**Supporting Information**

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

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**Table S1**. The calculated values of first hyperpolarizabilities (βtot, and βvec a. u.)a for compounds **1-3** at B3LYP and CAM-B3LYP/Genb levels of theory

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

a Conversion factors for *β*tot from a.u. to SI and esu units: 1 a. u. = 3.26361x10-53C3m2J-2 =8.639418x10-33 esu

bGen = LANL2DZ for I atoms.

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

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

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

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

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**Fig. S1**. The comparison of first hyperpolarizabilities ( βtot, and βvec a. u.)a for compounds **1-3** at B3LYP and CAM-B3LYP levels of theory.

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

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