



Supporting Information

for

Thermodynamics and polarity-driven properties of fluorinated cyclopropanes

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Standard orientations and Gibbs free energies for the studied compounds

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Pages S2–S12. Standard Cartesian coordinates for the optimized geometries of the studied compounds and their corresponding standard Gibbs free energies (ΔG°), calculated at the B3LYP-GD3BJ/6-311++G(d,p) level of theory.

Methane

0 1

C 0.00000000 0.00000000 0.00000000

H 0.62966400 0.62966400 0.62966400

H -0.62966400 -0.62966400 0.62966400

H -0.62966400 0.62966400 -0.62966400

H 0.62966400 -0.62966400 -0.62966400

$G^0 = -40.508639$ hartrees

Fluoromethane

0 1

C 0.00000000 0.00000000 -0.63952800

H 0.00000000 1.03485900 -0.98850500

H -0.89621400 -0.51743000 -0.98850500

H 0.89621400 -0.51743000 -0.98850500

F 0.00000000 0.00000000 0.75585400

$G^0 = -139.775939$ hartrees

Cyclopropane

0 1

C 0.75411800 0.43539000 0.00000000

C 0.00000000 -0.87076200 0.00000000

C -0.75411000 0.43538200 0.00000000

H 1.26312600 0.72925200 0.90980600

H 1.26312600 0.72925200 -0.90980600

H -0.00002000 -1.45850500 0.90980400

H -0.00002000 -1.45850500 -0.90980400

H -1.26313200 0.72922100 -0.90980300

H -1.26313200 0.72922100 0.90980300

$G^0 = -117.882098$ hartrees

Fluorocyclopropane (**1**)

0 1

C 0.24692800 0.00000000 0.48053200
C -0.87739100 -0.76228800 -0.13149200
C -0.87739000 0.76228800 -0.13149300
H 0.40406100 0.00000000 1.55230000
H -1.55828000 -1.29308600 0.52275800
H -0.67332300 -1.24793100 -1.07756100
H -0.67332100 1.24793100 -1.07756100
H -1.55827800 1.29308800 0.52275700
F 1.45625200 0.00000000 -0.19422000
 $G^0 = -217.156923$ hartrees

1,1-Difluorocyclopropane (**1.1**)

0 1

C 0.00000300 0.17413500 0.00000000
C 0.77587800 -1.07856600 0.00000000
C -0.77588700 -1.07855600 0.00000000
H 1.27525500 -1.35971000 0.91828700
H 1.27525500 -1.35971000 -0.91828700
H -1.27526800 -1.35969300 -0.91828700
H -1.27526800 -1.35969300 0.91828700
F 0.00000300 0.96315100 -1.10650200
F 0.00000300 0.96315100 1.10650200
 $G^0 = -316.438503$ hartrees

cis-1,2-Difluorocyclopropane (**1.2cis**)

0 1

C -0.74846400 0.25019400 0.42642800

C -0.00007800 1.19722800 -0.47032600

C 0.74847100 0.25024400 0.42635200

H -0.00006200 2.25840000 -0.25267700

H -0.00017100 0.92914400 -1.52048900

H 1.29450800 0.60533100 1.29255800

F -1.38142500 -0.81024900 -0.17258600

F 1.38148900 -0.81019000 -0.17260000

H -1.29443000 0.60509000 1.29256100

$G^0 = -316.423836$ hartrees

trans-1,2-Difluorocyclopropane (**1.2trans**)

0 1

C 0.59911800 -0.09939500 -0.43630100

C -0.00000100 1.20962200 0.00000000

C -0.59911800 -0.09939500 0.43630200

H -0.51790200 1.78398100 -0.75847200

H 0.51789800 1.78398300 0.75847200

F 1.79933000 -0.48955100 0.11824100

H 0.50313900 -0.41051800 -1.46924300

H -0.50313700 -0.41051700 1.46924300

F -1.79932900 -0.48955200 -0.11824100

$G^0 = -316.428603$ hartrees

1,1,2-Trifluorocyclopropane (**1.1.2**)

0 1

C 0.53173000 0.02593400 0.03698700

C -0.18607400 -0.88368100 0.96767600

C -0.79910900 -0.48320500 -0.37536200

H -0.61782700 -0.41459800 1.84403600

H 0.16170600 -1.90273600 1.08350500

F 1.63176300 -0.41724200 -0.61970700

H -0.86427900 -1.21343300 -1.17334700

F -1.86083100 0.37863400 -0.35804600

F 0.67808000 1.32488300 0.36330900

$G^0 = -415.704493$ hartrees

All-*cis*-1,2,3-trifluorocyclopropane (**1.2.3ciscis**)

0 1

C 0.48174600 0.72777400 0.59736800

C -0.87128800 0.05340700 0.59725000

C 0.38928800 -0.78110300 0.59739100

H -1.50253100 0.09210400 1.47819500

H 0.67136500 -1.34735100 1.47828700

F 0.70788500 -1.41963200 -0.56241700

F 0.87591000 1.32260400 -0.56245400

F -1.58359300 0.09696400 -0.56255000

H 0.83086300 1.25535800 1.47825200

$G^0 = -415.682905$ hartrees

cis,trans,trans-1,2,3-Trifluorocyclopropane (**1.2.3cistrans**)

0 1

C 0.21119500 0.75722000 0.44411500
C -0.76528100 0.00001000 -0.39558600
C 0.21117900 -0.75721500 0.44411900
H -0.12334300 -1.25907800 1.34501900
F 1.20898900 -1.42848200 -0.20575600
F 1.20902700 1.42845500 -0.20575800
H -0.12331800 1.25909700 1.34501100
H -0.59336900 0.00000800 -1.46643600
F -2.09607500 0.00001400 -0.05287300
 $G^0 = -415.692053$ hartrees

1,1,2,2-Tetrafluorocyclopropane (**1.1.2.2**)

0 1

C 0.03579800 0.74370000 0.00000000
C 1.34914300 0.00000200 0.00000000
C 0.03580000 -0.74370000 0.00000000
F -0.34311600 -1.40934600 1.10649500
F -0.34311600 1.40934500 1.10649600
H 1.91386200 0.00000400 0.92500600
F -0.34311600 1.40934500 -1.10649600
F -0.34311600 -1.40934600 -1.10649500
H 1.91386200 0.00000400 -0.92500600
 $G^0 = -514.979693$ hartrees

cis-1,1,2,3-Tetrafluorocyclopropane (**1.1.2.3cis**)

0 1

C -0.69861800 0.00000000 0.02762700

C 0.40351700 -0.77000400 -0.62913100

C 0.40351600 0.77000300 -0.62913200

F -1.92691800 -0.00000100 -0.54083800

H 0.21411500 -1.28396800 -1.56538900

F -0.78125300 0.00000100 1.36271500

F 1.29415600 1.40720100 0.17320500

H 0.21411400 1.28396600 -1.56539100

F 1.29415700 -1.40720000 0.17320700

$G^0 = -514.962693$ hartrees

trans-1,1,2,3-Tetrafluorocyclopropane (**1.1.2.3trans**)

0 1

C 0.00000200 0.63889700 0.00000000

C -0.53444500 -0.65315000 0.53837800

C 0.53444000 -0.65315400 -0.53837700

F -0.75251600 1.39810900 -0.81538600

F 0.75252400 1.39810600 0.81538600

F 1.78994200 -1.07390700 -0.21391500

H 0.22640200 -0.91562700 -1.54548400

F -1.78994700 -1.07389800 0.21391400

H -0.22640600 -0.91562600 1.54548500

$G^0 = -514.967122$ hartrees

Pentafluorocyclopropane (1.1.2.2.3)

0 1

C -0.75152400 -0.26979000 0.07083900

C 0.75153300 -0.26977100 0.07083700

C -0.00000900 0.65316300 -0.87621900

F -1.42573700 -1.30776600 -0.45158800

F -1.38803000 0.25536900 1.12197000

F -0.00003100 1.98628400 -0.63678000

H -0.00000900 0.38432900 -1.92854100

F 1.42577000 -1.30773100 -0.45159100

F 1.38802800 0.25540600 1.12196600

$G^0 = -614.237180$ hartrees

Hexafluorocyclopropane (1.1.2.2.3.3)

0 1

C 0.44053600 -0.76302800 0.00000000

C -0.88110900 -0.00000700 0.00000000

C 0.44049500 0.76305900 0.00000000

F 0.81335100 -1.40868700 1.10782300

F 0.81335100 -1.40868700 -1.10782300

F 0.81335100 1.40870000 -1.10781100

F -1.62667700 -0.00002200 1.10781600

F -1.62667700 -0.00002200 -1.10781600

F 0.81335100 1.40870000 1.10781100

$G^0 = -713.506980$ hartrees

Bis-all-*cis*-1,2,3-trifluorocyclopropane

0 1 0 1 0 1

C(Fragment=2) -2.74761000 -0.85790700 -0.14971100

C(Fragment=2) -2.74663400 0.56099700 -0.66758100

C(Fragment=2) -2.74512200 0.30006800 0.82023100

H(Fragment=2) -3.62079700 -1.49025500 -0.25978300

H(Fragment=2) -3.61884800 0.97499800 -1.15977900

H(Fragment=2) -3.61609700 0.52172700 1.42577000

F(Fragment=2) -1.57461800 1.00927500 -1.20554600

F(Fragment=2) -1.57175400 0.53861500 1.47619600

F(Fragment=2) -1.57659700 -1.54892600 -0.27216800

C(Fragment=1) 1.54142000 -0.30317700 -0.81705000

C(Fragment=1) 1.54415400 0.86043300 0.14561100

C(Fragment=1) 1.54193800 -0.55511300 0.67197800

H(Fragment=1) 0.65810800 -0.52044900 -1.40446500

H(Fragment=1) 0.66299100 1.48085000 0.25079800

H(Fragment=1) 0.65908400 -0.95351400 1.15600200

F(Fragment=1) 2.70867300 1.56378300 0.26420800

F(Fragment=1) 2.70468800 -1.01318400 1.22252800

F(Fragment=1) 2.70368400 -0.55458200 -1.48848500

$G^0 = -831.359838$ hartrees

1.2.3ciscis–Na⁺

1 1 0 1 1 1

C(Fragment=1) -1.08821500 0.87050800 -0.00468900

C(Fragment=1) -1.08658400 -0.43013200 0.75882000

C(Fragment=1) -1.08953500 -0.44100600 -0.74945700

H(Fragment=1) -1.92232200 1.55926600 -0.00774900

H(Fragment=1) -1.91851500 -0.77051600 1.36058400

H(Fragment=1) -1.92378800 -0.79023800 -1.34288600

F(Fragment=1) 0.13807300 1.51590200 -0.01182200

F(Fragment=1) 0.13640800 -0.76736100 -1.30721300

F(Fragment=1) 0.14167300 -0.74841500 1.31650800

Na(Fragment=2) 1.96411300 0.00037600 -0.00138700

G⁰ = -577.823964 hartrees

1.2.3ciscis–Cl[−]

-1 1 0 1 -1 1

C(Fragment=1) 0.39521700 -0.58492500 -0.64525300

C(Fragment=1) 0.39640800 -0.26734600 0.82956400

C(Fragment=1) 0.39430700 0.85105600 -0.18290200

H(Fragment=1) -0.49798300 -0.99559800 -1.09750800

H(Fragment=1) -0.49556100 -0.45551600 1.41262900

H(Fragment=1) -0.49983200 1.44703800 -0.31071600

F(Fragment=1) 1.57699800 -1.06384700 -1.17621500

F(Fragment=1) 1.57519300 1.55130500 -0.33449700

F(Fragment=1) 1.57938000 -0.48546900 1.50853900

Cl(Fragment=2) -2.83566800 -0.00038500 0.00039400

G⁰ = -876.026513 hartrees

1.2.3ciscis–Na⁺–1.2.3ciscis

1 1 0 1 0 1 1 1

C(Fragment=1) 3.11230800 0.34094400 -0.78304200

C(Fragment=1) 3.10770200 0.46719100 0.72000600

C(Fragment=1) 3.06587000 -0.89686100 0.07761200

H(Fragment=1) 3.95547500 0.82896000 1.28629700

H(Fragment=1) 3.88212400 -1.60414500 0.13950900

F(Fragment=1) 1.82627100 -1.50442900 0.12486000

F(Fragment=1) 1.90629800 0.65887800 -1.37816900

F(Fragment=1) 1.89824400 0.87928900 1.24637500

H(Fragment=1) 3.96370400 0.60356800 -1.39658400

C(Fragment=2) -3.10584800 0.45908500 0.72732800

C(Fragment=2) -3.06242400 -0.90020900 0.07496600

C(Fragment=2) -3.11729300 0.34358300 -0.77651100

H(Fragment=2) -3.95243500 0.81357500 1.29993300

H(Fragment=2) -3.87523900 -1.61145700 0.13605200

H(Fragment=2) -3.97329000 0.60745000 -1.38309000

F(Fragment=2) -1.89557300 0.87189700 1.25132300

F(Fragment=2) -1.91598400 0.66985300 -1.37587900

F(Fragment=2) -1.81995100 -1.50354900 0.11145600

Na(Fragment=3) 0.00036600 0.07565500 -0.01308800

G⁰ = -993.531128 hartrees

1.2.3ciscis-Cl⁻-1.2.3ciscis

-1 1 0 1 0 1 -1 1

C(Fragment=1) 3.24887600 -0.68483600 -0.53832100

C(Fragment=1) 3.26082800 -0.12303300 0.86194400

C(Fragment=1) 3.28124200 0.80847900 -0.32483000

H(Fragment=1) 2.36876600 -0.19067900 1.47028800

H(Fragment=1) 2.40368900 1.39827900 -0.55391000

F(Fragment=1) 4.47372300 1.44589900 -0.59066400

F(Fragment=1) 4.41430600 -1.27282300 -0.97955800

F(Fragment=1) 4.43645000 -0.24948100 1.56964800

H(Fragment=1) 2.34819000 -1.14858800 -0.91811300

C(Fragment=2) -3.26190000 -0.08935600 0.86628900

C(Fragment=2) -3.28138200 0.79555900 -0.35558600

C(Fragment=2) -3.24805600 -0.70478200 -0.51126100

H(Fragment=2) -2.37065700 -0.13269900 1.47806700

H(Fragment=2) -2.40331700 1.37565300 -0.60609500

H(Fragment=2) -2.34703300 -1.18270000 -0.87217000

F(Fragment=2) -4.43833800 -0.18967900 1.57676100

F(Fragment=2) -4.41308600 -1.30962400 -0.93046500

F(Fragment=2) -4.47334600 1.42219500 -0.64762300

Cl(Fragment=3) 0.00031300 0.07353900 0.00174300

$G^0 = -1291.728312$ hartrees

Na⁺

$G^0 = -162.101996$ hartrees

Cl⁻

$G^0 = -460.318750$ hartrees