-3.59301200	-0.71431400	0.03065400
C	4.78620100	-6.70613200	-0.65967500
H	5.01839600	-6.13271100	-1.56010600
H	3.98548000	-7.42539800	-0.85580600
H	5.67708200	-7.24262900	-0.33506300
C	1.38150100	-7.93501500	0.17601600
H	1.66019200	-7.84703400	-0.87969900

H	0.30712200	-7.77838600	0.27930200
H	1.65164600	-8.92707300	0.53704200
C	7.08478100	2.29459900	-1.10566900
H	8.01788700	2.78247500	-1.37926900
C	6.75994900	-3.10300400	-1.10660600
H	7.62728600	-3.69910500	-1.38227300
C	-0.34445900	-5.68376700	2.41717900
H	-0.42713300	-4.67253600	2.82678100
H	0.50342400	-6.20317600	2.87120700
H	-1.26431800	-6.23230500	2.61776500
C	-3.58477700	3.79401800	-0.18164600
C	-4.58618100	4.46829900	-0.28417000
C	-4.02293900	-3.30823500	-0.00893200
C	-5.10127500	-3.85810700	-0.06320500
C	-5.75310800	5.26189300	-0.40597600
C	-5.66835600	6.65379800	-0.56115100
C	-7.03110700	4.68387100	-0.37701900
C	-6.80394700	7.42998600	-0.68313300
H	-4.69056400	7.12341100	-0.58885100
C	-8.16871100	5.45753800	-0.49764400
H	-7.12219800	3.60910800	-0.25851400
C	-8.07879800	6.84750500	-0.65562300
H	-6.70930400	8.50667800	-0.79867300
H	-9.14681500	4.98432500	-0.46622000
C	-6.36060300	-4.50331800	-0.12897000
C	-6.45527000	-5.90087900	-0.20879000
C	-7.55463800	-3.76681500	-0.11837100
C	-7.68180600	-6.53176100	-0.27632800
H	-5.54525400	-6.49178300	-0.22044100
C	-8.78282200	-4.39466800	-0.18503400

H	-7.50691800	-2.68448100	-0.05787100
C	-8.87209900	-5.79120600	-0.26777800
H	-7.72632900	-7.61636500	-0.33330800
H	-9.69246100	-3.79975900	-0.16983000
N	-10.09959000	-6.42336500	-0.28206100
N	-9.21589500	7.62792100	-0.72406100
H	-10.88064400	-5.86868900	-0.59129100
H	-10.11300600	-7.35748800	-0.65701900
H	-9.10634300	8.53499400	-1.14665900
H	-10.05748600	7.16055300	-1.01844900