

Supporting Information

Structural, Electronic and Nonlinear Optical Properties of Novel Derivatives of 9,12-diido-1,2-dicarba-closo-dodecaborane: Density Functional Theory Approach

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Table S1. The calculated values of first hyperpolarizabilities (β_{tot} , and β_{vec} a. u.)^a for compounds **1-3** at B3LYP and CAM-B3LYP/Gen^b levels of theory

Compounds	Hyperpolarizability	B3LYP 6-31G**	CAM-B3LYP 6-31+G**	Diff.	% Diff.
1	β_{tot}	827	562	265	32
	β_{vec}	496	337	159	32
2	β_{tot}	6391	3160	3231	50
	β_{vec}	4808	1896	2912	60
3	β_{tot}	6789	5773	1016	14
	β_{vec}	4074	3464	610	14

^a Conversion factors for β_{tot} from a.u. to SI and esu units: 1 a. u. = $3.26361 \times 10^{-53} \text{C}^3 \text{m}^2 \text{J}^{-2}$ = 8.639418×10^{-33} esu

^b Gen = LANL2DZ for I atoms.

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Table S2: Optimized geometries of the molecules (Cartesian coordinates) of ground state for compounds **1** at the B3LYP/Gen^b and CAM-B3LYP/Gen^c methods levels of theory

B3LYP/6-31G**				CAM-B3LYP/6-31+G**			
I	-2.12915800	-1.35435900	-0.00000700	I	-2.10703800	-1.34544300	-0.00000200
I	2.13043100	-1.35239300	-0.00000100	I	2.10717100	-1.34523600	0.00000000
C	-0.81435800	3.19851900	0.00013800	C	-0.80729800	3.18012900	0.00006800
H	-1.29611500	4.16787800	0.00021200	H	-1.28890400	4.14889600	0.00011000
C	0.81138100	3.19926800	0.00001600	C	0.80700600	3.18019700	0.00001800
H	1.29223000	4.16907900	-0.00005800	H	1.28852800	4.14900500	0.00000600
B	-0.00120100	2.77842900	1.45473800	B	-0.00007700	2.76312900	1.44671400
H	-0.00153100	3.56271100	2.33600300	H	-0.00009000	3.54725700	2.32723900
B	-1.44063300	1.89944400	0.89461900	B	-1.43258000	1.88890400	0.88947800
H	-2.45465800	2.05217400	1.48000800	H	-2.44671700	2.04110100	1.47364600
B	-1.44064600	1.89951300	-0.89441900	B	-1.43261500	1.88894500	-0.88937000
H	-2.45471100	2.05238800	-1.47971500	H	-2.44678700	2.04121400	-1.47346400
B	-0.00140500	2.77861200	-1.45458000	B	-0.00018200	2.76322900	-1.44664700
H	-0.00181500	3.56294800	-2.33579600	H	-0.00023700	3.54739000	-2.32714200
B	1.43892600	1.90073600	0.89441300	B	1.43244000	1.88901600	0.88937000
H	2.45289900	2.05435000	1.47966600	H	2.44661100	2.04128000	1.47346300
B	-0.00036900	1.01368400	1.45836400	B	-0.00000100	1.00672400	1.45068300
H	-0.00004200	0.41318200	2.47608800	H	0.00005200	0.40471800	2.46712800
B	-0.89414200	0.46384500	-0.00001400	B	-0.88863400	0.45973500	-0.00001400
B	-0.00059000	1.01389600	-1.45841700	B	-0.00011200	1.00682100	-1.45073300
H	-0.00035000	0.41356800	-2.47625300	H	-0.00011600	0.40491000	-2.46723600
B	1.43879800	1.90085500	-0.89461600	B	1.43238100	1.88906900	-0.88947600
H	2.45264300	2.05468000	-1.48003800	H	2.44649400	2.04142500	-1.47364700
B	0.89363400	0.46461900	-0.00021000	B	0.88855600	0.45979500	-0.00010300

^bGen = 6-31G** for H, C, B and O atoms, while Gen = LANL2DZ for I atoms

^cGen = 6-31+G** for H, C, B and O atoms, while Gen = LANL2DZ for I atoms

Table S3: Optimized geometries of the molecules (Cartesian coordinates) of ground state for compound **2** at the B3LYP/Gen^b at B3LYP and CAM-B3LYP/Gen^c methods levels of theory, respectively.

B3LYP/6-31G**				CAM-B3LYP/6-31+G**			
I	-5.20437100	2.12696000	0.01819400	I	-5.18288300	-2.10585300	-0.01981100
I	-5.20428200	-2.12700500	-0.01822700	I	-5.18287500	2.10585800	0.01977100
C	-0.62860500	0.87365100	0.00800300	C	-0.63311900	-0.84296800	-0.00841600
C	-0.62856300	-0.87350600	-0.00813700	C	-0.63311600	0.84295400	0.00849400
B	-1.06607800	-0.01193500	1.43812800	B	-1.07393000	0.01338200	-1.44137400
H	-0.29582200	-0.01993100	2.32952500	H	-0.29617000	0.02210400	-2.32489500
B	-1.95994900	1.43799000	0.90840500	B	-1.95460800	-1.42701300	-0.90356200
H	-1.81449800	2.43699900	1.51949800	H	-1.80154800	-2.42952200	-1.50531900
B	-1.95887400	1.45312000	-0.88303700	B	-1.95378500	-1.44367600	0.87577900
H	-1.81363200	2.46257800	-1.47683900	H	-1.80094000	-2.45751600	1.45838500
B	-1.06610600	0.01206900	-1.43822300	B	-1.07396700	-0.01339400	1.44144100
H	-0.29589400	0.02008300	-2.32966000	H	-0.29623000	-0.02212000	2.32498100
B	-1.95876800	-1.45301000	0.88295500	B	-1.95375600	1.44366700	-0.87573600
H	-1.81349700	-2.46244700	1.47678700	H	-1.80089100	2.45750700	-1.45833800
B	-2.83127400	-0.01260100	1.45324900	B	-2.82764500	0.01383900	-1.44577900
H	-3.42225400	-0.02185000	2.47654300	H	-3.42198300	0.02393400	-2.46658600
B	-3.39045400	0.89247200	0.00757700	B	-3.38040200	-0.88850500	-0.00840300
B	-2.83131200	0.01265700	-1.45330600	B	-2.82768300	-0.01384300	1.44579900
H	-3.42231000	0.02187900	-2.47659000	H	-3.42204800	-0.02393700	2.46659100
B	-1.95991800	-1.43792100	-0.90848500	B	-1.95462500	1.42700400	0.90360600
H	-1.81446000	-2.43694700	-1.51954500	H	-1.80157700	2.42951300	1.50536600
B	-3.39041300	-0.89245000	-0.00762600	B	-3.38039800	0.88850300	0.00840900
C	0.63493500	1.53504900	0.01376500	C	0.63325100	-1.51281300	-0.01449400
C	0.63500800	-1.53484400	-0.01385900	C	0.63325700	1.51279400	0.01460500
C	1.70236800	2.11004800	0.01951000	C	1.69246400	-2.08769400	-0.01943000
C	1.70243600	-2.10985200	-0.01959100	C	1.69247000	2.08767300	0.01955700
C	2.95401900	2.79305900	0.02432100	C	2.94817700	-2.77464200	-0.02373200
C	3.66931100	2.95486600	1.22831500	C	3.65759500	-2.93469400	-1.22223100
C	3.48294500	3.31104800	-1.17542600	C	3.47012500	-3.29063600	1.17069500
C	4.88995900	3.61850000	1.23432300	C	4.87456900	-3.59917600	-1.22953900
H	3.25907100	2.55845500	2.15051100	H	3.24888500	-2.53729600	-2.14417600
C	4.70254000	3.97656400	-1.17393300	C	4.68588800	-3.95733200	1.17072300
H	2.92954200	3.18783000	-2.09980500	H	2.91675900	-3.16763600	2.09462400
C	5.38693600	4.11840200	0.03195300	C	5.36614800	-4.09805900	-0.03108600
H	5.45974000	3.75650600	2.14453800	H	5.44175600	-3.73606400	-2.14139300
H	5.13069100	4.38476600	-2.08070600	H	5.10978000	-4.36593600	2.07917200
C	2.95405700	-2.79292700	-0.02432800	C	2.94817700	2.77463200	0.02380800
C	3.67025100	-2.95322900	-1.22799400	C	3.65760500	2.93475600	1.22229300
C	3.48204300	-3.31251300	1.17513900	C	3.47011000	3.29056500	-1.17065200
C	4.89083900	-3.61696500	-1.23394700	C	4.87457400	3.59924800	1.22955200
H	3.26073500	-2.55559100	-2.14998400	H	3.24890700	2.53740600	2.14426400
C	4.70159400	-3.97811600	1.17370000	C	4.68586800	3.95727000	-1.17072800
H	2.92795800	-3.19046200	2.09926400	H	2.91673700	3.16750900	-2.09456900
C	5.38687900	-4.11846400	-0.03185200	C	5.36613800	4.09806800	0.03106700
H	5.46127100	-3.75387600	-2.14392000	H	5.44176900	3.73619100	2.14139300
H	5.12903900	-4.38749300	2.08027700	H	5.10974900	4.36582700	-2.07920300
N	6.68242900	4.82226000	0.03579400	N	6.65771000	-4.80355100	-0.03481800
O	7.09700400	5.25183000	-1.03900200	O	7.07091800	-5.23345500	1.03199900
O	7.26387900	4.93298100	1.11341400	O	7.23829900	-4.91583800	-1.10437900
N	6.68230800	-4.82242800	-0.03563900	N	6.65769400	4.80357100	0.03474800
O	7.09621900	-5.25311200	1.03896800	O	7.07089500	5.23340300	-1.03210100
O	7.26436800	-4.93213900	-1.11303500	O	7.23829900	4.91590400	1.10429500

^bGen = 6-31G** for H, C, B and O atoms, while Gen = LANL2DZ for I atoms

^cGen = 6-31+G** for H, C, B and O atoms, while Gen = LANL2DZ for I atoms

Table S4: Optimized geometries of the molecules (Cartesian coordinates) of ground state for compound **3** at the B3LYP/Gen^b at B3LYP and CAM-B3LYP/Gen^c methods levels of theory, respectively.

B3LYP/6-31G**				CAM-B3LYP/6-31+G**			
I	-4.54624000	2.12307800	0.01222400	I	4.51834100	2.10467100	-0.02031100
I	-4.54623800	-2.12307200	-0.01228800	I	4.51848400	-2.10457900	0.02027800
C	0.03465700	0.91877700	0.00646700	C	-0.03771300	0.85513600	-0.00961600
C	0.03466200	-0.91875300	-0.00645800	C	-0.03765400	-0.85535300	0.00968500
B	-0.38394400	-0.00759900	1.41176900	B	0.39941300	-0.01325900	-1.43138200
H	0.37279300	-0.01381600	2.31540600	H	-0.37048000	-0.02314900	-2.32182900
B	-1.29682600	1.44518700	0.90445700	B	1.28691400	1.42722900	-0.90328600
H	-1.16978000	2.43916800	1.52873600	H	1.14259600	2.42823700	-1.51011800
B	-1.29516500	1.45549300	-0.88613300	B	1.28482100	1.44442900	0.87354000
H	-1.16828300	2.45662100	-1.49896000	H	1.14071400	2.45713300	1.46077900
B	-0.38394400	0.00761500	-1.41177300	B	0.39944400	0.01307200	1.43144200
H	0.37280900	0.01383900	-2.31539700	H	-0.37043000	0.02290900	2.32190600
B	-1.29516800	-1.45549300	0.88614700	B	1.28490000	-1.44455600	-0.87350000
H	-1.16826100	-2.45662200	1.49896600	H	1.14084900	-2.45727000	-1.46073600
B	-2.15704400	-0.00877500	1.45124300	B	2.15626800	-0.01456100	-1.44464300
H	-2.74756100	-0.01578200	2.47558800	H	2.75153300	-0.02576500	-2.46556700
B	-2.72375700	0.88908000	0.00525200	B	2.71053700	0.88672200	-0.00877600
B	-2.15704400	0.00878100	-1.45123200	B	2.15629900	0.01449300	1.44466300
H	-2.74758400	0.01578300	-2.47556500	H	2.75158600	0.02573800	2.46557400
B	-1.29680800	-1.44516600	-0.90444700	B	1.28703100	-1.42735500	0.90332600
H	-1.16976200	-2.43914400	-1.52873100	H	1.14279500	-2.42837300	1.51016100
B	-2.72375200	-0.88907800	-0.00524700	B	2.71059800	-0.88675200	0.00878300
C	1.29514900	1.56788600	0.00922200	C	-1.30192800	1.52115000	-0.01452500
C	1.29515700	-1.56786400	-0.00921000	C	-1.30182300	-1.52145700	0.01462300
C	2.37954700	2.11746100	0.01039900	C	-2.36772000	2.08846800	-0.01686600
C	2.37954900	-2.11744800	-0.01037200	C	-2.36763500	-2.08873700	0.01698100
C	3.63796100	2.77471200	0.01028800	C	-3.62366400	2.76528900	-0.01889100
C	4.31865600	3.03734400	1.21759100	C	-4.33452700	2.95661600	-1.21252000
C	4.23972600	3.18608100	-1.19744400	C	-4.17552000	3.25766100	1.17262900
C	5.54463900	3.68266300	1.21849300	C	-5.55100400	3.61550700	-1.21645400
H	3.86939800	2.72989300	2.15639700	H	-3.92131300	2.58232800	-2.14314200
C	5.46512100	3.83253300	-1.19920900	C	-5.39113600	3.91824600	1.17244700
H	3.72882500	2.99448300	-2.13554200	H	-3.63770700	3.11906800	2.10457400
C	6.14179900	4.09392900	0.00953400	C	-6.09945600	4.10976300	-0.02340300
H	6.05495800	3.87378600	2.15887100	H	-6.08933500	3.75016600	-2.15013400
H	5.91320200	4.14055400	-2.14025700	H	-5.80406400	4.28999100	2.10570500
C	3.63795700	-2.77470200	-0.01024600	C	-3.62367500	-2.76537900	0.01894200
C	4.31933000	-3.03607300	-1.21744100	C	-4.33458000	-2.95668800	1.21254900
C	4.23902900	-3.18735100	1.19739300	C	-4.17555500	-3.25764900	-1.17260900
C	5.54530600	-3.68140500	-1.21832400	C	-5.55111500	-3.61547300	1.21643300
H	3.87060600	-2.72762800	-2.15617600	H	-3.92134100	-2.58249300	2.14319700
C	5.46440700	-3.83383500	1.19917100	C	-5.39122900	-3.91812700	-1.17247800
H	3.72760200	-2.99672900	2.13540300	H	-3.63770200	-3.11908200	-2.10453600
C	6.14176700	-4.09396800	-0.00946200	C	-6.09959000	-4.10962800	0.02335000
H	6.05616200	-3.87153600	-2.15861200	H	-6.08947100	-3.75013200	2.15009800
H	5.91194600	-4.14285800	2.14014900	H	-5.80416800	-4.28980500	-2.10575800
N	7.38724100	4.69605400	0.00605600	N	-7.33365600	4.73333000	-0.01994100
N	7.38720300	-4.69610800	-0.00591600	N	-7.33384400	-4.73308700	0.01984000
H	7.63590100	5.22697700	-0.81556600	H	-7.56661600	5.30312300	0.77854500
H	7.69107900	5.12208000	0.86916300	H	-7.67877400	5.08998400	-0.89755200
H	7.69151700	-5.12123500	-0.86929800	H	-7.67900900	-5.08974700	0.89743000
H	7.63539400	-5.22789700	0.81528700	H	-7.56683900	-5.30282700	-0.77867400

^bGen = 6-31G** for H, C, B and O atoms, while Gen = LANL2DZ for I atoms

^cGen = 6-31+G** for H, C, B and O atoms, while Gen = LANL2DZ for I atoms

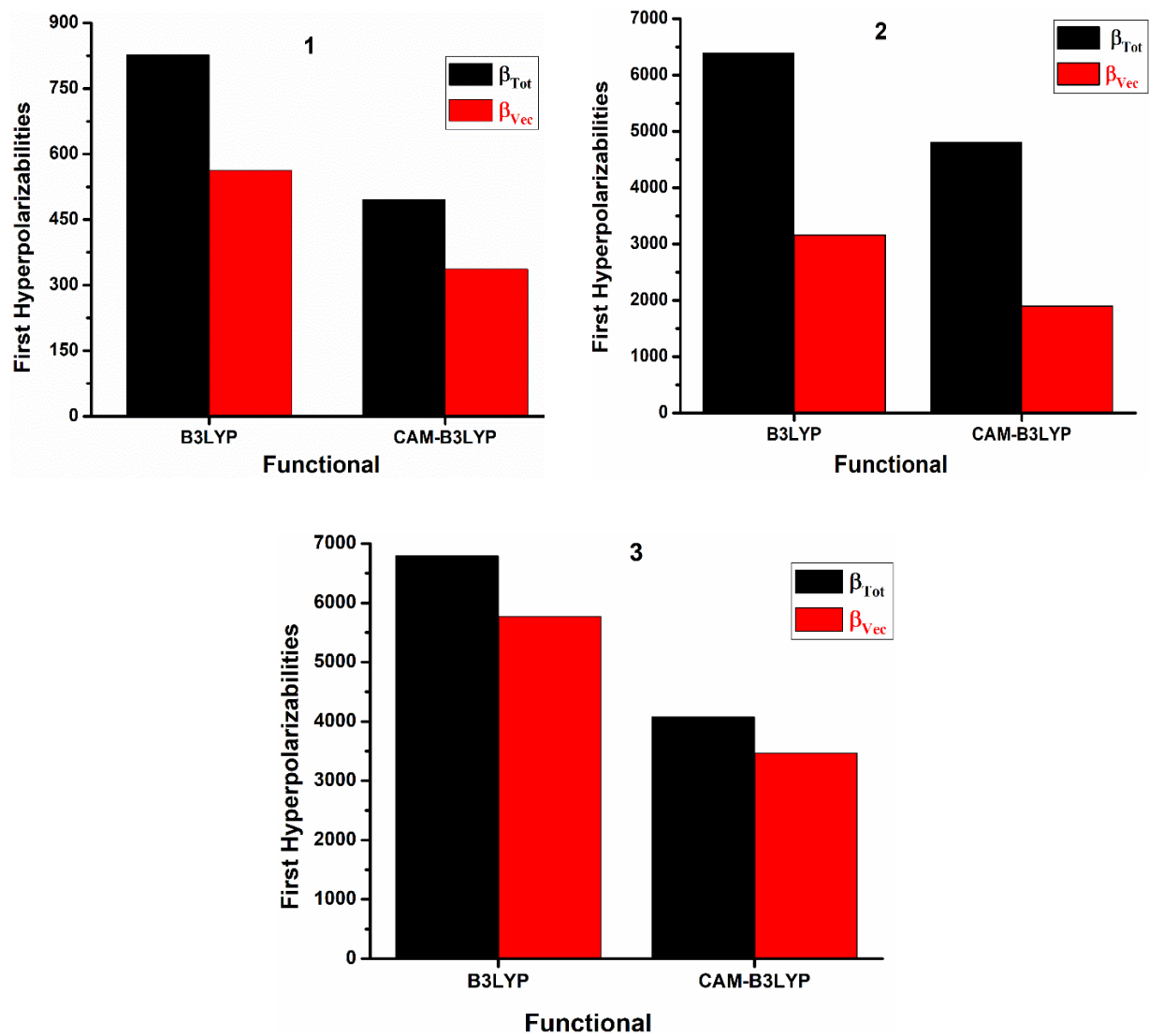


Fig. S1. The comparison of first hyperpolarizabilities (β_{tot} , and β_{vec} a. u.)^a for compounds **1-3** at B3LYP and CAM-B3LYP levels of theory.

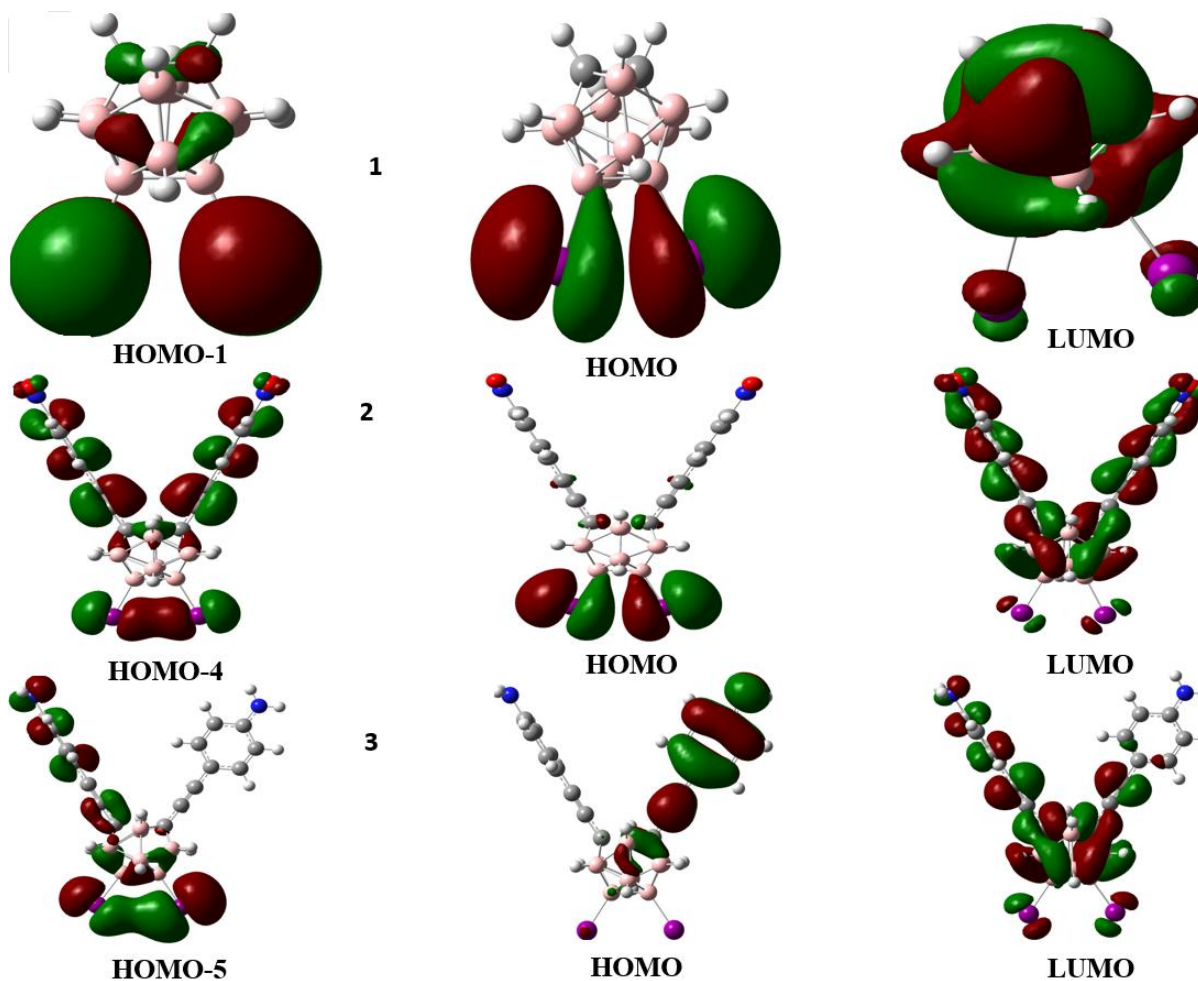


Fig. S2: Distribution patterns of the HOMOs and LUMOs of derivatives under study at the first excited states.