# Electronic Supporting Information

*for*

# Apical functionalization of the [*closo*-$B_{10}H_{10}$]$^{2-}$ anion: Building blocks for modern materials

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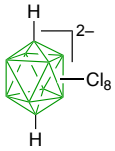
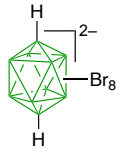
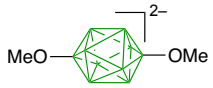
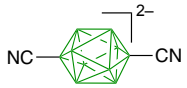
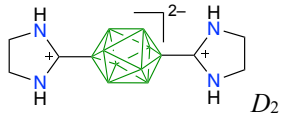
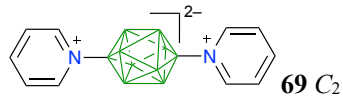
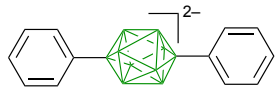
## 1. Computational Details

***General***. Quantum-mechanical calculations were carried out with the B3LYP[1, 2] method using Gaussian 16 package.[3]

***Geometry optimization and FMO energies***. Geometry optimizations of compounds in appropriate symmetry constraints were undertaken at the using the Def2TZVP basis sets[4, 5] with tight convergence limits in PhCl dielectric medium requested with SCRF(PCM, Solvent=C6H5Cl). The presence of a weak dielectric medium was demonstrated to be particularly effective for obtaining accurate molecular geometries.[6] The nature of the stationary points was verified with frequency calculations. The resulting energies of the HOMO and the LUMO are listed in Table S1.

**Table S1**. FMO energies for selected compounds obtained in PhCl dielectric medium.[a]

| compound | $E_{HOMO}$ /eV | $E_{LUMO}$ /eV |
|---|---|---|
|  $D_{6h}$ symmetry | -7.125 | -0.458 |
|  $C_5$ | -7.062 | 0.836 |
|  $C_{4v}$ | -6.262 | 0.761 |
|  $D_{5d}$ | -5.436 | 1.801 |
|  **A** $C_{4v}$ | -4.143 | 1.969 |
|  **A-Cl$_8$** $C_{4v}$ | -5.097 | 0.580 |

| | | |
|---|---|---|
|  **A-Br8** $C_{4v}$ | -5.216 | -0.115 |
|  $C_2$ | -3.432 | 2.010 |
|  **8** $C_{4v}$ | -4.911 | 1.092 |
|  $D_2$ | -6.096 | -0.956 |
|  **69** $C_2$ | -6.012 | -2.320 |
|  $C_2$ | -3.891 | 0.719 |

[a] Obtained with B3LYP/def2TZVP method in $CH_2Cl_2$ dielectric medium for model compounds. [b.] . [c] Ref.

***Electronic excitations.*** Electronic excitation energies in $CH_2Cl_2$ dielectric medium were obtained at the TD-B3LYP/def2TZVP ($CH_2Cl_2$)//B3LYP/def2TZVP (PhCl) level of theory using the time-dependent TD-DFT method[7] supplied in the Gaussian 16 package. Solvation models in calculations were implemented with the PCM model[8] using the SCRF(solvent=CH2Cl2) keyword. Partial outputs for dinitrogen **I**, **II**, dicarbonyl **7** and dinitrile **8** are provided below.

```
#P B3LYP/Def2TZVP TD(NStates=20) SCF=tight Geom(NoAngle, noDistance) #
 P SCRF(Solvent=CH2CL2)
I
Excited State   1:      Singlet-E      3.6344 eV  341.14 nm  f=0.0000
<S**2>=0.000
      42 -> 45        -0.49733
      43 -> 44         0.49733
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -472.498653328
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-E      3.6770 eV  337.19 nm  f=0.0000
<S**2>=0.000
      42 -> 45         0.49775
      43 -> 44         0.49775
```

```
 Excited State   3:      Singlet-E      3.6770 eV  337.19 nm  f=0.0000
<S**2>=0.000
      42 -> 44         0.49775
      43 -> 45        -0.49775

 Excited State   4:      Singlet-E      4.2177 eV  293.96 nm  f=0.0000
<S**2>=0.000
      40 -> 45        -0.49817
      41 -> 44         0.50065

 Excited State   5:      Singlet-E      4.2177 eV  293.96 nm  f=0.0000
<S**2>=0.000
      40 -> 44         0.49817
      41 -> 45         0.50065

 Excited State   6:      Singlet-E      4.2857 eV  289.29 nm  f=0.0120
<S**2>=0.000
      40 -> 45         0.49863
      41 -> 44         0.49615

 Excited State   7:      Singlet-E      4.2857 eV  289.29 nm  f=0.0120
<S**2>=0.000
      40 -> 44         0.49863
      41 -> 45        -0.49615

 Excited State   8:      Singlet-E      4.3970 eV  281.98 nm  f=0.0000
<S**2>=0.000
      38 -> 44        -0.22968
      39 -> 45         0.22968
      42 -> 47        -0.44261
      43 -> 46         0.44261

 Excited State   9:      Singlet-E      4.4552 eV  278.29 nm  f=0.0000
<S**2>=0.000
      38 -> 45        -0.25548
      39 -> 44         0.25548
      42 -> 46        -0.42831
      43 -> 47         0.42831

 Excited State  10:      Singlet-E      4.4552 eV  278.29 nm  f=0.0000
<S**2>=0.000
      38 -> 44        -0.25548
      39 -> 45        -0.25548
      42 -> 47         0.42831
      43 -> 46         0.42831

 Excited State  11:      Singlet-E      4.8066 eV  257.95 nm  f=0.0000
<S**2>=0.000
      38 -> 44         0.44258
      39 -> 45        -0.44258
      42 -> 47        -0.22955
      43 -> 46         0.22955
```

```
 Excited State  12:      Singlet-E      4.8410 eV  256.11 nm  f=0.0000
<S**2>=0.000
      38 -> 45        -0.42834
      39 -> 44         0.42834
      42 -> 46         0.25544
      43 -> 47        -0.25544

 Excited State  13:      Singlet-E      4.8411 eV  256.11 nm  f=0.0000
<S**2>=0.000
      38 -> 44         0.42834
      39 -> 45         0.42834
      42 -> 47         0.25544
      43 -> 46         0.25544

 Excited State  14:      Singlet-E      4.8639 eV  254.91 nm  f=1.2468
<S**2>=0.000
      42 -> 44         0.48884
      43 -> 45         0.48884

 Excited State  15:      Singlet-E      4.8675 eV  254.72 nm  f=0.0070
<S**2>=0.000
      38 -> 45         0.45028
      39 -> 44         0.45028
      42 -> 46         0.21148
      43 -> 47         0.21148
```

**II**

```
Excited State   1:      Singlet-E      3.3415 eV  371.04 nm  f=0.0000
<S**2>=0.000
      36 -> 38        -0.49461
      37 -> 39         0.49461
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -363.704315254
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-E      3.4143 eV  363.14 nm  f=0.0000
<S**2>=0.000
      36 -> 38         0.49464
      37 -> 39         0.49464

 Excited State   3:      Singlet-E      3.4225 eV  362.26 nm  f=0.0000
<S**2>=0.000
      36 -> 39        -0.49580
      37 -> 38         0.49580

 Excited State   4:      Singlet-E      4.2208 eV  293.75 nm  f=0.0007
<S**2>=0.000
      34 -> 39         0.11615
      35 -> 38         0.69669
```

```
 Excited State   5:      Singlet-E      4.2208 eV  293.75 nm  f=0.0007
<S**2>=0.000
      34 -> 38        -0.11615
      35 -> 39         0.69669

 Excited State   6:      Singlet-E      4.3528 eV  284.84 nm  f=0.0063
<S**2>=0.000
      34 -> 38         0.69579
      35 -> 39         0.11524

 Excited State   7:      Singlet-E      4.3528 eV  284.84 nm  f=0.0063
<S**2>=0.000
      34 -> 39         0.69579
      35 -> 38        -0.11524

 Excited State   8:      Singlet-E      4.4065 eV  281.36 nm  f=0.3294
<S**2>=0.000
      32 -> 39         0.24980
      33 -> 38        -0.24980
      36 -> 39         0.43220
      37 -> 38         0.43220

 Excited State   9:      Singlet-E      4.7228 eV  262.52 nm  f=0.0000
<S**2>=0.000
      32 -> 38         0.49208
      33 -> 39         0.49208

 Excited State  10:      Singlet-E      4.7316 eV  262.03 nm  f=0.0000
<S**2>=0.000
      32 -> 39         0.49269
      33 -> 38         0.49269

 Excited State  11:      Singlet-E      4.7731 eV  259.76 nm  f=0.0000
<S**2>=0.000
      32 -> 38        -0.49329
      33 -> 39         0.49329

 Excited State  12:      Singlet-E      5.4389 eV  227.96 nm  f=0.7517
<S**2>=0.000
      32 -> 39        -0.42425
      33 -> 38         0.42425
      36 -> 39         0.24975
      37 -> 38         0.24975

7
Excited State   1:      Singlet-E      3.8226 eV  324.34 nm  f=0.0000
<S**2>=0.000
      42 -> 45        -0.49791
      43 -> 44         0.49791
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -480.144477690
 Copying the excited state density for this state as the 1-particle RhoCI
density.
```

```
 Excited State   2:      Singlet-E      3.8679 eV  320.55 nm  f=0.0000
<S**2>=0.000
      42 -> 44        -0.49817
      43 -> 45         0.49817

 Excited State   3:      Singlet-E      3.8679 eV  320.55 nm  f=0.0000
<S**2>=0.000
      42 -> 45         0.49817
      43 -> 44         0.49817

 Excited State   4:      Singlet-E      4.2367 eV  292.65 nm  f=0.0000
<S**2>=0.000
      40 -> 44        -0.49921
      41 -> 45         0.49954

 Excited State   5:      Singlet-E      4.2367 eV  292.65 nm  f=0.0000
<S**2>=0.000
      40 -> 45         0.49921
      41 -> 44         0.49954

 Excited State   6:      Singlet-E      4.3324 eV  286.18 nm  f=0.0141
<S**2>=0.000
      40 -> 44         0.49730
      41 -> 45         0.49697

 Excited State   7:      Singlet-E      4.3324 eV  286.18 nm  f=0.0141
<S**2>=0.000
      40 -> 45         0.49730
      41 -> 44        -0.49697

 Excited State   8:      Singlet-E      4.6744 eV  265.24 nm  f=0.0000
<S**2>=0.000
      38 -> 45         0.45898
      39 -> 44         0.45898
      42 -> 46        -0.19553
      43 -> 47        -0.19553
Excited State   9:      Singlet-E      4.7024 eV  263.66 nm  f=0.0000
<S**2>=0.000
      38 -> 44         0.46311
      39 -> 45         0.46311
      42 -> 47         0.18572
      43 -> 46         0.18572

 Excited State  10:      Singlet-E      4.7024 eV  263.66 nm  f=0.0000
<S**2>=0.000
      38 -> 45        -0.46311
      39 -> 44         0.46311
      42 -> 46         0.18571
      43 -> 47        -0.18571

 Excited State  11:      Singlet-E      4.9812 eV  248.90 nm  f=0.0000
<S**2>=0.000
```

```
      38 -> 44        -0.47836
      39 -> 45         0.47836
      42 -> 47         0.13981
      43 -> 46        -0.13981

 Excited State  12:      Singlet-E      5.1427 eV  241.09 nm  f=0.0000
<S**2>=0.000
      38 -> 45         0.19542
      39 -> 44         0.19542
      42 -> 46         0.45832
      43 -> 47         0.45832

 Excited State  13:      Singlet-E      5.1981 eV  238.52 nm  f=1.2712
<S**2>=0.000
      42 -> 44         0.48507
      43 -> 45         0.48507

 Excited State  14:      Singlet-E      5.2164 eV  237.68 nm  f=0.0000
<S**2>=0.000
      38 -> 45        -0.18577
      39 -> 44         0.18577
      42 -> 46        -0.46184
      43 -> 47         0.46184
```

**8**

```
Excited State   1:      Singlet-E      4.9175 eV  252.13 nm  f=0.0000
<S**2>=0.000
      42 -> 44         0.49815
      43 -> 45        -0.49815
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -439.452521048
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-E      4.9664 eV  249.65 nm  f=0.0000
<S**2>=0.000
      42 -> 45         0.49825
      43 -> 44        -0.49825

 Excited State   3:      Singlet-E      4.9664 eV  249.65 nm  f=0.0000
<S**2>=0.000
      42 -> 44         0.49825
      43 -> 45         0.49825

 Excited State   4:      Singlet-E      5.8918 eV  210.44 nm  f=1.3248
<S**2>=0.000
      42 -> 45         0.49024
      43 -> 44         0.49024

 Excited State   5:      Singlet-E      5.9716 eV  207.62 nm  f=0.0172
<S**2>=0.000
      42 -> 46         0.69226
```

```
 Excited State   6:      Singlet-E      5.9716 eV  207.62 nm  f=0.0172
<S**2>=0.000
      43 -> 46         0.69226

 Excited State   7:      Singlet-E      5.9889 eV  207.02 nm  f=0.0000
<S**2>=0.000
      40 -> 45        -0.49620
      41 -> 44         0.49869

 Excited State   8:      Singlet-E      5.9889 eV  207.02 nm  f=0.0000
<S**2>=0.000
      40 -> 44         0.49620
      41 -> 45         0.49869
```

## 2. Archive for DFT

```
B3LYP/Def2TZVP FOpt geom(noangle, nodistance) fcheck
#P freq(noraman, readIso) SCRF(Solvent=C6H5Cl)
```

```
1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H6\PIOTR\14-Feb-2021\0\\#P B
 3LYP/Def2TZVP FOpt geom(noangle, nodistance) fcheck #P freq(noraman, r
 eadIso) SCRF(Solvent=C6H5Cl)\\Benzene D6h in PhCl\\0,1\C,0.0000000899,
 1.391875,0.\C,1.2053991538,0.6959374222,0.\C,1.2053990639,-0.695937577
 8,0.\C,-0.0000000899,-1.391875,0.\C,-1.2053991538,-0.6959374222,0.\C,-
 1.2053990639,0.6959375778,0.\H,0.0000001598,2.474843,0.\H,2.1432769883
 ,1.2374213616,0.\H,2.1432768285,-1.2374216384,0.\H,-0.0000001598,-2.47
 4843,0.\H,-2.1432769883,-1.2374213616,0.\H,-2.1432768285,1.2374216384,
 0.\\Version=ES64L-G09RevD.01\State=1-A1G\HF=-232.3393054\RMSD=2.500e-0
 9\RMSF=9.747e-06\Dipole=0.,0.,0.\Quadrupole=2.0716327,2.0716327,-4.143
 2654,0.,0.,0.\PG=D06H [3C2'(H1C1.C1H1)]\\@
```

```
1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H12B11(1-)\PIOTR\27-Sep-2021
 \0\\#P B3LYP/Def2TZVP FOpt geom(noangle, nodistance) fcheck #P SCRF(So
 lvent=C6H5Cl)\\1-CB11H12 anion, C5v\\-1,1\B,-0.77054365,-1.30639172,0.
 76801534\B,1.0043412753,-1.1365278023,0.76801534\B,-1.4805634408,0.329
 1333165,0.76801534\B,1.3912606944,0.6039789088,0.76801534\B,-0.1444948
 789,1.5098072963,0.76801534\B,0.76693875,1.29977928,-0.73382942\B,1.47
 31606615,-0.3277482094,-0.73382942\B,-0.9991664467,1.1310559821,-0.733
 82942\B,0.1435246097,-1.5023388134,-0.73382942\B,-1.3844575745,-0.6007
 4824,-0.73382942\C,0.,-0.0000000001,-1.52058891\B,0.,-0.0000000001,1.7
 0054504\H,0.,-0.0000000001,2.89121839\H,0.,-0.0000000001,-2.59993438\H
 ,-1.31757552,-2.23303228,1.27628122\H,1.7165866738,-1.9431337076,1.276
 28122\H,-2.5308931279,0.5630438604,1.27628122\H,2.378484429,1.03210960
 38,1.27628122\H,-0.2466024549,2.5810125227,1.27628122\H,1.27173168,2.1
 5532841,-1.38238989\H,2.4428258306,-0.5434555942,-1.38238989\H,-1.6568
 524278,1.8755218083,-1.38238989\H,0.2380177119,-2.4912024388,-1.382389
 89\H,-2.2957227947,-0.996192186,-1.38238989\\Version=ES64L-G09RevD.01\
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 61,0.0000162,-1.4031538\Quadrupole=-1.6260872,-1.6263118,3.252399,-0.0
 000559,0.0031112,-0.0006908\PG=C05 [C5(H1B1C1H1),X(H10B10)]\\@
```

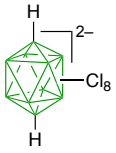
1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C1H10B9(1-)\PIOTR\10-Apr-2024\
0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P S
CRF(Solvent=C6H5Cl)\\1-CB9 anion, C4v\\-1,1\B,-1.3006576463,0.,-0.7365
95208\B,0.,-1.3006576463,-0.736595208\B,1.3006576463,0.,-0.736595208\B
,0.,1.3006576463,-0.736595208\B,-0.9187847767,-0.9187847767,0.76725623
55\B,0.9187847767,-0.9187847767,0.7672562355\B,0.9187847767,0.91878477
67,0.7672562355\B,-0.9187847767,0.9187847767,0.7672562355\B,0.,0.,1.85
81218311\C,0.,0.,-1.6681911273\H,-2.3774952998,0.,-1.2382968984\H,0.,-
2.3774952998,-1.2382968984\H,2.3774952998,0.,-1.2382968984\H,0.,2.3774
952998,-1.2382968984\H,-1.713169667,-1.713169667,1.1680155149\H,1.7131
69667,-1.713169667,1.1680155149\H,1.713169667,1.713169667,1.1680155149
\H,-1.713169667,1.713169667,1.1680155149\H,0.,0.,3.0462421471\H,0.,0.,
-2.7449274278\\Version=ES64L-G16RevC.01\State=1-A1\HF=-268.1441185\RMS
D=4.273e-09\RMSF=2.489e-06\Dipole=0.,0.,-1.4822589\Quadrupole=-0.51169
47,-0.5116947,1.0233894,0.,0.,0.\PG=C04V [C4(H1B1C1H1),2SGV(H2B2),2SGD
(H2B2)]\\@

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\B12H12(2-)\PIOTR\14-Feb-2021\0
\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SC
RF(Solvent=C6H5Cl)\\B12H12 dianion, D5d geom\\-2,1\B,0.,1.5119072135,0
.7562789558\B,-1.439763263,0.4674496268,0.7569794506\B,1.4397632626,0.
4674496282,0.7569794508\B,-0.8893934227,-1.2243089999,0.7572523537\B,0
.8893934238,-1.2243089983,0.7572523532\B,0.,-1.5119072135,-0.756278955
8\B,-1.4397632626,-0.4674496282,-0.7569794508\B,1.439763263,-0.4674496
268,-0.7569794506\B,-0.8893934238,1.2243089983,-0.7572523532\B,0.88939
34227,1.2243089999,-0.7572523537\B,0.,-0.0001337681,-1.6922347355\B,0.
,0.0001337681,1.6922347355\H,0.,2.5839353441,1.2929071827\H,-2.4587351
74,0.8008966951,1.2933086308\H,2.4587351734,0.800896697,1.293308631\H,
-1.5191540852,-2.0925902472,1.2924351868\H,1.5191540872,-2.0925902417,
1.2924351918\H,0.,-2.5839353441,-1.2929071827\H,-2.4587351734,-0.80089
6697,-1.293308631\H,2.458735174,-0.8008966951,-1.2933086308\H,-1.51915
40872,2.0925902417,-1.2924351918\H,1.5191540852,2.0925902472,-1.292435
1868\H,0.,-0.000458147,-2.8904932868\H,0.,0.000458147,2.8904932868\\Ve
rsion=ES64L-G09RevD.01\State=1-AG\HF=-306.0136123\RMSD=4.832e-09\RMSF=
1.195e-05\Dipole=0.,0.,0.\Quadrupole=-0.0005894,-0.0108378,0.0114272,0
.,0.,-0.0139893\PG=CI [X(B12H12)]\\@

**A**

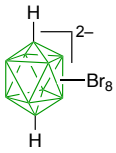
1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\B10H10(2-)\PIOTR\06-Oct-2020\0
\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SC
RF(Solvent=C6H5Cl)\\B10H10, D4d sym\\-2,1\B,-0.0000000005,1.2957092086
,-0.7581709109\B,0.0000000004,-1.2957092087,-0.7581709109\B,-1.2957092
087,-0.0000000005,-0.7581709109\B,1.2957092086,0.0000000004,-0.7581709
109\B,0.9159543786,0.9159543793,0.7583973801\B,-0.9159543794,0.9159543
786,0.7583973801\B,-0.9159543787,-0.9159543793,0.7583973801\B,0.915954
3792,-0.9159543787,0.7583973801\B,-0.0000000001,0.,1.852483092\B,-0.00

00000001,0.,-1.853192525\H,-0.0000000009,2.4276753168,-1.1606966772\H,
0.0000000008,-2.4276753169,-1.1606966772\H,-2.4276753169,-0.0000000009
,-1.1606966772\H,2.4276753168,0.0000000008,-1.1606966772\H,1.716524196
5,1.7165241978,1.1608053637\H,-1.7165241979,1.7165241966,1.1608053637\
H,-1.7165241967,-1.7165241978,1.1608053637\H,1.7165241977,-1.716524196
6,1.1608053637\H,-0.0000000001,0.,-3.0496046444\H,-0.0000000001,0.,3.0
489734512\\Version=ES64L-G09RevD.01\State=1-A1\HF=-254.9669623\RMSD=6.
060e-09\RMSF=1.276e-06\Dipole=0.,0.,0.0049907\Quadrupole=2.1625257,2.1
625257,-4.3250514,0.,0.,0.\PG=C04V [C4(H1B1B1H1),2SGV(B2H2),2SGD(B2H2)
]\\@



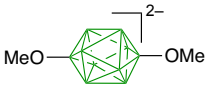

**A-Cl$_8$**

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\B10Cl8H2(2-)\PK\20-Aug-2025\0\
\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCR
F(Solvent=C6H5Cl)\\B10Cl8H2 anion, D4d sym\\-2,1\B,0.,1.2956923664,0.7
690564594\B,0.,-1.2956923664,0.7690564594\B,1.2956923664,0.,0.76905645
94\B,-1.2956923664,0.,0.7690564594\B,-0.9171603351,0.9171603351,-0.772
9621566\B,0.9171603351,0.9171603351,-0.7729621566\B,0.9171603351,-0.91
71603351,-0.7729621566\B,-0.9171603351,-0.9171603351,-0.7729621566\B,0
.,0.,-1.8469305435\B,0.,0.,1.8416876926\H,0.,0.,3.025209537\H,0.,0.,-3
.0305158616\Cl,-2.131564623,2.131564623,-1.3937612603\Cl,-3.0077029139
,0.,1.4005282362\Cl,-2.131564623,-2.131564623,-1.3937612603\Cl,0.,-3.0
077029139,1.4005282362\Cl,2.131564623,-2.131564623,-1.3937612603\Cl,3.
0077029139,0.,1.4005282362\Cl,2.131564623,2.131564623,-1.3937612603\Cl
,0.,3.0077029139,1.4005282362\\Version=ES64L-G16RevB.01\HF=-3932.36731
42\RMSD=4.097e-09\RMSF=5.230e-06\Dipole=0.,0.,-0.0082496\Quadrupole=-3
.6417254,-3.6417254,7.2834509,0.,0.,0.\PG=C04V [C4(H1B1B1H1),2SGV(B2Cl
2),2SGD(B2Cl2)]\\@

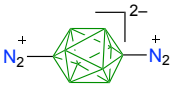



**A-Br$_8$**

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\B10Br8H2(2-)\PK\22-Aug-2025\0\
\#P B3LYP/Def2TZVP FOpt geom(noangle, nodistance) fcheck #P SCRF(Solve
nt=C6H5Cl) guess=check\\B10Br8H2 anion, D4d sym\\-2,1\B,0.,1.296707403
8,0.7741631227\B,0.,-1.2967074038,0.7741631227\B,1.2967074038,0.,0.774
1631227\B,-1.2967074038,0.,0.7741631227\B,-0.9175957203,0.9175957203,-
0.7619637797\B,0.9175957203,0.9175957203,-0.7619637797\B,0.9175957203,
-0.9175957203,-0.7619637797\B,-0.9175957203,-0.9175957203,-0.761963779
7\B,0.,0.,-1.8373743608\B,0.,0.,1.8493011656\H,0.,0.,3.0310440117\H,0.
,0.,-3.0191383403\Br,-2.2261135978,2.2261135978,-1.4943951098\Br,-3.14
79565245,0.,1.5065528795\Br,-2.2261135978,-2.2261135978,-1.4943951098\
Br,0.,-3.1479565245,1.5065528795\Br,2.2261135978,-2.2261135978,-1.4943
951098\Br,3.1479565245,0.,1.5065528795\Br,2.2261135978,2.2261135978,-1
.4943951098\Br,0.,3.1479565245,1.5065528795\\Version=ES64L-G16RevB.01\
HF=-20843.9828724\RMSD=6.047e-09\RMSF=3.413e-04\Dipole=0.,0.,-0.002348
\Quadrupole=-3.9468047,-3.9468047,7.8936095,0.,0.,0.\PG=C04V [C4(H1B1B
1H1),2SGV(B2Br2),2SGD(B2Br2)]\\@

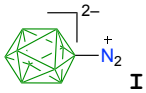



1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C2H14B10O2(2-)\PIOTR\06-Oct-20
20\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #
P SCRF(Solvent=C6H5Cl) guess=check\\MeO-B10-PhOMe C2 from Def2TZVP in
vacc\\-2,1\B,-0.9350313409,1.0671592168,-0.3609195349\B,-0.5700574229,
-1.2944985119,0.6369309023\B,-0.6632263246,-0.6008946666,-1.0681104557
\B,-0.814608059,0.3771280421,1.340460428\B,0.5700574229,1.2944985119,0
.6369309023\B,0.6632263246,0.6008946666,-1.0681104557\B,0.9350313409,-
1.0671592168,-0.3609195349\B,0.814608059,-0.3771280421,1.340460428\B,1
.8306517945,0.2837394753,0.1376193469\B,-1.8306517945,-0.2837394753,0.
1376193469\H,-1.4899997075,2.0403377494,-0.792726752\H,-0.8299703627,-
2.3870704538,1.0629411018\H,-1.0254505377,-1.0948688713,-2.1017821626\
H,-1.3083664023,0.7368702927,2.3746672301\H,0.8299703627,2.3870704538,
1.0629411018\H,1.0254505377,1.0948688713,-2.1017821626\H,1.4899997075,
-2.0403377494,-0.792726752\H,1.3083664023,-0.7368702927,2.3746672301\O
,-3.2444926452,-0.5637156447,0.1671486467\C,-4.1124970963,0.3534287903
,-0.4409858772\H,-5.138311985,-0.0186577559,-0.3483767561\H,-4.0621491
511,1.3445863589,0.0308940489\H,-3.8923122109,0.4877473702,-1.50978491
5\O,3.2444926452,0.5637156447,0.1671486467\C,4.1124970963,-0.353428790
3,-0.4409858772\H,3.8923122109,-0.4877473702,-1.509784915\H,5.13831198
5,0.0186577559,-0.3483767561\H,4.0621491511,-1.3445863589,0.0308940489
\\Version=ES64L-G09RevD.01\State=1-A\HF=-484.1768014\RMSD=1.918e-09\RM
SF=2.868e-06\Dipole=0.,0.,-0.8317182\Quadrupole=-6.2542912,2.5683863,3
.6859049,-6.3698246,0.,0.\PG=C02 [X(C2H14B10O2)]\\@




**I**

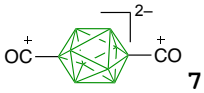
1\1\GINC-LOCALHOST\SP\RB3LYP TD-FC\def2TZVP\B10H8N4\PK\09-Sep-2025\0\\
#P B3LYP/Def2TZVP TD(NStates=20) SCF=tight Geom(NoAngle, noDistance) #
P SCRF(Solvent=CH2CL2)\\B10H8,10-(N2)2, D4d\\0,1\B,0,0.0000000001,1.32
87739086,0.7409533346\B,0,0.0000000001,-1.3287739087,0.7409533346\B,0,
1.3287739088,0.,0.7409533346\B,0,-1.3287739085,0.,0.7409533346\B,0,-0.
9395578436,0.9395578437,-0.7409730696\B,0,0.9395578439,0.9395578437,-0
.7409730696\B,0,0.9395578439,-0.9395578438,-0.7409730696\B,0,-0.939557
8436,-0.9395578438,-0.7409730696\B,0,0.0000000001,0.,-1.7661712733\B,0
,0.0000000001,0.,1.7661898943\H,0,0.0000000001,2.4266166505,1.18936049
8\H,0,0.0000000001,-2.4266166505,1.189360498\H,0,2.4266166506,0.,1.189
360498\H,0,-2.4266166504,0.,1.189360498\H,0,-1.7158453579,1.715845358,
-1.1893687949\H,0,1.7158453582,1.715845358,-1.1893687949\H,0,1.7158453
582,-1.7158453581,-1.1893687949\H,0,-1.7158453579,-1.7158453581,-1.189
3687949\N,0,0.0000000001,0.,3.2273415861\N,0,0.0000000001,0.,4.3263289
626\N,0,0.0000000001,0.,-3.2273016874\N,0,0.0000000001,0.,-4.326275328
6\\Version=ES64L-G16RevB.01\State=1-A1\HF=-472.6322156\RMSD=2.854e-09\
PG=C04V [C4(N1N1B1B1N1N1),2SGV(B2H2),2SGD(B2H2)]\\@




**II**

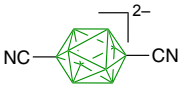
1\1\GINC-LOCALHOST\SP\RB3LYP TD-FC\def2TZVP\B10H9N2(1-)\PK\09-Sep-2025
\0\\#P B3LYP/Def2TZVP TD(NStates=20) SCF=tight Geom(NoAngle, noDistanc
e) #P SCRF(Solvent=CH2CL2)\\H-B10H8-10-N2, D4d\\-1,1\B,0,0.,1.30325034
8,0.7578077565\B,0,0.,-1.303250348,0.7578077565\B,0,1.303250348,0.,0.7
578077565\B,0,-1.303250348,0.,0.7578077565\B,0,-0.9344306959,0.9344306

959,-0.7345201049\B,0,0.9344306959,0.9344306959,-0.7345201049\B,0,0.93
44306959,-0.9344306959,-0.7345201049\B,0,-0.9344306959,-0.9344306959,-
0.7345201049\B,0,0.,0.,-1.7792050853\B,0,0.,0.,1.8479398357\H,0,0.,2.4
229499751,1.1706562573\H,0,0.,-2.4229499751,1.1706562573\H,0,2.4229499
751,0.,1.1706562573\H,0,-2.4229499751,0.,1.1706562573\H,0,-1.715221557
6,1.7152215576,-1.1805692249\H,0,1.7152215576,1.7152215576,-1.18056922
49\H,0,1.7152215576,-1.7152215576,-1.1805692249\H,0,-1.7152215576,-1.7
152215576,-1.1805692249\H,0,0.,0.,3.0360146733\N,0,0.,0.,-3.2182002661
\N,0,0.,0.,-4.3247905887\\Version=ES64L-G16RevB.01\State=1-A1\HF=-363.
8271147\RMSD=6.085e-09\PG=C04V [C4(H1B1B1N1N1),2SGV(B2H2),2SGD(B2H2)]\
\@



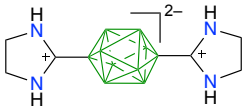

**7**

1\1\GINC-LOCALHOST\SP\RB3LYP TD-FC\def2TZVP\C2H8B10O2\PK\09-Sep-2025\0
\\#P B3LYP/Def2TZVP TD(NStates=20) SCF=tight Geom(NoAngle, noDistance)
#P SCRF(Solvent=CH2CL2) guess=check\\B10H8,10-(CO)2, D4d\\0,1\B,0,0.9
393721266,0.9393721266,0.7405719906\B,0,-0.9393721266,-0.9393721266,0.
7405719906\B,0,0.9393721266,-0.9393721266,0.7405719906\B,0,-0.93937212
66,0.9393721266,0.7405719906\B,0,0.,1.3284827653,-0.7405591798\B,0,1.3
284827653,0.,-0.7405591798\B,0,0.,-1.3284827653,-0.7405591798\B,0,-1.3
284827653,0.,-0.7405591798\B,0,0.,0.,-1.7808991332\B,0,0.,0.,1.7808711
175\H,0,1.7179271133,1.7179271133,1.1786753093\H,0,-1.7179271133,-1.71
79271133,1.1786753093\H,0,1.7179271133,-1.7179271133,1.1786753093\H,0,
-1.7179271133,1.7179271133,1.1786753093\H,0,0.,2.4295109533,-1.1786971
226\H,0,2.4295109533,0.,-1.1786971226\H,0,0.,-2.4295109533,-1.17869712
26\H,0,-2.4295109533,0.,-1.1786971226\C,0,0.,0.,3.2632073546\O,0,0.,0.
,4.390780306\C,0,0.,0.,-3.263216889\O,0,0.,0.,-4.3907917744\\Version=E
S64L-G16RevB.01\State=1-A1\HF=-480.2849561\RMSD=1.516e-09\PG=C04V [C4(
O1C1B1B1C1O1),2SGV(H2B2),2SGD(H2B2)]\\@

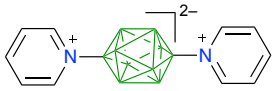



**8**

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C2H8B10N2(2-)\PIOTR\30-Nov-202
0\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl) guess=check freq(noraman, readIso)\\B10H01,10-(C
N)2, D4d\\-2,1\B,-0.0000438252,1.3051963072,0.7508880076\B,0.000043824
4,-1.3051963068,0.7508880076\B,1.3051963066,0.000043825,0.7508880076\B
,-1.3051963074,-0.0000438246,0.7508880076\B,-0.9226089021,0.9225812293
,-0.7508037712\B,0.9225812287,0.9226089019,-0.7508037712\B,0.922608901
3,-0.9225812289,-0.7508037712\B,-0.9225812295,-0.9226089015,-0.7508037
712\B,-0.0000000004,0.0000000002,-1.8282020846\B,-0.0000000004,0.00000
00002,1.8276166664\H,0.0000107758,2.4236390263,1.1715472522\H,-0.00001
07766,-2.4236390259,1.1715472522\H,2.4236390257,-0.000010776,1.1715472
522\H,-2.4236390265,0.0000107764,1.1715472522\H,-1.7136397659,1.713672
2452,-1.1711313593\H,1.7136722446,1.7136397657,-1.1711313593\H,1.71363
97651,-1.7136722448,-1.1711313593\H,-1.7136722454,-1.7136397653,-1.171
1313593\C,-0.0000000004,0.0000000002,3.3599257401\N,-0.0000000004,0.00
00000002,4.5183536076\C,-0.0000000004,0.0000000002,-3.3606401374\N,-0.
0000000004,0.0000000002,-4.5190543159\\Version=ES64L-G09RevD.01\State=
1-A\HF=-439.6175758\RMSD=5.357e-09\RMSF=4.188e-06\Dipole=0.,0.,-0.0057
249\Quadrupole=21.4948807,21.4948807,-42.9897613,0.,0.,0.\PG=C04 [C4(N
1C1B1B1C1N1),X(H8B8)]\\@



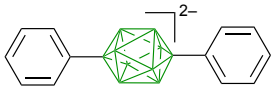
1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H20B10N4\PIOTR\16-Jun-2024\0
\\#P B3LYP/Def2TZVP FOpt geom(noangle, nodistance) fcheck #P SCRF(Solv
ent=C6H5Cl)\\B10H8-1,10-diImidazoleH2 symm\\0,1\B,-0.5048917573,1.2057
168343,-0.7516307947\B,0.5048917573,-1.2057168343,-0.7516307947\B,-1.2
099353923,-0.4957377841,-0.7477387749\B,1.2099353923,0.4957377841,-0.7
477387749\B,0.5048917573,1.2057168343,0.7516307947\B,-1.2099353923,0.4
957377841,0.7477387749\B,-0.5048917573,-1.2057168343,0.7516307947\B,1.
2099353923,-0.4957377841,0.7477387749\B,0.,0.,1.814963718\B,0.,0.,-1.8
14963718\H,-0.9302095968,2.2377491449,-1.1741720523\H,0.9302095968,-2.
2377491449,-1.1741720523\H,-2.2407004034,-0.9257717424,-1.1753277107\H
,2.2407004034,0.9257717424,-1.1753277107\H,0.9302095968,2.2377491449,1
.1741720523\H,-2.2407004034,0.9257717424,1.1753277107\H,-0.9302095968,
-2.2377491449,1.1741720523\H,2.2407004034,-0.9257717424,1.1753277107\C
,0.,0.,3.3690705284\C,0.,0.,-3.3690705284\N,-1.0238514156,-0.349235684
7,-4.1418035816\N,1.0238514156,0.3492356847,-4.1418035816\N,-1.0238514
156,0.3492356847,4.1418035816\N,1.0238514156,-0.3492356847,4.141803581
6\H,1.8625303319,-0.7508895957,3.7578350223\H,-1.8625303319,0.75088959
57,3.7578350223\H,1.8625303319,0.7508895957,-3.7578350223\H,-1.8625303
319,-0.7508895957,-3.7578350223\C,-0.6848755747,-0.3577018749,-5.56889
92794\H,-1.4326835642,0.1718154869,-6.1557425767\H,-0.6113725755,-1.38
30227743,-5.9360056999\C,0.6848755747,0.3577018749,-5.5688992794\H,0.6
113725755,1.3830227743,-5.9360056999\H,1.4326835642,-0.1718154869,-6.1
557425767\C,0.6848755747,-0.3577018749,5.5688992794\H,1.4326835642,0.1
718154869,6.1557425767\H,0.6113725755,-1.3830227743,5.9360056999\C,-0.
6848755747,0.3577018749,5.5688992794\H,-0.6113725755,1.3830227743,5.93
60056999\H,-1.4326835642,-0.1718154869,6.1557425767\\Version=ES64L-G16
RevC.01\State=1-A\HF=-708.6369982\RMSD=4.170e-09\RMSF=4.152e-06\Dipole
=0.,0.,0.\Quadrupole=-27.5079873,-36.9673864,64.4753737,0.,0.,0.\PG=D0
2 [C2(C1B1.B1C1),X(C4H20B8N4)]\\@



**69**

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C10H18B10N2\PIOTR\10-Jun-2020\
0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P S
CRF(Solvent=C6H5Cl)\\1-Pyridine-B10-1-Pyridine, C2 staggered\\0,1\B,0.
,0.,1.800181\B,1.211733,0.497672,-0.749867\B,0.50421,-1.208205,-0.7475
6\B,-1.211733,-0.497672,-0.749867\B,-0.50421,1.208205,-0.74756\B,0.504
374,1.208136,0.74756\B,1.211666,-0.497836,0.749866\B,-0.504374,-1.2081
36,0.74756\B,-1.211666,0.497836,0.749866\B,0.,0.,-1.80018\N,0.,0.,3.32
8038\C,1.122476,0.412099,5.389164\C,-1.122476,-0.412099,5.389164\C,1.0
92883,0.401217,4.009746\C,-1.092883,-0.401217,4.009746\C,0.,0.,6.09629
5\H,2.235313,0.925638,-1.190774\H,0.925812,-2.235906,-1.184386\H,-2.23
5313,-0.925638,-1.190774\H,-0.925812,2.235906,-1.184386\H,2.018661,0.7
41063,5.894909\H,-2.018661,-0.741063,5.894909\H,0.926117,2.23578,1.184
384\H,2.235187,-0.925942,1.190773\H,-0.926117,-2.23578,1.184384\H,-2.2
35187,0.925942,1.190773\H,1.933782,0.708773,3.407764\H,-1.933782,-0.70
8773,3.407764\H,0.,0.,7.177814\N,0.,0.,-3.328037\C,-1.092883,0.401217,
-4.009746\C,1.092883,-0.401217,-4.009746\C,-1.122476,0.412098,-5.38916
4\C,1.122476,-0.412098,-5.389164\C,0.,0.,-6.096295\H,-1.933783,0.70877
,-3.407763\H,1.933783,-0.70877,-3.407763\H,-2.018662,0.741061,-5.89490
9\H,2.018662,-0.741061,-5.894909\H,0.,0.,-7.177814\\Version=ES64L-G09R
evD.01\State=1-A\HF=-750.360128\RMSD=8.858e-09\RMSF=2.099e-07\Dipole=0

.,0.,0.0000051\Quadrupole=-25.7824445,-39.1612049,64.9436494,0.0000234
,0.,0.\PG=C02 [C2(H1C1N1B1B1N1C1H1),X(C8H16B8)]\\@




1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C12H18B10(2-)\PIOTR\29-Nov-202
0\0\\#P B3LYP/Def2TZVP FOpt=tight geom(noangle, nodistance) fcheck #P
SCRF(Solvent=C6H5Cl) freq(noraman, readIso)\\1-Ph-B10-10-PPh, staggere
d in PhCl\\-2,1\B,0.,0.,1.8348274386\B,-0.5066844658,1.1925218991,-0.7
802720674\B,1.1884513053,0.5147139823,-0.7764788178\B,0.5066844658,-1.
1925218991,-0.7802720674\B,-1.1884513053,-0.5147139823,-0.7764788178\B
,-1.2006736235,0.4855201836,0.7313653133\B,0.4773935452,1.2045469677,0
.7351586549\B,1.2006736235,-0.4855201836,0.7313653133\B,-0.4773935452,
-1.2045469677,0.7351586549\B,0.,0.,-1.8799410151\C,0.,0.,3.4126659631\
C,-0.453297254,1.1096979238,5.5525653262\C,0.453297254,-1.1096979238,5
.5525653262\C,-0.4502274684,1.1032486461,4.1606342462\C,0.4502274684,-
1.1032486461,4.1606342462\C,0.,0.,6.261331208\H,-0.9556997279,2.224242
3274,-1.1977500454\H,2.2246765061,0.9553470044,-1.1912759929\H,0.95569
97279,-2.2242423274,-1.1977500454\H,-2.2246765061,-0.9553470044,-1.191
2759929\H,-0.8102564444,1.9837803411,6.0870227184\H,0.8102564444,-1.98
37803411,6.0870227184\H,-2.2473565876,0.9007010285,1.1461620847\H,0.90
10642531,2.2469311695,1.1526367504\H,2.2473565876,-0.9007010285,1.1461
620847\H,-0.9010642531,-2.2469311695,1.1526367504\H,-0.8070995774,1.98
02169555,3.6317598027\H,0.8070995774,-1.9802169555,3.6317598027\H,0.,0
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057480351\C,0.4231257968,1.113924099,-4.2057480351\C,-0.4260369802,-1.
1204464657,-5.5976791245\C,0.4260369802,1.1204464657,-5.5976791245\C,0
.,0.,-6.3064450401\H,-0.7584553304,-1.9993537455,-3.6768739722\H,0.758
4553304,1.9993537455,-3.6768739722\H,-0.7615239075,-2.0029930646,-6.13
21364794\H,0.7615239075,2.0029930646,-6.1321364794\H,0.,0.,-7.39030563
63\\Version=ES64L-G09RevD.01\State=1-A\HF=-717.2611334\RMSD=3.037e-09\
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,-21.0561268,-0.0781015,0.,0.\PG=C02 [C2(H1C1C1B1B1C1C1H1),X(C8H16B8)]
\\@

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