Effects of Benzoheterocyclic Annelation on the *s*-Indacene Core: a Computational Analysis

Gabrielle I. Warren,[a,b] Katarzyna Młodzikowska-Pieńko,[b] Said Jalife,[c] Isabella S. Demachkie,[a] Judy I. Wu,[c] Michael M. Haley,[a] and Renana Gershoni-Poranne*[b]

[a]*Department of Chemistry & Biochemistry and the Materials Science Institute, University of Oregon, Eugene, Oregon 97403, United States*

[b]*Schulich Faculty of Chemistry and the Resnick Sustainability Center for Catalysis, Technion – Israel Institute of Technology, Haifa 32000, Israel*

[c]*Department of Chemistry, University of Houston, Houston, Texas 77204, United States*

1. Computational Details

Optimization

All structures were optimized using the following Gaussian[1] input:

```
#n CAM-B3LYP/def2tzvp opt=(MaxCycles=500,Tight) freq=noraman Integral=(UltraFineGrid)
empiricaldispersion=gd3bj

opt

0 1
@compound.xyz
```

where compound is the name of the XYZ file.

Wavefunction Stability

All structures were checked for wavefunction stability according to Gaussian instructions,[2] using the following input:

```
%oldchk=compound
%chk=compoundchk

#n CAM-B3LYP/def2tzvp opt=(MaxCycles=500, Tight) guess=read geom=check stable=opt
Integral=(UltraFineGrid) empiricaldispersion=gd3bj

Checking stability of compound
```

where %olchk is the name of the name of the checkpoint file from the optimization above. If the output file is stable, the original output from the optimization was used. If the wavefunction is not stable, structure was re-optimized based on the stable wavefunction from above:

```
%oldchk=compoundchk
%chk=compoundopt

#n CAM-B3LYP/def2tzvp opt=(MaxCycles=500, Tight) guess=read geom=allcheck freq=noraman
Integral=(UltraFineGrid) empiricaldispersion=gd3bj

Optimizing compound with new wfn
```

where %olchk is the name of the checkpoint file from the wavefunction stability check above. After successful optimization, the wavefunction stability was checked a final time:

```
%oldchk=compoundopt
%chk=compoundchkfinal

#n CAM-B3LYP/def2tzvp guess=read geom=allcheck stable=opt Integral=(UltraFineGrid)
empiricaldispersion=gd3bj

Checking the re-optimized wfn for stability
```

where %olchk is the name of the re-optimized checkpoint file. If the final check was stable, the re-optimized structure was used in further calculations.

NICS-Scans

The general input for NICS values generated by the Aroma package[3–5] is as follows:

```
geomfile=compound
run=nicsscan
center:VALUES
aromatic rings
VALUES
```

where compound specifies the optimized Gaussian output, center:VALUES specifies the bonds and rings to scan over (as outlined in the Aroma manual), and VALUES specifies the aromatic/antiaromatic rings (as outlined in the Aroma manual).

Note: the level of theory for the NICS calculations was changed to CAM-B3LYP/def2tzvp in aroma_constants.py

All plots and values were generated using the zz components of the chemical shielding tensor, calculated at 1 Å above the molecular plane.

NICS2BC

To ensure the correct orientation, BC-wizard was used to generate NICS values and then calculate the weights, bond current strengths, and finally to plot the bond currents.[6] The NICS input files were generated using the following:

```
1
1
compound.xyz
7
1
-1
5
1
compound
7
0 1
```

where compound is the basename of the optimized XYZ coordinates and sets the basename for BC-wizard.

Note: the level of theory for the NICS2BC calculations were changed to CAM-B3LYP/def2tzvp in bcwizard/fileman/gsn_inp_header.txt

The Gaussian outputs generated by BC-wizard were run, and then the following commands were used to calculate the ring weights, bond current strengths, and generate a pdf plot:

```
1
5
compound_nics.log
0,0,1
z
n
8
opt
-30.33
z

-1
3
1
z
-1
5
1
compound
5
6
-1
```

where compound is the basename as specified previously and -30.33 is the NICS value of benzene at 1 Å.

SYSMOIC

All SYSMOIC[7] inputs (CSGT calculations) were generated following the procedure outlined in the BC-wizard publication using the CAM-B3LYP/def2tzvp level of theory.[6] The SYSMOIC program was the used in the following way:

```
unpackwfx compound
TIPOMO
JBMAP -qf PIG -o compound < jbmap.inp
python plot.py compound.3d
```

where compound is the basename of the .wfx file (without .wfx extension) and plot.py is the python code for plotting the current densities from the BC-wizard SI. The jbmap.inp settings are as follows:

```
FATT 15
STEP 0.6
RI -20 -20 1
RF 20 20 1
y
n
n
```

The RI and RF x- and y-axes were set to be large enough to encompass any compound in the dataset and the z-axis value was set to 1 Å.

2. π-Density information

All the π-density calculations were computed using an Extended Hückel population analysis as implemented in Gaussian16 version C.01,[8] using the input provided below:

```
#ExtendedHuckel pop=full

Population analysis Extended Huckel Calculation

0  1
```

3. Calculated HOMO-LUMO Gaps

Table S1. Frontier Molecular orbital energies for compounds **1a-1c**, **2a-2c**, **3a-3c** (in eV).

	HOMO-1	HOMO	LUMO	LUMO+1	E_{Gap}
1a	-6.39	-5.65	-0.94	0.88	4.71
1b	-6.72	-6.29	-1.39	0.63	4.90
1c	-6.98	-6.56	-1.91	0.37	4.64
2a	-6.30	-6.03	-1.46	0.71	4.57
2b	-6.92	-6.48	-1.94	0.24	4.54
2c	-6.77	-6.66	-2.01	-0.01	4.65
3a	-6.16	-6.06	-1.60	-0.02	4.45
3b	-6.74	-6.45	-1.98	-0.32	4.47
3c	-6.63	-6.50	-2.13	-0.32	4.36

Table S2. Frontier Molecular orbital energies for compounds **1d-1f**, **2d-2f**, **3d-3f** (in eV).

	HOMO-1	HOMO	LUMO	LUMO+1	E_{Gap}
1d	-6.99	-5.64	-1.36	1.59	4.28
1e	-7.37	-6.41	-1.90	1.06	4.51
1f	-7.50	-6.73	-2.26	0.36	4.47
2d	-6.91	-6.04	-1.50	1.26	4.54
2e	-6.69	-6.59	-2.07	0.84	4.52
2f	-6.72	-6.64	-2.09	0.62	4.54
3d	-6.49	-6.01	-1.95	0.79	4.06
3e	-6.86	-6.54	-2.38	0.49	4.16
3f	-6.81	-6.52	-2.35	0.31	4.17
s-indacene	-7.14	-6.87	-2.06	0.56	4.80

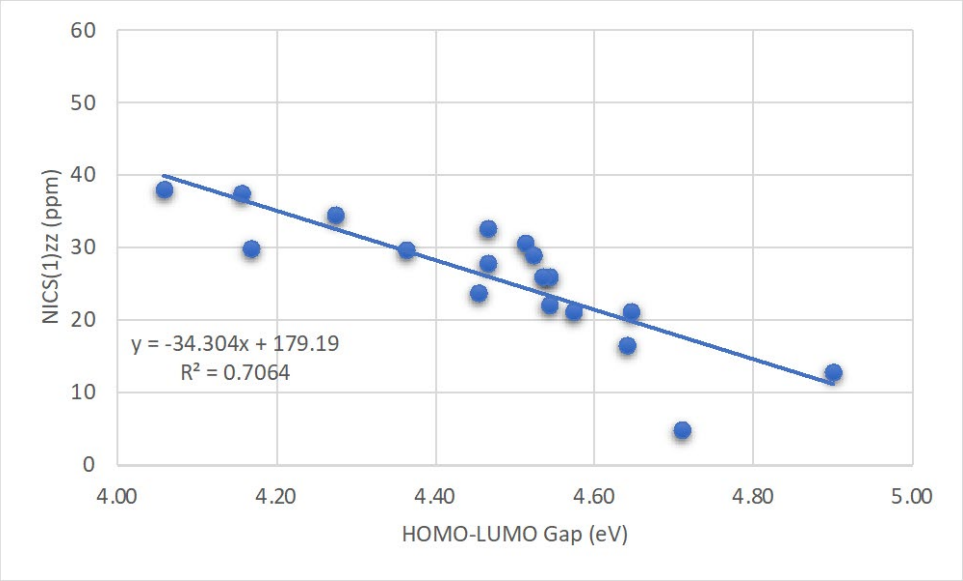

Figure S1. Scatter plot of the HOMO-LUMO gap (in eV) of all molecules versus the NICS(1)zz value (in ppm) of the 6-membered ring in the s-Indacene core.

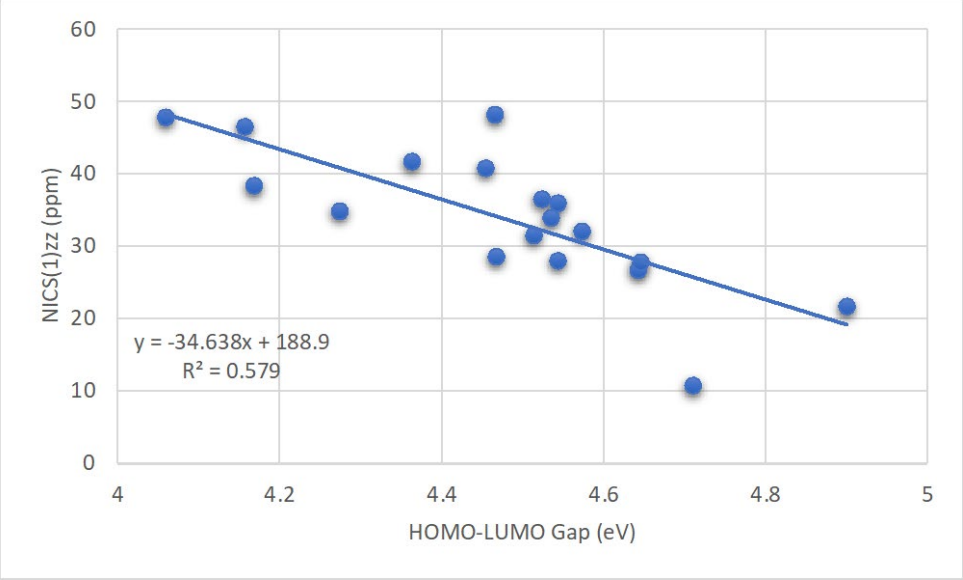

Figure S2. Scatter plot of the HOMO-LUMO gap (in eV) of all molecules versus the NICS(1)zz value (in ppm) of the 5-membered ring in the s-Indacene core.

4. Hammett Plots

The σ_p values for NH_2 (-0.66), OH (-0.37), and SH (0.15)[9] were plotted versus the NICS values for the corresponding acyclic compounds **1a-f**.

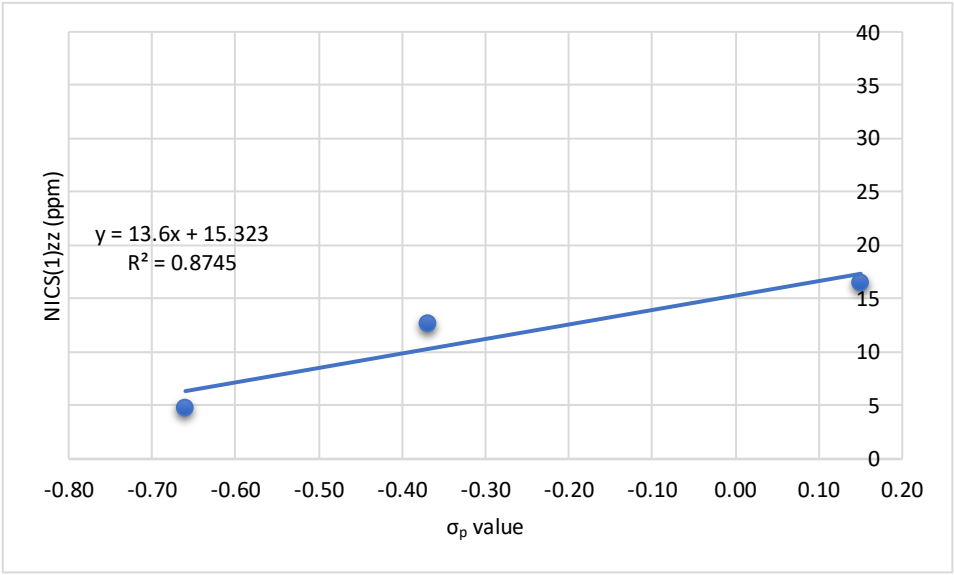

Figure S3. σ_p Values for NH_2, OH, and SH plotted versus the NICS values for **1a-c**.

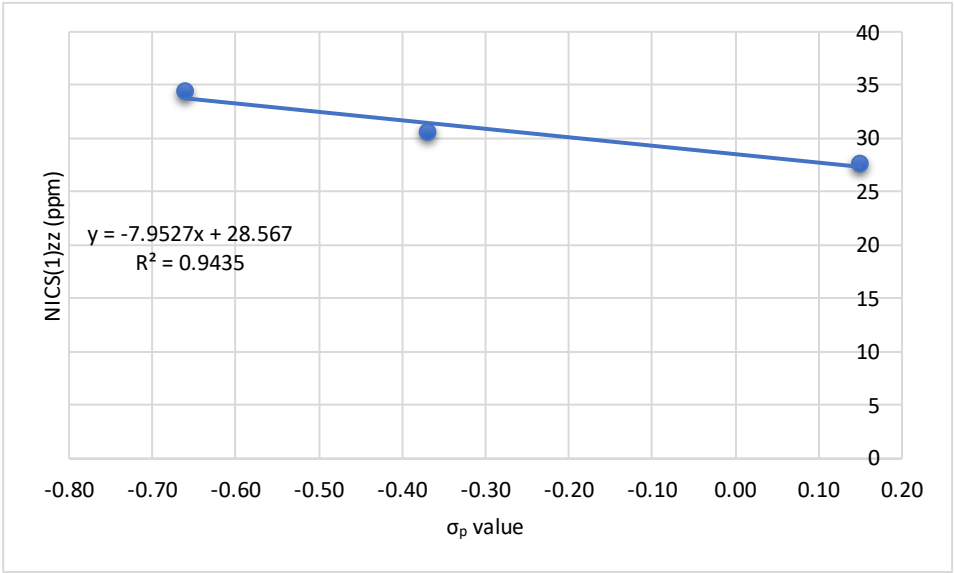

Figure S4. σ_p Values for NH_2, OH, and SH plotted versus the NICS values for **1d-f**.

5. Coordinates of optimized dataset

_s_-Indacene
Zero-point correction = 0.156531 (Hartree/Particle)
Thermal correction to Energy = 0.164909
Thermal correction to Enthalpy = 0.165853
Thermal correction to Gibbs Free Energy = 0.123342
Sum of electronic and zero-point Energies = -461.777297
Sum of electronic and thermal Energies = -461.768918
Sum of electronic and thermal Enthalpies = -461.767974
Sum of electronic and thermal Free Energies = -461.810485

C	0.5892700000	-1.2684440000	0.0000000000
C	1.4231800000	-0.1925380000	0.0000000000
C	0.8428380000	1.1001210000	0.0000000000
C	1.4076740000	2.3645950000	0.0000000000
C	0.3566920000	3.3423440000	0.0000000000
C	-0.8428380000	2.6975010000	0.0000000000
C	-0.5892700000	1.2684440000	0.0000000000
C	-1.4231800000	0.1925380000	0.0000000000
C	-0.8428380000	-1.1001210000	0.0000000000
C	-1.4076740000	-2.3645950000	0.0000000000
C	-0.3566920000	-3.3423440000	0.0000000000
C	0.8428380000	-2.6975010000	0.0000000000
H	2.5007420000	-0.3097330000	0.0000000000
H	2.4654630000	2.5849440000	0.0000000000
H	0.5058320000	4.4105870000	0.0000000000
H	-1.8201420000	3.1557820000	0.0000000000
H	-2.5007420000	0.3097330000	0.0000000000
H	-2.4654630000	-2.5849440000	0.0000000000
H	-0.5058320000	-4.4105870000	0.0000000000
H	1.8201420000	-3.1557820000	0.0000000000

1a; *anti*-NH2
Zero-point correction = 0.191128 (Hartree/Particle)
Thermal correction to Energy = 0.202362
Thermal correction to Enthalpy = 0.203307
Thermal correction to Gibbs Free Energy = 0.155001
Sum of electronic and zero-point Energies = -572.483421
Sum of electronic and thermal Energies = -572.472187
Sum of electronic and thermal Enthalpies = -572.471243
Sum of electronic and thermal Free Energies = -572.519548

N	3.5789190000	1.4015910000	-0.0282550000
C	2.7671850000	0.3092590000	0.0009090000

C	3.2022430000	-1.0439980000	-0.0071630000
C	2.0988590000	-1.8622280000	-0.0097480000
C	0.9180440000	-1.0463460000	-0.0047690000
C	1.3460860000	0.3238590000	-0.0020230000
C	0.4219490000	1.3661920000	-0.0053590000
C	-0.9180430000	1.0463460000	-0.0047690000
C	-2.0988580000	1.8622280000	-0.0097480000
C	-3.2022430000	1.0439980000	-0.0071630000
C	-2.7671850000	-0.3092590000	0.0009090000
N	-3.5789190000	-1.4015910000	-0.0282550000
C	-1.3460860000	-0.3238590000	-0.0020230000
C	-0.4219480000	-1.3661920000	-0.0053590000
H	4.5509400000	1.2806080000	0.1935270000
H	3.1899370000	2.2957380000	0.2125690000
H	4.2345960000	-1.3600880000	-0.0118640000
H	2.1110220000	-2.9417100000	-0.0129860000
H	0.7358810000	2.4046320000	-0.0145420000
H	-2.1110210000	2.9417100000	-0.0129860000
H	-4.2345960000	1.3600890000	-0.0118650000
H	-4.5509400000	-1.2806070000	0.1935260000
H	-3.1899380000	-2.2957380000	0.2125680000
H	-0.7358810000	-2.4046320000	-0.0145430000

1b; *anti*-OH

Zero-point correction= 0.166522 (Hartree/Particle)
Thermal correction to Energy= 0.176988
Thermal correction to Enthalpy= 0.177932
Thermal correction to Gibbs Free Energy= 0.130843
Sum of electronic and zero-point Energies= -612.252596
Sum of electronic and thermal Energies= -612.242130
Sum of electronic and thermal Enthalpies= -612.241186
Sum of electronic and thermal Free Energies= -612.288275

O	-3.4779190000	-1.4698850000	-0.0000010000
C	-2.7469400000	-0.3453900000	0.0000000000
C	-3.2213010000	0.9868800000	-0.0000050000
C	-2.1289780000	1.8269860000	0.0000060000
C	-0.9335160000	1.0325160000	0.0000010000
C	-1.3336080000	-0.3448350000	0.0000000000
C	-0.4000870000	-1.3784220000	0.0000000000
C	0.9335160000	-1.0325160000	0.0000010000
C	2.1289780000	-1.8269860000	0.0000060000
C	3.2213010000	-0.9868800000	-0.0000040000
C	2.7469400000	0.3453900000	0.0000000000
O	3.4779190000	1.4698850000	-0.0000010000

C	1.3336080000	0.3448350000	0.0000000000
C	0.4000860000	1.3784220000	0.0000000000
H	-4.4164020000	-1.2551550000	-0.0000040000
H	-4.2601910000	1.2813880000	-0.0000090000
H	-2.1602290000	2.9059340000	0.0000090000
H	-0.7167660000	-2.4141490000	0.0000010000
H	2.1602290000	-2.9059340000	0.0000080000
H	4.2601910000	-1.2813880000	-0.0000090000
H	4.4164030000	1.2551550000	-0.0000040000
H	0.7167660000	2.4141490000	0.0000010000

1c; *anti*-SH

Zero-point correction= 0.155933 (Hartree/Particle)
Thermal correction to Energy= 0.167855
Thermal correction to Enthalpy= 0.168800
Thermal correction to Gibbs Free Energy= 0.117499
Sum of electronic and zero-point Energies= -1258.227851
Sum of electronic and thermal Energies= -1258.215929
Sum of electronic and thermal Enthalpies= -1258.214985
Sum of electronic and thermal Free Energies= -1258.266285

S	4.1042410000	0.8912760000	-0.0000010000
C	2.7757570000	-0.2088380000	-0.0000010000
C	2.9540010000	-1.6224330000	-0.0000020000
C	1.7230750000	-2.2194370000	0.0000010000
C	0.7112460000	-1.1925250000	0.0000010000
C	1.3840970000	0.0709120000	0.0000010000
C	0.6620150000	1.2652580000	0.0000010000
C	-0.7112460000	1.1925250000	0.0000010000
C	-1.7230750000	2.2194370000	0.0000010000
C	-2.9540020000	1.6224330000	-0.0000020000
C	-2.7757570000	0.2088380000	0.0000000000
S	-4.1042410000	-0.8912760000	-0.0000010000
C	-1.3840970000	-0.0709120000	0.0000010000
C	-0.6620150000	-1.2652580000	0.0000010000
H	3.3938650000	2.0255210000	0.0000030000
H	3.9097170000	-2.1225680000	-0.0000030000
H	1.5329310000	-3.2819910000	0.0000030000
H	1.1580950000	2.2289050000	0.0000010000
H	-1.5329310000	3.2819910000	0.0000030000
H	-3.9097170000	2.1225680000	-0.0000030000
H	-3.3938650000	-2.0255210000	0.0000030000
H	-1.1580950000	-2.2289050000	0.0000010000

1d; *syn*-NH2

Zero-point correction= 0.190615 (Hartree/Particle)
Thermal correction to Energy= 0.201225
Thermal correction to Enthalpy= 0.202169
Thermal correction to Gibbs Free Energy= 0.154729
Sum of electronic and zero-point Energies= -572.465620
Sum of electronic and thermal Energies= -572.455010
Sum of electronic and thermal Enthalpies= -572.454066
Sum of electronic and thermal Free Energies= -572.501505

N	4.7078810000	0.0835880000	-0.0000060000
C	3.3529830000	-0.0511820000	-0.0000010000
C	2.5989070000	-1.1769880000	0.0000000000
C	1.2045600000	-0.7647790000	0.0000000000
C	0.0510550000	-1.4497320000	0.0000000000
C	-1.1900010000	-0.7115110000	0.0000000000
C	-2.4689440000	-1.1301570000	0.0000010000
C	-3.3529830000	0.0511820000	0.0000000000
N	-4.7078810000	-0.0835880000	0.0000020000
C	-2.5989070000	1.1769880000	0.0000000000
C	-1.2045600000	0.7647790000	0.0000000000
C	-0.0510550000	1.4497320000	0.0000000000
C	1.1900010000	0.7115110000	0.0000000000
C	2.4689440000	1.1301570000	-0.0000010000
H	5.3067650000	-0.7190900000	0.0000190000
H	5.1329200000	0.9893260000	0.0000280000
H	2.9526580000	-2.1955240000	0.0000000000
H	0.0275040000	-2.5328360000	0.0000000000
H	-2.8174090000	-2.1537530000	0.0000010000
H	-5.1329200000	-0.9893260000	-0.0000090000
H	-5.3067650000	0.7190900000	-0.0000060000
H	-2.9526580000	2.1955240000	0.0000010000
H	-0.0275040000	2.5328360000	0.0000000000
H	2.8174090000	2.1537530000	-0.0000020000

1e; *syn*-OH

Zero-point correction= 0.167977 (Hartree/Particle)
Thermal correction to Energy= 0.178395
Thermal correction to Enthalpy= 0.179339
Thermal correction to Gibbs Free Energy= 0.132241
Sum of electronic and zero-point Energies= -612.240323
Sum of electronic and thermal Energies= -612.229905
Sum of electronic and thermal Enthalpies= -612.228960
Sum of electronic and thermal Free Energies= -612.276059

O	4.6751300000	-0.1624530000	0.0000000000
C	3.3385510000	0.0164010000	0.0000000000
C	2.6097660000	1.1507990000	0.0000000000
C	1.2076970000	0.7463070000	0.0000000000
C	0.0643800000	1.4472730000	0.0000000000
C	-1.1840900000	0.7237070000	0.0000000000
C	-2.4620970000	1.1566990000	0.0000000000
C	-3.3385520000	-0.0164050000	0.0000000000
O	-4.6751310000	0.1624430000	0.0000000000
C	-2.6097620000	-1.1507970000	0.0000000000
C	-1.2076960000	-0.7463020000	0.0000000000
C	-0.0643800000	-1.4472680000	0.0000000000
C	1.1840880000	-0.7237030000	0.0000000000
C	2.4620930000	-1.1566970000	0.0000000000
H	5.1194570000	0.6915890000	0.0000020000
H	2.9740830000	2.1661020000	0.0000000000
H	0.0544720000	2.5304930000	0.0000000000
H	-2.8175430000	2.1760900000	0.0000000000
H	-5.1194530000	-0.6916020000	0.0000020000
H	-2.9740740000	-2.1661030000	0.0000000000
H	-0.0544690000	-2.5304870000	0.0000000000
H	2.8175350000	-2.1760900000	0.0000000000

1f; *syn*-SH

Zero-point correction= 0.157290 (Hartree/Particle)
Thermal correction to Energy= 0.169335
Thermal correction to Enthalpy= 0.170279
Thermal correction to Gibbs Free Energy= 0.118437
Sum of electronic and zero-point Energies= -1258.213853
Sum of electronic and thermal Energies= -1258.201808
Sum of electronic and thermal Enthalpies= -1258.200864
Sum of electronic and thermal Free Energies= -1258.252706

S	-5.0980330000	-0.0231330000	-0.0815880000
C	-3.3519350000	-0.0617470000	0.0210490000
C	-2.5865830000	-1.1753850000	0.0252450000
C	-1.1932700000	-0.7547540000	0.0164230000
C	-0.0401910000	-1.4468340000	0.0149500000
C	1.1941560000	-0.7078310000	0.0164430000
C	2.4842760000	-1.1184020000	0.0115520000
C	3.3519350000	0.0617470000	0.0210490000
S	5.0980330000	0.0231330000	-0.0815880000
C	2.5865840000	1.1753850000	0.0252450000
C	1.1932700000	0.7547540000	0.0164230000
C	0.0401910000	1.4468340000	0.0149500000

C	-1.1941560000	0.7078310000	0.0164430000
C	-2.4842760000	1.1184020000	0.0115520000
H	-5.2769320000	1.1005150000	0.6254980000
H	-2.9344500000	-2.1960940000	0.0396220000
H	-0.0217330000	-2.5300260000	0.0108790000
H	2.8399800000	-2.1382820000	-0.0045610000
H	5.2769320000	-1.1005150000	0.6254970000
H	2.9344500000	2.1960940000	0.0396220000
H	0.0217330000	2.5300260000	0.0108790000
H	-2.8399800000	2.1382820000	-0.0045610000

2a; *anti*-IDP

Zero-point correction= 0.218650 (Hartree/Particle)
Thermal correction to Energy= 0.230825
Thermal correction to Enthalpy= 0.231769
Thermal correction to Gibbs Free Energy= 0.180244
Sum of electronic and zero-point Energies= -724.829177
Sum of electronic and thermal Energies= -724.817002
Sum of electronic and thermal Enthalpies= -724.816057
Sum of electronic and thermal Free Energies= -724.867583

C	1.3379550000	0.4370520000	0.0000000000
C	0.3884380000	1.3916450000	0.0000000000
C	-0.9868190000	0.9962790000	0.0000000000
C	-2.1261270000	1.7484040000	0.0000000000
C	-3.2669590000	0.8556890000	0.0000000000
C	-2.7866350000	-0.4408540000	0.0000000000
N	-3.8416280000	-1.2913980000	0.0000000000
C	-5.0043740000	-0.5481480000	0.0000000000
C	-4.6840020000	0.7848850000	0.0000000000
C	-1.3379550000	-0.4370520000	0.0000000000
C	-0.3884380000	-1.3916450000	0.0000000000
C	0.9868190000	-0.9962780000	0.0000000000
C	2.1261270000	-1.7484040000	0.0000000000
C	3.2669590000	-0.8556890000	0.0000000000
C	2.7866350000	0.4408540000	0.0000000000
N	3.8416280000	1.2913980000	0.0000000000
C	5.0043740000	0.5481480000	0.0000000000
C	4.6840020000	-0.7848850000	0.0000000000
H	0.6364390000	2.4469490000	0.0000000000
H	-2.1621350000	2.8281220000	0.0000000000
H	-3.8024090000	-2.2938450000	0.0000000000
H	-5.9651800000	-1.0327700000	0.0000000000
H	-5.3943420000	1.5943260000	0.0000000000
H	-0.6364400000	-2.4469490000	0.0000000000

H	2.1621350000	-2.8281230000	0.0000000000
H	3.8024090000	2.2938450000	0.0000000000
H	5.9651800000	1.0327700000	0.0000000000
H	5.3943420000	-1.5943260000	0.0000000000

2b; *anti*-IDF

Zero-point correction= 0.193699 (Hartree/Particle)
Thermal correction to Energy= 0.205296
Thermal correction to Enthalpy= 0.206240
Thermal correction to Gibbs Free Energy= 0.155602
Sum of electronic and zero-point Energies= -764.575045
Sum of electronic and thermal Energies= -764.563448
Sum of electronic and thermal Enthalpies= -764.562504
Sum of electronic and thermal Free Energies= -764.613142

C	-1.3339590000	-0.4327080000	-0.0000010000
C	-0.3910180000	-1.3944700000	-0.0000010000
C	0.9834260000	-0.9995150000	-0.0000020000
C	2.1221410000	-1.7564470000	-0.0000030000
C	3.2594290000	-0.8583390000	0.0000000000
C	2.7757470000	0.4184790000	-0.0000020000
O	3.7592450000	1.3272970000	0.0000020000
C	4.9249680000	0.6012340000	-0.0000100000
C	4.6824460000	-0.7310640000	0.0000140000
C	1.3339590000	0.4327080000	-0.0000010000
C	0.3910180000	1.3944700000	0.0000000000
C	-0.9834260000	0.9995150000	-0.0000010000
C	-2.1221410000	1.7564470000	-0.0000030000
C	-3.2594290000	0.8583390000	0.0000000000
C	-2.7757470000	-0.4184790000	-0.0000010000
O	-3.7592450000	-1.3272970000	0.0000020000
C	-4.9249680000	-0.6012340000	-0.0000090000
C	-4.6824460000	0.7310640000	0.0000130000
H	-0.6512620000	-2.4458780000	-0.0000010000
H	2.1570420000	-2.8357050000	-0.0000010000
H	5.8301530000	1.1809240000	-0.0000190000
H	5.4340660000	-1.5019270000	0.0000250000
H	0.6512620000	2.4458780000	0.0000000000
H	-2.1570420000	2.8357050000	-0.0000010000
H	-5.8301530000	-1.1809240000	-0.0000160000
H	-5.4340660000	1.5019270000	0.0000220000

2c; *anti*-IDT

Zero-point correction= 0.187659 (Hartree/Particle)

Thermal correction to Energy= 0.200194
Thermal correction to Enthalpy= 0.201138
Thermal correction to Gibbs Free Energy= 0.148021
Sum of electronic and zero-point Energies= -1410.596776
Sum of electronic and thermal Energies= -1410.584241
Sum of electronic and thermal Enthalpies= -1410.583297
Sum of electronic and thermal Free Energies= -1410.636415

C	-1.3653190000	-0.3401970000	0.0000000000
C	-0.4896040000	-1.3613330000	0.0000000000
C	0.9116890000	-1.0595790000	0.0000000000
C	1.9957920000	-1.8826060000	0.0000000000
C	3.1960700000	-1.0651270000	0.0000000000
C	2.8145270000	0.2620830000	0.0000000000
S	4.1567980000	1.3039280000	-0.0000010000
C	5.2450130000	-0.0326770000	0.0000010000
C	4.6032370000	-1.2320450000	0.0000000000
C	1.3653190000	0.3401970000	0.0000000000
C	0.4896040000	1.3613330000	0.0000000000
C	-0.9116890000	1.0595790000	0.0000000000
C	-1.9957920000	1.8826060000	0.0000000000
C	-3.1960700000	1.0651270000	0.0000000000
C	-2.8145270000	-0.2620830000	0.0000000000
S	-4.1567980000	-1.3039280000	-0.0000010000
C	-5.2450130000	0.0326770000	0.0000020000
C	-4.6032370000	1.2320460000	0.0000000000
H	-0.8159200000	-2.3944090000	0.0000000000
H	1.9700090000	-2.9624560000	0.0000000000
H	6.3070420000	0.1478770000	0.0000020000
H	5.1195570000	-2.1804280000	0.0000000000
H	0.8159200000	2.3944090000	0.0000000000
H	-1.9700090000	2.9624560000	0.0000000000
H	-6.3070420000	-0.1478770000	0.0000030000
H	-5.1195570000	2.1804280000	0.0000000000

2d; *syn*-IDP
Zero-point correction= 0.218703 (Hartree/Particle)
Thermal correction to Energy= 0.230878
Thermal correction to Enthalpy= 0.231822
Thermal correction to Gibbs Free Energy= 0.180314
Sum of electronic and zero-point Energies= -724.830834
Sum of electronic and thermal Energies= -724.818659
Sum of electronic and thermal Enthalpies= -724.817715
Sum of electronic and thermal Free Energies= -724.869223

C	-1.3355930000	-0.4688090000	-0.0000020000
C	-0.3638070000	-1.3975840000	-0.0000030000
C	1.0048660000	-0.9677870000	-0.0000020000
C	2.1559810000	-1.7029270000	-0.0000010000
C	3.2505140000	-0.7672800000	0.0000000000
C	2.7940410000	0.5369930000	0.0000000000
C	3.9244050000	1.3824890000	0.0000040000
C	5.0275580000	0.5590740000	0.0000010000
N	4.6120220000	-0.7502440000	0.0000030000
C	1.3355930000	0.4688090000	-0.0000010000
C	0.3638070000	1.3975840000	-0.0000020000
C	-1.0048660000	0.9677870000	-0.0000020000
C	-2.1559810000	1.7029270000	-0.0000020000
C	-3.2505140000	0.7672800000	-0.0000010000
C	-2.7940410000	-0.5369930000	-0.0000020000
C	-3.9244050000	-1.3824890000	-0.0000020000
C	-5.0275580000	-0.5590740000	0.0000100000
N	-4.6120220000	0.7502440000	-0.0000010000
H	-0.5918800000	-2.4569040000	-0.0000030000
H	2.2204960000	-2.7809200000	-0.0000010000
H	3.9569240000	2.4590130000	0.0000060000
H	6.0753610000	0.8048590000	0.0000000000
H	5.2214580000	-1.5469030000	0.0000040000
H	0.5918800000	2.4569040000	-0.0000020000
H	-2.2204960000	2.7809200000	-0.0000020000
H	-3.9569240000	-2.4590130000	-0.0000040000
H	-6.0753610000	-0.8048590000	0.0000180000
H	-5.2214580000	1.5469030000	0.0000000000

2e; *syn*-IDF

Zero-point correction= 0.193697 (Hartree/Particle)
Thermal correction to Energy= 0.205294
Thermal correction to Enthalpy= 0.206238
Thermal correction to Gibbs Free Energy= 0.155592
Sum of electronic and zero-point Energies= -764.578360
Sum of electronic and thermal Energies= -764.566763
Sum of electronic and thermal Enthalpies= -764.565819
Sum of electronic and thermal Free Energies= -764.616465

C	-1.3311230000	-0.4744190000	0.0000000000
C	-0.3552620000	-1.3999500000	0.0000010000
C	1.0098740000	-0.9633770000	0.0000000000
C	2.1654970000	-1.6965410000	-0.0000010000
C	3.2359470000	-0.7428790000	-0.0000010000
C	2.7880490000	0.5465030000	-0.0000010000

C	3.9537130000	1.3603950000	0.0000030000
C	4.9998670000	0.4929030000	-0.0000020000
O	4.5805610000	-0.8063250000	0.0000010000
C	1.3311230000	0.4744190000	-0.0000010000
C	0.3552620000	1.3999500000	-0.0000010000
C	-1.0098740000	0.9633770000	0.0000000000
C	-2.1654970000	1.6965410000	0.0000010000
C	-3.2359470000	0.7428790000	0.0000000000
C	-2.7880490000	-0.5465030000	0.0000010000
C	-3.9537130000	-1.3603950000	0.0000030000
C	-4.9998670000	-0.4929030000	-0.0000040000
O	-4.5805610000	0.8063250000	0.0000010000
H	-0.5778980000	-2.4601750000	0.0000010000
H	2.2497200000	-2.7720330000	-0.0000010000
H	4.0356510000	2.4339320000	0.0000050000
H	6.0652540000	0.6380300000	-0.0000030000
H	0.5778980000	2.4601750000	-0.0000010000
H	-2.2497200000	2.7720330000	0.0000010000
H	-4.0356510000	-2.4339320000	0.0000050000
H	-6.0652540000	-0.6380300000	-0.0000060000

2f; *syn*-IDT

Zero-point correction= 0.187688 (Hartree/Particle)
Thermal correction to Energy= 0.200215
Thermal correction to Enthalpy= 0.201159
Thermal correction to Gibbs Free Energy= 0.148074
Sum of electronic and zero-point Energies= -1410.597962
Sum of electronic and thermal Energies= -1410.585436
Sum of electronic and thermal Enthalpies= -1410.584491
Sum of electronic and thermal Free Energies= -1410.637577

C	1.3203520000	-0.4926970000	0.0000000000
C	0.3326720000	-1.4062090000	0.0000010000
C	-1.0246340000	-0.9447790000	0.0000010000
C	-2.1963010000	-1.6441310000	0.0000020000
C	-3.2755720000	-0.6876770000	0.0000010000
C	-2.7758490000	0.6006420000	0.0000000000
C	-3.7902110000	1.5812100000	-0.0000010000
C	-5.0312350000	1.0145690000	-0.0000010000
S	-4.9812790000	-0.7038970000	0.0000000000
C	-1.3203520000	0.4926970000	0.0000000000
C	-0.3326720000	1.4062090000	0.0000000000
C	1.0246340000	0.9447790000	-0.0000010000
C	2.1963010000	1.6441310000	-0.0000010000
C	3.2755720000	0.6876770000	0.0000000000

C	2.7758490000	-0.6006420000	0.0000000000
C	3.7902110000	-1.5812100000	0.0000000000
C	5.0312350000	-1.0145690000	-0.0000070000
S	4.9812790000	0.7038970000	0.0000030000
H	0.5388550000	-2.4698060000	0.0000020000
H	-2.2977000000	-2.7188240000	0.0000020000
H	-3.6301070000	2.6491050000	-0.0000020000
H	-5.9830140000	1.5193690000	-0.0000020000
H	-0.5388550000	2.4698060000	0.0000000000
H	2.2977000000	2.7188240000	-0.0000010000
H	3.6301070000	-2.6491050000	0.0000000000
H	5.9830140000	-1.5193690000	-0.0000110000

3a; *anti*-IDI

Zero-point correction= 0.311542 (Hartree/Particle)
Thermal correction to Energy= 0.329140
Thermal correction to Enthalpy= 0.330085
Thermal correction to Gibbs Free Energy= 0.266294
Sum of electronic and zero-point Energies= -1031.988801
Sum of electronic and thermal Energies= -1031.971203
Sum of electronic and thermal Enthalpies= -1031.970258
Sum of electronic and thermal Free Energies= -1032.034049

N	-3.7268790000	-1.4734030000	0.0000000000
C	-4.9557930000	-0.8149110000	0.0000020000
C	-4.7238520000	0.5805830000	0.0000000000
C	-5.8155800000	1.4396960000	0.0000000000
C	-7.0922890000	0.9092110000	0.0000020000
C	-7.2978440000	-0.4693080000	0.0000030000
C	-6.2302620000	-1.3496340000	0.0000030000
C	-2.7378460000	-0.5441050000	-0.0000010000
C	-3.2933300000	0.7435150000	0.0000000000
C	-2.2413490000	1.6741290000	-0.0000010000
C	-1.0219810000	0.9538200000	0.0000000000
C	-1.3079740000	-0.4659920000	-0.0000020000
C	-0.2996840000	-1.4010740000	-0.0000030000
C	1.0219820000	-0.9538200000	-0.0000040000
C	2.2413490000	-1.6741290000	-0.0000080000
C	3.2933300000	-0.7435150000	-0.0000030000
C	2.7378460000	0.5441050000	-0.0000020000
N	3.7268790000	1.4734030000	-0.0000020000
C	4.9557930000	0.8149110000	-0.0000010000
C	4.7238520000	-0.5805830000	0.0000020000
C	5.8155810000	-1.4396950000	0.0000060000
C	7.0922890000	-0.9092110000	0.0000060000

C	7.2978440000	0.4693080000	0.0000030000
C	6.2302620000	1.3496340000	0.0000000000
C	1.3079740000	0.4659910000	-0.0000020000
C	0.2996840000	1.4010740000	0.0000010000
H	-5.6682370000	2.5116120000	0.0000000000
H	-7.9467350000	1.5724340000	0.0000020000
H	-8.3069480000	-0.8584720000	0.0000040000
H	-6.3912910000	-2.4199480000	0.0000040000
H	-2.3259520000	2.7504220000	-0.0000010000
H	-0.5134130000	-2.4638450000	-0.0000050000
H	2.3259520000	-2.7504220000	-0.0000110000
H	5.6682370000	-2.5116120000	0.0000070000
H	7.9467360000	-1.5724340000	0.0000090000
H	8.3069470000	0.8584720000	0.0000040000
H	6.3912910000	2.4199480000	-0.0000020000
H	0.5134130000	2.4638440000	0.0000020000
H	3.6106050000	2.4699170000	0.0000000000
H	-3.6106060000	-2.4699170000	0.0000010000

3b; *anti*-IDBF

Zero-point correction= 0.286703 (Hartree/Particle)
Thermal correction to Energy= 0.303596
Thermal correction to Enthalpy= 0.304540
Thermal correction to Gibbs Free Energy= 0.241856
Sum of electronic and zero-point Energies= -1071.739690
Sum of electronic and thermal Energies= -1071.722797
Sum of electronic and thermal Enthalpies= -1071.721853
Sum of electronic and thermal Free Energies= -1071.784537

C	1.3113000000	-0.4362020000	0.0000040000
C	0.3208340000	-1.3993990000	0.0000040000
C	-1.0014150000	-0.9757330000	0.0000020000
C	-2.2160820000	-1.7255430000	0.0000000000
C	-3.2744010000	-0.8123890000	0.0000000000
C	-2.7293260000	0.4723430000	0.0000000000
O	-3.6594700000	1.4407290000	-0.0000010000
C	-4.8768180000	0.7756990000	-0.0000010000
C	-4.7046990000	-0.6165800000	-0.0000010000
C	-5.8343760000	-1.4220090000	-0.0000010000
C	-7.0820140000	-0.8208600000	-0.0000010000
C	-7.2166150000	0.5639960000	-0.0000010000
C	-6.1031000000	1.3918840000	-0.0000010000
C	-1.3113000000	0.4362020000	-0.0000020000
C	-0.3208340000	1.3993990000	-0.0000030000
C	1.0014150000	0.9757330000	0.0000010000

C	2.2160820000	1.7255430000	0.0000070000
C	3.2744010000	0.8123890000	0.0000030000
C	2.7293260000	-0.4723430000	0.0000020000
O	3.6594700000	-1.4407290000	0.0000010000
C	4.8768180000	-0.7756990000	-0.0000010000
C	4.7046990000	0.6165800000	0.0000000000
C	5.8343760000	1.4220090000	-0.0000010000
C	7.0820140000	0.8208600000	-0.0000030000
C	7.2166150000	-0.5639960000	-0.0000040000
C	6.1031000000	-1.3918840000	-0.0000020000
H	0.5672560000	-2.4539860000	0.0000050000
H	-2.2791570000	-2.8028980000	0.0000010000
H	-5.7432140000	-2.4996910000	-0.0000010000
H	-7.9700030000	-1.4383430000	-0.0000010000
H	-8.2042080000	1.0043660000	-0.0000010000
H	-6.1885690000	2.4691440000	-0.0000010000
H	-0.5672560000	2.4539860000	-0.0000030000
H	2.2791570000	2.8028980000	0.0000080000
H	5.7432140000	2.4996910000	0.0000000000
H	7.9700030000	1.4383420000	-0.0000040000
H	8.2042080000	-1.0043660000	-0.0000050000
H	6.1885690000	-2.4691440000	-0.0000030000

3c; *anti*-IDBT

Zero-point correction= 0.280886 (Hartree/Particle)
Thermal correction to Energy= 0.298988
Thermal correction to Enthalpy= 0.299932
Thermal correction to Gibbs Free Energy= 0.234313
Sum of electronic and zero-point Energies= -1717.753891
Sum of electronic and thermal Energies= -1717.735788
Sum of electronic and thermal Enthalpies= -1717.734844
Sum of electronic and thermal Free Energies= -1717.800464

C	1.3028240000	-0.4958820000	0.0000000000
C	0.2897110000	-1.4078170000	0.0000000000
C	-1.0372740000	-0.9295510000	0.0000010000
C	-2.2522450000	-1.6120380000	0.0000010000
C	-3.3053580000	-0.6516980000	0.0000000000
C	-2.7424260000	0.6140950000	0.0000000000
S	-3.8996540000	1.8744320000	0.0000000000
C	-5.2072840000	0.7073160000	0.0000000000
C	-4.7399820000	-0.6205960000	0.0000000000
C	-5.6710510000	-1.6576680000	0.0000000000
C	-7.0180700000	-1.3655840000	-0.0000010000
C	-7.4631030000	-0.0439630000	-0.0000010000

C	-6.5616660000	1.0012130000	-0.0000010000
C	-1.3028250000	0.4958820000	0.0000010000
C	-0.2897120000	1.4078170000	0.0000010000
C	1.0372730000	0.9295510000	0.0000010000
C	2.2522440000	1.6120400000	0.0000000000
C	3.3053580000	0.6516980000	0.0000000000
C	2.7424250000	-0.6140950000	0.0000000000
S	3.8996540000	-1.8744320000	0.0000000000
C	5.2072840000	-0.7073160000	0.0000000000
C	4.7399820000	0.6205960000	0.0000000000
C	5.6710520000	1.6576680000	0.0000000000
C	7.0180710000	1.3655840000	-0.0000010000
C	7.4631030000	0.0439630000	-0.0000010000
C	6.5616660000	-1.0012130000	-0.0000010000
H	0.4858200000	-2.4733780000	0.0000000000
H	-2.3686330000	-2.6857470000	0.0000010000
H	-5.3338090000	-2.6859190000	0.0000000000
H	-7.7406070000	-2.1705850000	-0.0000010000
H	-8.5240690000	0.1655280000	-0.0000010000
H	-6.9056480000	2.0268600000	-0.0000010000
H	-0.4858200000	2.4733780000	0.0000010000
H	2.3686330000	2.6857500000	0.0000000000
H	5.3338090000	2.6859190000	0.0000000000
H	7.7406070000	2.1705840000	-0.0000010000
H	8.5240690000	-0.1655290000	-0.0000010000
H	6.9056470000	-2.0268610000	-0.0000010000

3d; *syn*-IDI

Zero-point correction= 0.313146 (Hartree/Particle)
Thermal correction to Energy= 0.330769
Thermal correction to Enthalpy= 0.331713
Thermal correction to Gibbs Free Energy= 0.267688
Sum of electronic and zero-point Energies= -1031.984466
Sum of electronic and thermal Energies= -1031.966844
Sum of electronic and thermal Enthalpies= -1031.965899
Sum of electronic and thermal Free Energies= -1032.029925

N	-4.2706820000	1.9209040000	0.0000000000
C	-5.0322400000	0.7680740000	0.0000010000
C	-4.1570390000	-0.3519770000	0.0000000000
C	-4.7114430000	-1.6336540000	0.0000010000
C	-6.0811370000	-1.7743750000	0.0000030000
C	-6.9245300000	-0.6570900000	0.0000040000
C	-6.4117900000	0.6228680000	0.0000030000
C	-2.8379110000	0.1858330000	-0.0000030000

C	-2.9530430000	1.5551890000	-0.0000030000
C	-1.6548930000	2.1874930000	-0.0000020000
C	-0.7279710000	1.1878670000	-0.0000020000
C	-1.4136820000	-0.1192310000	-0.0000030000
C	-0.7068080000	-1.2619600000	-0.0000030000
C	0.7279710000	-1.1878690000	-0.0000020000
C	1.6548890000	-2.1874950000	-0.0000020000
C	2.9530410000	-1.5551880000	-0.0000020000
C	2.8379090000	-0.1858310000	-0.0000020000
C	4.1570360000	0.3519800000	0.0000000000
C	4.7114490000	1.6336550000	0.0000020000
C	6.0811440000	1.7743710000	0.0000040000
C	6.9245350000	0.6570870000	0.0000050000
C	6.4117870000	-0.6228700000	0.0000040000
C	5.0322390000	-0.7680680000	0.0000020000
N	4.2706770000	-1.9209010000	0.0000010000
C	1.4136840000	0.1192310000	-0.0000020000
C	0.7068070000	1.2619580000	-0.0000020000
H	-4.0716700000	-2.5060610000	0.0000000000
H	-6.5172690000	-2.7643050000	0.0000040000
H	-7.9965670000	-0.8004620000	0.0000050000
H	-7.0660860000	1.4852120000	0.0000040000
H	-1.4494550000	3.2474560000	-0.0000020000
H	-1.1905880000	-2.2309860000	-0.0000030000
H	1.4494540000	-3.2474580000	-0.0000020000
H	4.0716830000	2.5060690000	0.0000010000
H	6.5172750000	2.7643030000	0.0000050000
H	7.9965730000	0.8004570000	0.0000070000
H	7.0660730000	-1.4852210000	0.0000050000
H	1.1905860000	2.2309840000	-0.0000030000
H	4.6350050000	-2.8551920000	-0.0000020000
H	-4.6349990000	2.8552010000	-0.0000020000

3e; *syn*-IDBF

Zero-point correction= 0.288934 (Hartree/Particle)
Thermal correction to Energy= 0.305586
Thermal correction to Enthalpy= 0.306530
Thermal correction to Gibbs Free Energy= 0.244339
Sum of electronic and zero-point Energies= -1071.769607
Sum of electronic and thermal Energies= -1071.752956
Sum of electronic and thermal Enthalpies= -1071.752011
Sum of electronic and thermal Free Energies= -1071.814202

C	1.3736390000	0.3008620000	0.0000000000
C	0.5306380000	1.3450940000	0.0000000000

C	-0.8821420000	1.0817290000	0.0000000000
C	-1.9399740000	1.9285130000	0.0000000000
C	-3.1761060000	1.1617860000	0.0000000000
C	-2.8375040000	-0.2216980000	0.0000000000
C	-3.7987960000	-1.2004560000	0.0000000000
C	-5.1356880000	-0.7886270000	0.0000000000
C	-6.4076090000	-1.4588690000	0.0000000000
C	-7.3397330000	-0.4907280000	-0.0000010000
O	-6.7849160000	0.7547210000	0.0000000000
C	-5.4370480000	0.5751790000	0.0000000000
C	-4.4893030000	1.5842080000	0.0000000000
C	-1.3736390000	-0.3008620000	0.0000000000
C	-0.5306380000	-1.3450940000	0.0000000000
C	0.8821420000	-1.0817290000	0.0000000000
C	1.9399740000	-1.9285130000	0.0000000000
C	3.1761060000	-1.1617860000	0.0000000000
C	2.8375040000	0.2216980000	0.0000000000
C	3.7987960000	1.2004560000	0.0000000000
C	5.1356880000	0.7886270000	0.0000000000
C	6.4076090000	1.4588690000	0.0000000000
C	7.3397330000	0.4907280000	-0.0000010000
O	6.7849160000	-0.7547210000	0.0000000000
C	5.4370480000	-0.5751790000	0.0000000000
C	4.4893030000	-1.5842080000	0.0000000000
H	0.8853640000	2.3686310000	0.0000000000
H	-1.8886310000	3.0078470000	0.0000000000
H	-3.5398440000	-2.2513890000	0.0000000000
H	-6.5928770000	-2.5193720000	0.0000000000
H	-8.4152630000	-0.5179650000	-0.0000020000
H	-4.7710330000	2.6279070000	0.0000000000
H	-0.8853640000	-2.3686310000	0.0000000000
H	1.8886310000	-3.0078470000	0.0000000000
H	3.5398440000	2.2513890000	0.0000000000
H	6.5928770000	2.5193720000	0.0000000000
H	8.4152630000	0.5179650000	-0.0000010000
H	4.7710330000	-2.6279070000	0.0000000000

3f; *syn*-IDBT

Zero-point correction= 0.282945 (Hartree/Particle)
Thermal correction to Energy= 0.300874
Thermal correction to Enthalpy= 0.301818
Thermal correction to Gibbs Free Energy= 0.236420
Sum of electronic and zero-point Energies= -1717.751036
Sum of electronic and thermal Energies= -1717.733108
Sum of electronic and thermal Enthalpies= -1717.732164

Sum of electronic and thermal Free Energies= -1717.797562

C	1.4092970000	0.1076220000	-0.0000020000
C	0.7101360000	1.2581970000	-0.0000030000
C	-0.7216940000	1.1887020000	-0.0000020000
C	-1.6524180000	2.1858500000	-0.0000020000
C	-2.9549700000	1.5652760000	-0.0000020000
C	-2.8349820000	0.1982510000	-0.0000010000
C	-4.0937860000	-0.4715090000	0.0000010000
C	-4.4046620000	-1.8346750000	0.0000030000
C	-5.7204420000	-2.2346490000	0.0000050000
C	-6.7551250000	-1.2954440000	0.0000050000
C	-6.4793740000	0.0544870000	0.0000030000
C	-5.1526100000	0.4631460000	0.0000010000
S	-4.5864580000	2.1121910000	-0.0000030000
C	-1.4092970000	-0.1076220000	-0.0000020000
C	-0.7101360000	-1.2581970000	-0.0000020000
C	0.7216940000	-1.1887020000	-0.0000020000
C	1.6524180000	-2.1858500000	-0.0000020000
C	2.9549700000	-1.5652760000	-0.0000030000
C	2.8349820000	-0.1982510000	-0.0000020000
C	4.0937860000	0.4715090000	0.0000010000
C	4.4046620000	1.8346750000	0.0000030000
C	5.7204410000	2.2346490000	0.0000050000
C	6.7551250000	1.2954440000	0.0000050000
C	6.4793740000	-0.0544870000	0.0000030000
C	5.1526100000	-0.4631460000	0.0000010000
S	4.5864580000	-2.1121910000	-0.0000030000
H	1.1958310000	2.2256750000	-0.0000030000
H	-1.4534860000	3.2467830000	-0.0000020000
H	-3.6121830000	-2.5703400000	0.0000040000
H	-5.9599790000	-3.2894710000	0.0000070000
H	-7.7832650000	-1.6309160000	0.0000060000
H	-7.2803860000	0.7815570000	0.0000020000
H	-1.1958310000	-2.2256750000	-0.0000020000
H	1.4534860000	-3.2467830000	-0.0000030000
H	3.6121830000	2.5703390000	0.0000030000
H	5.9599790000	3.2894710000	0.0000070000
H	7.7832650000	1.6309160000	0.0000070000
H	7.2803860000	-0.7815570000	0.0000030000

6. References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, J. V. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Going, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, T. Throssell, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brother, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 09, Revision E.01 (version A.1.).
2. Modeling Antiferromagnetic Coupling in Gaussian, https://gaussian.com/afc/.
3. A. Stanger, *J. Org. Chem.*, 2006, **71**, 883–893.
4. A. Stanger, *J. Org. Chem.*, 2010, **75**, 2281–2288.
5. R. Gershoni-Poranne and A. Stanger, *Chem. Eur. J.*, 2014, **20**, 5673–5688.
6. E. Paenurk and R. Gershoni-Poranne, *Phys. Chem. Chem. Phys.*, 2022, **24**, 8631–8644.
7. G. Monaco, F. F. Summa and R. Zanasi, *J. Chem. Inf. Model.*, 2021, **61**, 270–283.
8. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, J. V. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Going, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, T. Throssell, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brother, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16, Revision C.01.
9. C. Hansch, A. Leo and R. W. Taft, *Chem. Rev.*, 1991, **91**, 165–195.