Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Palladium-catalysed Directed C-H Activation by Anilides and Ureas; Water Participation in a General Base Mechanism

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Variation of functional for the 7 –> 8 TS step

Substrate	Functional	GS Hartrees	TS Hartrees	Delta G (kcal/mol)a
Amide 3a	M06-2x	-1614.825928	-1614.812134	-8.66
Urea 3e	M06-2x	-1709.416016	-1709.401123	-9.35
4-MeAmide 3c	M06-2x	-1654.099854	-1654.084839	-9.42
Amide 3a	wB97xD	-1615.091064	-1615.081421	-6.05
Urea 3e	wB97xD	-1709.696655	-1709.682617	-8.81
4-MeAmide 3c	wB97xD	-1654.379395	-1654.367310	-7.58
Amide 3a	B3LYP	-1615.460938	-1615.449585	-7.12

[a]Difference in free energy between complex 7 and the 7–>8 transition state.

Summary of free energies for Fig 1 in kcal mol^{-1}

A	Anilide 3a	4-Cl AA 3b	4-Me AA 3c	4-F AA 3d	Urea 3e
3	0.0000	-0.10000	0.0000	0.0000	0.0000
4	-0.52000	0.75600	-3.1400	-2.1450	-5.3600
8	5.6800	8.4100	4.2200	4.3900	1.1770
TS	14.324	18.537	13.635	14.860	10.494
9					
	-5.8200	-5.8200	-7.6500	-7.3500	-8.5790

H_2O - M06-2x

Zero-point correction= 0.021629 (Hartree/Particle)
Thermal correction to Energy= 0.024465
Thermal correction to Enthalpy= 0.025409
Thermal correction to Gibbs Free Energy= 0.003979
Sum of electronic and zero-point Energies= -76.369263
Sum of electronic and thermal Energies= -76.366428
Sum of electronic and thermal Enthalpies= -76.365484
Sum of electronic and thermal Free Energies= -76.386914

rm062x

Water

0 1

O	0.00000000	0.00000000	0.11887400
H	0.00000000	0.75785900	-0.47549700
H	0.00000000	-0.75785900	-0.47549700

H_3O^+ M06-2x

- Zero-point correction= 0.035148 (Hartree/Particle)
- Thermal correction to Energy= 0.038033
- Thermal correction to Enthalpy= 0.038977
- Thermal correction to Gibbs Free Energy= 0.017058
- Sum of electronic and zero-point Energies= -76.752791
- Sum of electronic and thermal Energies= -76.749906
- Sum of electronic and thermal Enthalpies= -76.748962
- Sum of electronic and thermal Free Energies= -76.770881

- rm062x

- H3OM06

- 1 1
- H 0.00000000 0.93135100 -0.21783900
- H -0.80657300 -0.46567500 -0.21783900
- H 0.80657300 -0.46567500 -0.21783900
- O 0.00000000 0.00000000 0.08168900

Acetanilide **3a**

- Zero-point correction= 0.156612 (Hartree/Particle)
- Thermal correction to Energy= 0.165793
- Thermal correction to Enthalpy= 0.166737
- Thermal correction to Gibbs Free Energy= 0.120301
- Sum of electronic and zero-point Energies= -439.936545
- Sum of electronic and thermal Energies= -439.927364
- Sum of electronic and thermal Enthalpies= -439.926419
- Sum of electronic and thermal Free Energies= -439.972855

- rm062x

- Amide
- 0 1
- C -2.16761700 0.16674100 -0.00704300
- O -2.11217100 1.38707600 0.01418200
- N -1.06541400 -0.64616000 -0.03005200
- H -1.24815800 -1.64032200 -0.04092700
- C 0.29549500 -0.28698700 -0.01376500
- C 0.74629900 1.03867400 -0.01527300
- C 1.22935000 -1.33155900 0.00054300
- C 2.11616500 1.29361200 -0.00161400
- H 0.03213300 1.84835400 -0.02688900
- C 2.59095400 -1.05919200 0.01348900
- H 0.88103700 -2.36092600 0.00191200
- C 3.04552300 0.25828300 0.01276800
- H 2.45520600 2.32494300 -0.00293900
- H 3.29734900 -1.88303200 0.02464100
- H 4.10872400 0.47257100 0.02296300
- C -3.48146500 -0.58543200 0.01534100
- H -3.49202000 -1.39797700 -0.71450300
- H -3.64114800 -1.01672100 1.00750300
- H -4.28608500 0.11478200 -0.20153100

Acetanilide (3a) H^+ *syn*

- Zero-point correction= 0.170106 (Hartree/Particle)
- Thermal correction to Energy= 0.178401
- Thermal correction to Enthalpy= 0.179345
- Thermal correction to Gibbs Free Energy= 0.136443
- Sum of electronic and zero-point Energies= -440.346103
- Sum of electronic and thermal Energies= -440.337808
- Sum of electronic and thermal Enthalpies= -440.336864
- Sum of electronic and thermal Free Energies= -440.379766

- rm062x

- UreaHsyn

- 1 1
- C -2.06264900 0.03355000 -0.09617300
- O -1.82667500 0.76677400 -1.14087900
- N -1.09592900 -0.44758000 0.63669900
- H -1.35168200 -1.02716600 1.43105500
- C 0.30337500 -0.23254000 0.35870800
- C 0.84807700 1.03625300 0.54642900
- C 1.06726600 -1.30462400 -0.09440000
- C 2.19735000 1.23136800 0.26073300
- H 0.23099700 1.84627000 0.92287200
- C 2.41528600 -1.09559400 -0.36327100
- H 0.60854600 -2.27772500 -0.23209400
- C 2.97691400 0.16918000 -0.18973500
- H 2.63677100 2.21246900 0.40030700
- H 3.02516400 -1.92049600 -0.71390500
- H 4.02802500 0.32643700 -0.40558600
- C -3.49157200 -0.21620100 0.20774800
- H -3.61041300 -0.90391500 1.04214400
- H -3.96673500 0.73992300 0.43935900
- H -3.96645000 -0.62298300 -0.68696900
- H -0.87359800 0.89770900 -1.30727700

AmideHanti^{+}

- Zero-point correction= 0.170641 (Hartree/Particle)
- Thermal correction to Energy= 0.179564
- Thermal correction to Enthalpy= 0.180508
- Thermal correction to Gibbs Free Energy= 0.136244
- Sum of electronic and zero-point Energies= -440.345710
- Sum of electronic and thermal Energies= -440.336787
- Sum of electronic and thermal Enthalpies= -440.335843
- Sum of electronic and thermal Free Energies= -440.380107

- rm062x

- UreaHanti

- 1 1
- C -2.08565000 0.02727100 -0.05636500
- O -1.85571500 1.13602300 -0.69791800
- N -1.05231000 -0.64321100 0.36745900
- H -1.25000800 -1.52111000 0.83748200
- C 0.33341700 -0.30187000 0.19479300
- C 0.78359300 0.99421200 0.42961500
- C 1.20430300 -1.32410800 -0.17143900
- C 2.13837400 1.26789600 0.27127600
- H 0.09424400 1.77120200 0.73730800
- C 2.55672400 -1.03524900 -0.31989600
- H 0.82649700 -2.32673300 -0.34374900
- C 3.02327100 0.25930300 -0.10334700
- H 2.50191400 2.27370300 0.45011900
- H 3.24270400 -1.82418400 -0.60732700
- H 4.07825500 0.48107700 -0.22200400
- C -3.47507000 -0.44678000 0.17127400
- H -3.49592400 -1.37682700 0.73535200
- H -4.02705600 0.32362300 0.71571800
- H -3.95656900 -0.59643300 -0.79860500
- H -2.67592800 1.56593500 -0.98862400

4-chloroacetanilide **3b**

- Zero-point correction= 0.147063 (Hartree/Particle)
- Thermal correction to Energy= 0.156552
- Thermal correction to Enthalpy= 0.157497
- Thermal correction to Gibbs Free Energy= 0.110817
- Sum of electronic and zero-point Energies= -899.515472
- Sum of electronic and thermal Energies= -899.505983
- Sum of electronic and thermal Enthalpies= -899.505038
- Sum of electronic and thermal Free Energies= -899.551718

- rm062x

- Amide4Cl

- 0 1
- C 3.02508900 -0.25679100 -0.00500300
- O 2.88329500 -1.46938100 -0.00341300
- N 1.97831400 0.63002800 -0.01454600
- C 0.60020300 0.36001700 -0.00912200
- C 0.06163200 -0.93255700 -0.00750700
- C -0.26534300 1.46204200 -0.00595900
- C -1.31945400 -1.10608500 -0.00222800
- H 0.71698300 -1.79007100 -0.01015100
- C -1.64155700 1.28809200 -0.00085900
- H 0.14266500 2.46856300 -0.00728400
- C -2.16047000 -0.00176000 0.00108100
- H -2.30302200 2.14686000 0.00167100
- C 4.38495100 0.40664600 0.01944400
- H 4.47647600 1.14829900 -0.77758700
- H 4.53483900 0.91512700 0.97571500
- H 5.14780000 -0.35947700 -0.10409200
- H 2.22634600 1.61026100 -0.01391400
- H -1.73718700 -2.10679600 -0.00082500
- Cl -3.89586900 -0.23562000 0.00744200

4-methylacetanilide **3c**

- Zero-point correction= 0.184328 (Hartree/Particle)
- Thermal correction to Energy= 0.194431
- Thermal correction to Enthalpy= 0.195375
- Thermal correction to Gibbs Free Energy= 0.147669
- Sum of electronic and zero-point Energies= -479.207301
- Sum of electronic and thermal Energies= -479.197197
- Sum of electronic and thermal Enthalpies= -479.196253
- Sum of electronic and thermal Free Energies= -479.243960

- Rm062x
- Amide4Me

- 0 1
- C 2.63818200 -0.22751700 -0.00155500
- O 2.52763700 -1.44465200 0.01395300
- N 1.57454300 0.63322000 -0.02753500
- C 0.19764100 0.33557100 -0.01776900
- C -0.32009700 -0.96401900 -0.02582900
- C -0.68929100 1.41917100 -0.00714100
- C -1.70060800 -1.15068500 -0.01958800
- H 0.35036500 -1.81009000 -0.03986400
- C -2.06099100 1.20912900 -0.00141600
- H -0.29817500 2.43320300 -0.00688800
- C -2.59684000 -0.08182000 -0.00409100
- H -2.72773900 2.06729600 0.00355500
- C 3.98454700 0.46546600 0.02798600
- H 4.05082100 1.24175200 -0.73782700
- H 4.13764400 0.93615100 1.00305800
- H 4.76207700 -0.27835500 -0.13553600
- H 1.80082800 1.61852400 -0.03255400
- H -2.08736200 -2.16666600 -0.02947000
- C -4.08644500 -0.30805900 0.03417400
- H -4.35247300 -1.26253300 -0.42633300
- H -4.45487500 -0.32562600 1.06534500
- H -4.62059400 0.48760600 -0.49098300

4-fluoroacetanilide **3d**

- Zero-point correction= 0.148280 (Hartree/Particle)
- Thermal correction to Energy= 0.157431
- Thermal correction to Enthalpy= 0.158375
- Thermal correction to Gibbs Free Energy= 0.112594
- Sum of electronic and zero-point Energies= -539.148668
- Sum of electronic and thermal Energies= -539.139517
- Sum of electronic and thermal Enthalpies= -539.138573
- Sum of electronic and thermal Free Energies= -539.184354

- rm062x

- Amide4F

- 0 1
- C 2.59530800 -0.21650000 -0.00612200
- O 2.48747300 -1.43367200 0.00036900
- N 1.52763200 0.64075500 -0.02060000
- C 0.15336900 0.33417200 -0.01180800
- C -0.34948600 -0.97286900 -0.01061200
- C -0.73987800 1.41357200 -0.00548900
- C -1.72605100 -1.18430800 -0.00202800
- H 0.33116000 -1.81051500 -0.01587600
- C -2.11208200 1.20375200 0.00277100
- H -0.35628400 2.42969100 -0.00660300
- C -2.58489800 -0.09921400 0.00465100
- H -2.80931800 2.03355500 0.00812700
- C 3.93871500 0.48108500 0.02079500
- H 4.00335000 1.24962200 -0.75297000
- H 4.08796700 0.96224100 0.99126900
- H 4.71879700 -0.26179000 -0.13426600
- H 1.74930500 1.62703300 -0.02187700
- H -2.13323200 -2.18920300 -0.00067600
- F -3.91499200 -0.31274200 0.01346400

N,N-Dimethyl-N'-phenylurea **3e**

- Zero-point correction= 0.202822 (Hartree/Particle)
- Thermal correction to Energy= 0.214588
- Thermal correction to Enthalpy= 0.215533
- Thermal correction to Gibbs Free Energy= 0.164026
- Sum of electronic and zero-point Energies= -534.517005
- Sum of electronic and thermal Energies= -534.505238
- Sum of electronic and thermal Enthalpies= -534.504294
- Sum of electronic and thermal Free Energies= -534.555801

- rm062x

- Urea

- 0 1
- C 1.38832500 -0.39767600 0.07117400
- O 1.17763600 -1.58204200 0.32246900
- N 0.36489600 0.51975500 -0.11422700
- H 0.59700800 1.49887600 -0.03837100
- C -1.01085500 0.23630200 -0.04971300
- C -1.54855900 -1.01850900 -0.36002500
- C -1.87357200 1.28668500 0.28689800
- C -2.92743300 -1.20453700 -0.31508200
- H -0.88913200 -1.83215700 -0.62550800
- C -3.24870500 1.08849400 0.31820800
- H -1.45890000 2.26220000 0.52684100
- C -3.78675900 -0.16159900 0.02150900
- H -3.33203700 -2.18315600 -0.55493100
- H -3.89870600 1.91675000 0.58174200
- H -4.85934900 -0.32011000 0.05070700
- N 2.64489600 0.12356700 -0.06643600
- C 3.79046200 -0.68662400 0.30847700
- H 3.44223200 -1.67837600 0.58626300
- H 4.48714000 -0.76939600 -0.53142000
- H 4.31754700 -0.23593600 1.15641800
- C 2.90491500 1.50664500 -0.42634200
- H 2.75532300 2.19630300 0.41445400
- H 3.94467000 1.58687500 -0.74587100
- H 2.27766300 1.81612600 -1.26607200

Urea (**3e**) H^+ *syn*

- Zero-point correction= 0.216008 (Hartree/Particle)
- Thermal correction to Energy= 0.228038
- Thermal correction to Enthalpy= 0.228982
- Thermal correction to Gibbs Free Energy= 0.176690
- Sum of electronic and zero-point Energies= -534.935599
- Sum of electronic and thermal Energies= -534.923569
- Sum of electronic and thermal Enthalpies= -534.922625
- Sum of electronic and thermal Free Energies= -534.974917

- rm062x

- UreaHsyn

- 1 1
- H -1.40840200 2.04539800 -1.08573100
- C -1.83794800 1.18424100 -0.58475600
- C -2.89789600 -1.06455400 0.69110100
- C -1.01943800 0.33690100 0.15972800
- C -3.19717900 0.90519600 -0.67330800
- C -3.72597900 -0.22123400 -0.04440800
- C -1.53925400 -0.78170100 0.81120000
- H -3.84134900 1.56267200 -1.24660600
- H -4.78524600 -0.43904000 -0.12606200
- H -3.30786100 -1.93613900 1.18909900
- N 0.37793900 0.63626500 0.26672800
- H 0.63923800 1.57463600 0.54105800
- C 1.34286900 -0.20007400 -0.13123800
- H -0.89275100 -1.40780800 1.41873000
- O 1.03909000 -1.35074600 -0.68856600
- H 0.08549300 -1.42465500 -0.86645100
- N 2.61832400 0.07905400 0.02937400
- C 3.67678900 -0.79183500 -0.48991400
- H 4.25964900 -1.18061200 0.34698600
- H 4.32151300 -0.20352800 -1.14451200
- H 3.24277600 -1.61530000 -1.04897900
- C 3.02530600 1.30197600 0.72204400
- H 4.10109100 1.25494200 0.87632300
- H 2.53835900 1.36764500 1.69775000
- H 2.79730400 2.18703900 0.12152000

Urea (**3e**) H^+*anti*

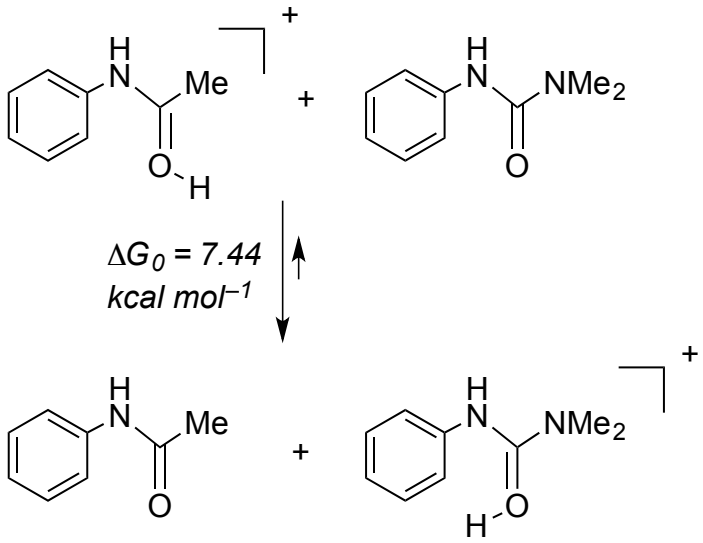
- Zero-point correction= 0.216083 (Hartree/Particle)
- Thermal correction to Energy= 0.227983
- Thermal correction to Enthalpy= 0.228927
- Thermal correction to Gibbs Free Energy= 0.177615
- Sum of electronic and zero-point Energies= -534.931353
- Sum of electronic and thermal Energies= -534.919453
- Sum of electronic and thermal Enthalpies= -534.918509
- Sum of electronic and thermal Free Energies= -534.969821

- rm062x

- UreaHanti

- 1 1
- H -1.49526500 2.08245000 -1.04842300
- C -1.89556400 1.19529600 -0.56789200
- C -2.88894900 -1.10225200 0.65809700
- C -1.03760300 0.30677800 0.07403400
- C -3.26137100 0.92880300 -0.58740400
- C -3.75941500 -0.22157900 0.01857100
- C -1.52400000 -0.83866200 0.70019900
- H -3.93325200 1.62044400 -1.08387800
- H -4.82342600 -0.43046000 -0.00333900
- H -3.27311100 -1.99533800 1.13897800
- N 0.35493100 0.63347000 0.11912100
- H 0.58983800 1.61143200 0.23000500
- C 1.35383100 -0.20892000 -0.13952600
- H -0.84471200 -1.51022600 1.21322600
- O 1.00699500 -1.37760300 -0.63260800
- H 1.70367800 -2.04594500 -0.54967100
- N 2.61659100 0.11640800 0.06467500
- C 3.70834700 -0.69225200 -0.48914100
- H 4.03652400 -1.44717900 0.22955600
- H 4.53875600 -0.02362400 -0.71080300
- H 3.40125000 -1.15938500 -1.42574000
- C 2.97414200 1.33163100 0.80030300
- H 3.95195100 1.17380300 1.25231300
- H 2.25280400 1.50888600 1.59880100
- H 3.02185200 2.19376100 0.12980900

Isodesmic proton transfer between **3a** and **3e (DFT)**



Isodesmic reaction for proton transfer;
more stable isomers of protonated states

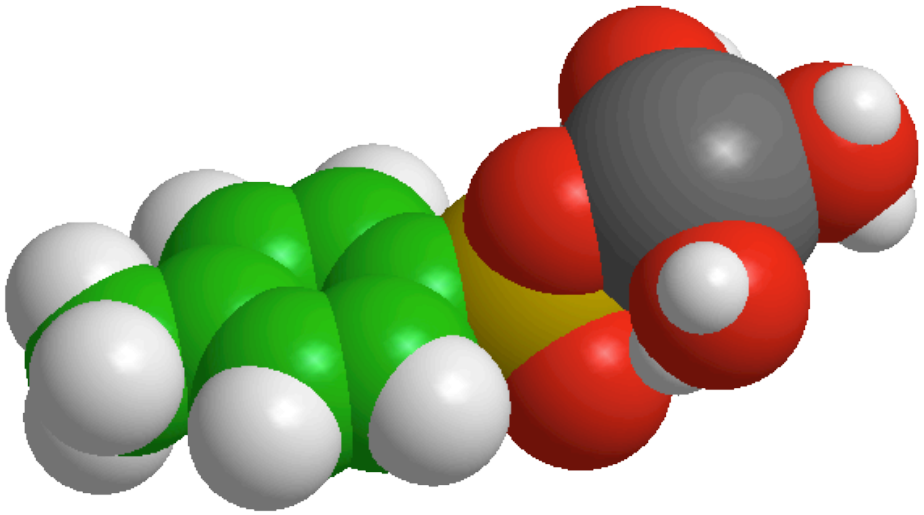
- Structures and DFT energies for the species in Scheme 3,4

AUPRECF (4)

Zero-point correction= 0.213778 (Hartree/Particle)
Thermal correction to Energy= 0.232020
Thermal correction to Enthalpy= 0.232964
Thermal correction to Gibbs Free Energy= 0.167068
Sum of electronic and zero-point Energies= -1251.202300
Sum of electronic and thermal Energies= -1251.184059
Sum of electronic and thermal Enthalpies= -1251.183114
Sum of electronic and thermal Free Energies= -1251.249010

1 1

O	-4.41340000	0.12360000	-0.01570000
Pd	-2.34810000	-0.00270000	-0.36480000
O	-0.35930000	-0.03930000	-0.69400000
O	-2.16170000	2.08090000	-0.31560000
H	-1.40160000	2.21860000	0.28820000
H	-2.93000000	2.52340000	0.07630000
S	0.35300000	-0.01130000	0.68510000
O	0.01280000	1.24890000	1.36410000
O	0.02880000	-1.25610000	1.40220000
C	2.06530000	-0.00470000	0.28050000
C	2.71010000	-1.21740000	0.04770000
C	2.73550000	1.21310000	0.20000000
C	4.06090000	-1.19910000	-0.27460000
H	2.16610000	-2.15220000	0.13160000
C	4.08690000	1.20690000	-0.12210000
H	2.20940000	2.14030000	0.39960000
C	4.76630000	0.00700000	-0.36050000
H	4.62530000	2.14760000	-0.18450000
H	4.57900000	-2.13570000	-0.45680000
C	6.23910000	0.01170000	-0.66830000
H	6.52940000	0.92360000	-1.19390000
H	6.81850000	-0.03540000	0.25940000
H	6.51840000	-0.84990000	-1.27780000
O	-2.28450000	-2.06810000	-0.03970000
H	-1.47540000	-2.17990000	0.50460000
H	-2.16570000	-2.59030000	-0.84720000
H	-4.95280000	-0.06490000	-0.79840000
H	-4.72410000	-0.46320000	0.69030000

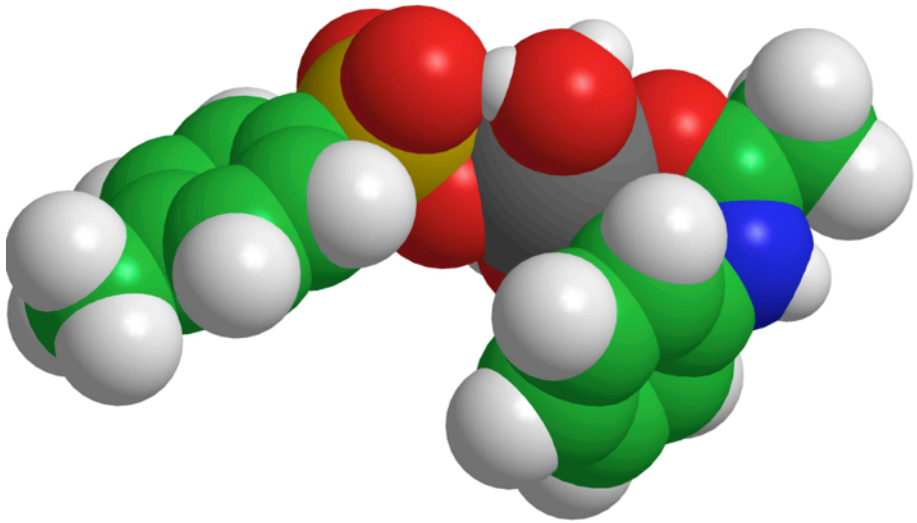


ARCOTF (**5a**)

- Zero-point correction= 0.346059 (Hartree/Particle)
- Thermal correction to Energy= 0.372275
- Thermal correction to Enthalpy= 0.373220
- Thermal correction to Gibbs Free Energy= 0.287712
- Sum of electronic and zero-point Energies= -1614.777451
- Sum of electronic and thermal Energies= -1614.751235
- Sum of electronic and thermal Enthalpies= -1614.750291
- Sum of electronic and thermal Free Energies= -1614.835799

- ARCOTF

- 1 1
- H -2.67060900 0.99489200 2.11808300
- C -2.44214400 1.65221700 1.28444800
- C -3.25653200 1.64611900 0.15326700
- C -1.33669700 2.50135200 1.32252400
- C -1.06433900 3.34515200 0.24796400
- H -0.69317800 2.50176200 2.19545100
- N -4.36952800 0.74968600 0.08722500
- H -5.29691800 1.15531300 0.04538700
- C -4.28792700 -0.57832100 0.04320900
- O -3.21090000 -1.22774200 0.01926700
- Pd -1.22168100 -0.73449400 -0.15002400
- H -0.20372600 4.00402000 0.28089400
- C -3.01028400 2.50680000 -0.91717000
- O 0.76415200 -0.31846600 -0.33249000
- O -0.98573800 -1.48265000 1.76599100
- H -0.02650900 -1.75979000 1.82230200
- H -1.54098000 -2.26328300 1.91044700
- C -1.90680100 3.35789900 -0.86487900
- H -1.70841900 4.03036200 -1.69238400
- S 1.79352000 -1.42140000 -0.00841700
- O 1.54392400 -1.91470900 1.36824100
- O 1.84033100 -2.44290200 -1.04890300
- C 3.31185100 -0.52290000 0.00537200
- C 4.21303000 -0.69059200 -1.03955800
- C 3.56272700 0.35741600 1.05676900
- C 5.39327200 0.04653100 -1.02686100
- H 3.99128500 -1.38748200 -1.84035500
- C 4.74459800 1.08434200 1.04891000
- H 2.84720700 0.46486300 1.86567100
- C 5.67409100 0.93990600 0.01041300
- H 4.95326900 1.77558000 1.85996200
- H 6.10722500 -0.07463500 -1.83581700
- C 6.96416300 1.71487700 0.03090000
- H 6.82240800 2.70281100 0.47446600
- H 7.71442300 1.18852200 0.62968800
- H 7.36844500 1.83757000 -0.97569800
- O -1.45714000 0.06238400 -2.07553400
- H -0.65204000 -0.09758700 -2.59290800
- H -1.56687800 1.02801600 -2.01970000
- H -3.67455800 2.50183700 -1.77623200
- C -5.56605400 -1.36114100 0.02829600
- H -6.44760600 -0.72211400 0.02142400
- H -5.56564700 -2.00437600 -0.85306000
- H -5.58422300 -2.00018800 0.91337200

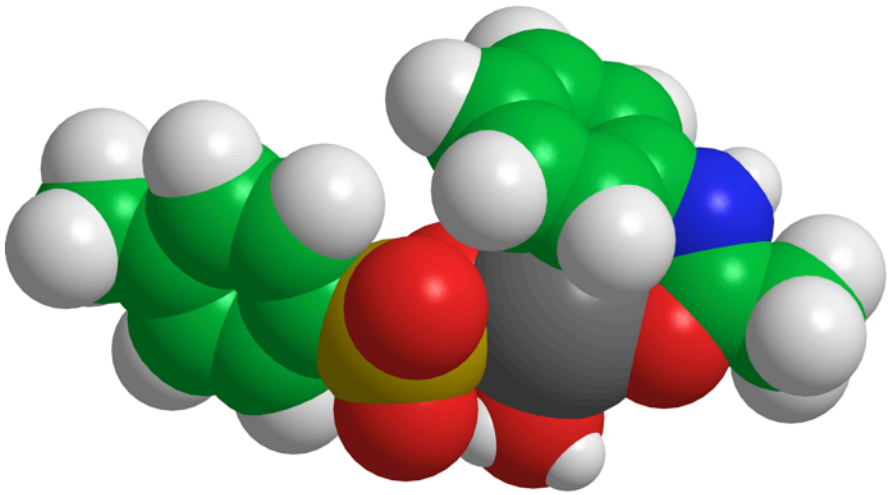


AWCOTS (**6a**)

- Zero-point correction= 0.320599 (Hartree/Particle)
- Thermal correction to Energy= 0.344212
- Thermal correction to Enthalpy= 0.345156
- Thermal correction to Gibbs Free Energy= 0.266012
- Sum of electronic and zero-point Energies= -1538.382273
- Sum of electronic and thermal Energies= -1538.358660
- Sum of electronic and thermal Enthalpies= -1538.357716
- Sum of electronic and thermal Free Energies= -1538.436860
- rm062x

- AWCOTS

- 1 1
- H 2.94210900 2.85539900 -1.89710300
- C 2.35599900 2.60123100 -1.02110400
- C 2.82864800 1.65065600 -0.11998500
- C 1.12864400 3.21080800 -0.77547800
- C 0.36132300 2.87098300 0.34278100
- H 0.75914700 3.95179000 -1.47596600
- N 4.11334400 1.06698100 -0.32037800
- H 4.87994900 1.69096800 -0.54441200
- C 4.36924400 -0.23832600 -0.22979700
- O 3.45842800 -1.09333800 -0.06297900
- Pd 1.47344900 -0.63614100 -0.10652200
- H -0.59814200 3.34746300 0.50681000
- C 2.07836200 1.30512100 1.02970400
- O -0.50312000 -0.23480300 -0.31068400
- O 1.02698400 -2.58025300 -0.83425000
- H 0.14704300 -2.79756700 -0.44187400
- H 1.66267400 -3.24551100 -0.53321200
- C 0.83272500 1.93009400 1.24462700
- H 0.25211100 1.65401000 2.11767800
- S -1.42914500 -0.96655700 0.69015200
- O -1.34790500 -2.42160000 0.44063700
- O -1.15916100 -0.53563000 2.06108300
- C -3.03297300 -0.40531100 0.21920800
- C -3.48596000 0.81384300 0.71883100
- C -3.80884300 -1.18057100 -0.63686700
- C -4.74819600 1.25777300 0.34712400
- H -2.86411700 1.39298500 1.39413600
- C -5.07067800 -0.71925100 -0.99339700
- H -3.43265600 -2.12980100 -1.00228300
- C -5.55759500 0.49853100 -0.50645100
- H -5.69047000 -1.31658200 -1.65523000
- H -5.11683900 2.20452000 0.73016700
- C -6.94256300 0.96703600 -0.86324400
- H -7.23623500 0.61567300 -1.85444100
- H -7.67020100 0.57682900 -0.14431700
- H -7.00903800 2.05669400 -0.84261200
- H 2.54284200 0.72866500 1.82741600
- C 5.78358700 -0.70804300 -0.32654800
- H 5.82206300 -1.55554500 -1.01127300
- H 6.45682400 0.07884000 -0.66283600
- H 6.09501500 -1.05274600 0.66267800



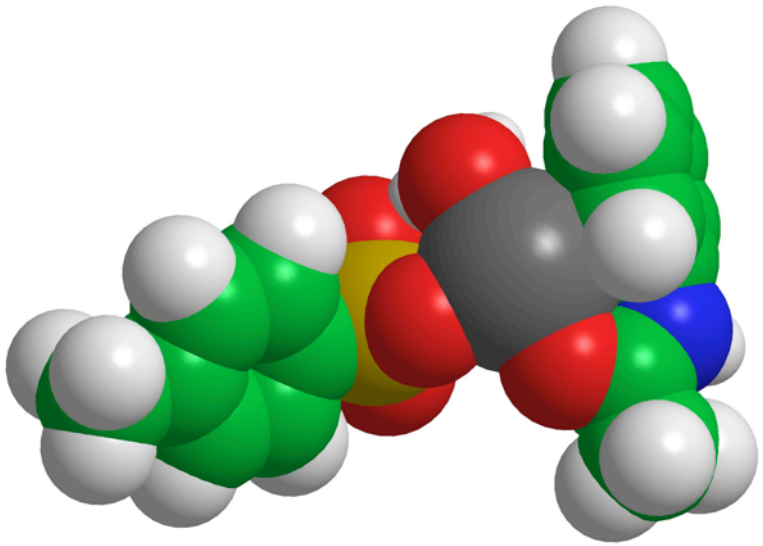
AWTOTF2 (6b)

- Zero-point correction= 0.319172 (Hartree/Particle)
- Thermal correction to Energy= 0.341942
- Thermal correction to Enthalpy= 0.342886
- Thermal correction to Gibbs Free Energy= 0.265120
- Sum of electronic and zero-point Energies= -1538.381163
- Sum of electronic and thermal Energies= -1538.358393
- Sum of electronic and thermal Enthalpies= -1538.357449
- Sum of electronic and thermal Free Energies= -1538.435214
- m062x

- AWTOTF2

- 1 1

H	4.27479600	0.11115100	2.19257800
C	4.09299000	-0.42661700	1.26865300
C	3.71160900	0.27553500	0.12266600
C	4.23398000	-1.80664500	1.19721600
C	3.99113500	-2.49703200	0.00145100
H	4.53115200	-2.35588500	2.08369100
N	3.65382800	1.70066000	0.15916600
H	4.45746900	2.19038300	0.53599800
C	2.62032600	2.41828900	-0.28042800
O	1.54479500	1.88147800	-0.65953200
Pd	1.20105400	-0.10710500	-0.47544600
H	4.11452100	-3.57348200	-0.03608000
C	3.47481200	-0.39811400	-1.09604600
O	-0.82026800	0.31990700	-0.28923500
O	0.70546500	-2.09712000	-0.27470900
H	-0.08856600	-2.06801600	0.35499100
H	1.40262000	-2.63239300	0.13480400
C	3.62002900	-1.79965400	-1.13859700
H	3.45442700	-2.31652700	-2.07742800
S	-1.59128600	-0.12678700	0.96009000
O	-1.25851100	-1.55117500	1.24247300
O	-1.41611200	0.78424400	2.08450400
C	-3.27131900	-0.07151800	0.41906300
C	-4.10341800	0.93938000	0.88434900
C	-3.72023300	-1.03246500	-0.48642600
C	-5.41754800	0.98598600	0.42760400
H	-3.72569200	1.66917900	1.59191200
C	-5.03265800	-0.96686500	-0.93055400
H	-3.05470200	-1.81859200	-0.82900200
C	-5.89808700	0.03996100	-0.48111900
H	-5.39722100	-1.70736600	-1.63637500
H	-6.07904800	1.77001500	0.78319300
C	-7.32593900	0.07735000	-0.95586400
H	-7.39153300	-0.16634200	-2.01892600
H	-7.92701100	-0.65908500	-0.41300000
H	-7.77271900	1.05998200	-0.79435700
H	3.35977200	0.16594500	-2.01861900
C	2.72940300	3.90663600	-0.32443900
H	1.89261400	4.33121000	0.23213300
H	3.67310400	4.26556500	0.08272800
H	2.63789600	4.22102100	-1.36649700

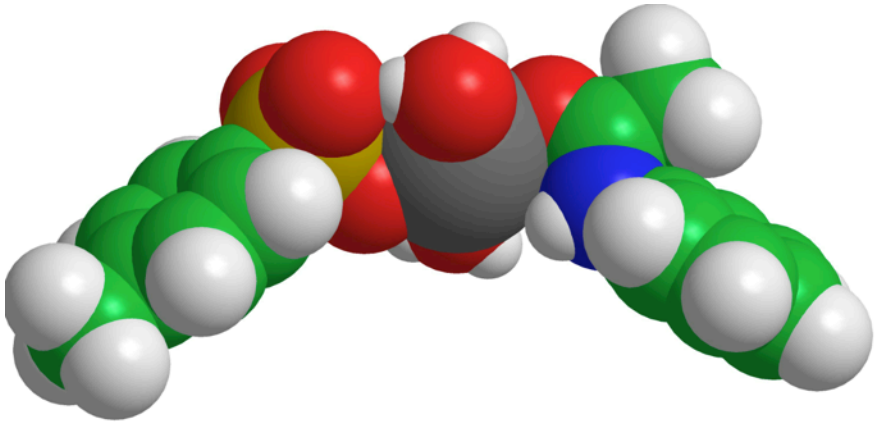


ARCOTFiso (**6c**)

- Zero-point correction= 0.347262 (Hartree/Particle)
- Thermal correction to Energy= 0.373342
- Thermal correction to Enthalpy= 0.374286
- Thermal correction to Gibbs Free Energy= 0.288191
- Sum of electronic and zero-point Energies= -1614.770252
- Sum of electronic and thermal Energies= -1614.744173
- Sum of electronic and thermal Enthalpies= -1614.743228
- Sum of electronic and thermal Free Energies= -1614.829323
- rm062x

- ARCOTFiso

- 1 1
- H 5.35286000 0.09106600 1.79261300
- C 5.49584200 0.86644000 1.04686300
- C 4.54940100 1.05057200 0.04163100
- C 6.61235900 1.69685500 1.08754600
- C 6.76493600 2.71301700 0.14673600
- H 7.35601300 1.55519500 1.86400000
- N 3.37837500 0.22473100 -0.00892200
- H 2.48734200 0.71270200 0.02666400
- C 3.35221900 -1.09931200 -0.13099800
- O 2.27430900 -1.76007100 -0.11653200
- Pd 0.37113100 -1.05940700 0.10009000
- H 7.63260700 3.36249400 0.18712800
- C 4.69091600 2.06316200 -0.90394700
- O -1.51811500 -0.35454200 0.39069000
- O 0.18322200 -0.93183100 -1.96084400
- H -0.80255000 -1.00238000 -2.11851500
- H 0.61692600 -1.67323600 -2.40842100
- C 5.80212300 2.89842600 -0.84376400
- H 5.91798800 3.68927000 -1.57660000
- S -2.70956500 -1.01457800 -0.33665500
- O -2.40191100 -1.07920400 -1.78647500
- O -3.09610600 -2.27400700 0.28810800
- C -3.99501400 0.17183900 -0.10984100
- C -4.98437600 -0.06866900 0.83671600
- C -3.97581700 1.33987200 -0.87066100
- C -5.97572300 0.88999600 1.02351400
- H -4.97684900 -0.99028800 1.40819800
- C -4.97308800 2.28320400 -0.66791300
- H -3.20000600 1.49810600 -1.61270600
- C -5.98414000 2.07282500 0.27934400
- H -4.97147400 3.19778300 -1.25327300
- H -6.75449800 0.71578500 1.75965600
- C -7.07308100 3.09466000 0.46820300
- H -6.67773600 4.10950900 0.38447100
- H -7.84310300 2.97655000 -0.30070700
- H -7.55352400 2.98503600 1.44225400
- O 0.44479700 -1.20009600 2.19083300
- H -0.43098300 -0.95344000 2.52992600
- H 1.08704600 -0.61489400 2.61924300
- H 3.93907900 2.18855800 -1.67649600
- C 4.62427300 -1.87509600 -0.28998800
- H 5.40940500 -1.27975100 -0.75385500
- H 4.96545100 -2.20696900 0.69429100
- H 4.40382800 -2.75699800 -0.88995200



ARTOTF (*trans*-isomer of 5)

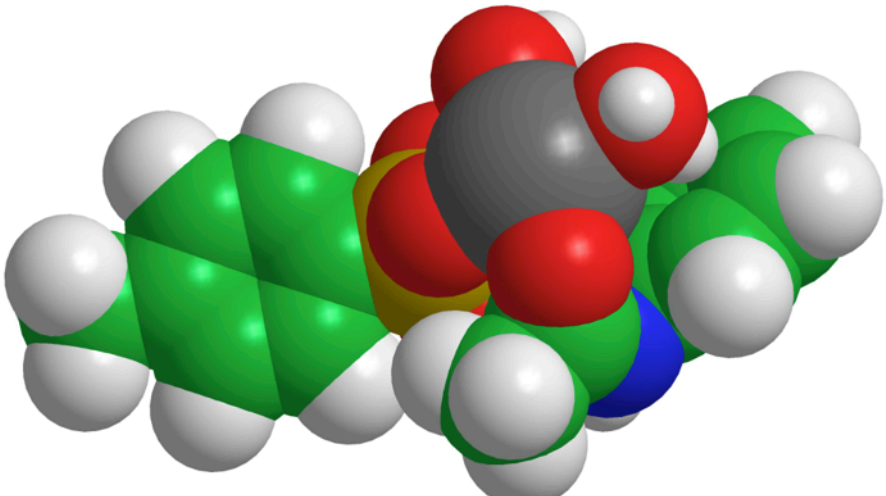
Zero-point correction= 0.345856 (Hartree/Particle)
Thermal correction to Energy= 0.372015
Thermal correction to Enthalpy= 0.372960
Thermal correction to Gibbs Free Energy= 0.288254
Sum of electronic and zero-point Energies= -1614.778572
Sum of electronic and thermal Energies= -1614.752412
Sum of electronic and thermal Enthalpies= -1614.751468
Sum of electronic and thermal Free Energies= -1614.836173

rm062x

ARTOTF

1 1

H	1.43744400	0.50396600	2.25828300
C	2.43876300	0.44535800	1.84217700
C	2.78827100	1.28636200	0.78817300
C	3.37718900	-0.46905000	2.32021000
C	4.64683700	-0.53356300	1.75036600
H	3.11227500	-1.12932300	3.13869400
N	1.82194100	2.20996400	0.27443800
H	1.49453200	2.94916600	0.88560700
C	1.24628400	2.08725900	-0.91389100
O	1.51049500	1.12455200	-1.69773900
Pd	1.17889300	-0.78657500	-1.00497000
H	5.37398100	-1.24548900	2.12521800
C	4.06019500	1.24390100	0.21737800
O	-0.74961300	-0.21145000	-0.72573200
O	0.68502500	-2.68529900	-0.29958600
H	1.44891100	-3.15401800	0.06785500
H	0.05251800	-2.49450200	0.43826700
C	4.99193400	0.32658400	0.70442200
H	5.98714000	0.29131300	0.27402800
S	-1.28319100	-0.16600900	0.72356400
O	-0.97294400	-1.45160500	1.38828800
O	-0.82853100	1.03828900	1.41584000
C	-3.02870400	-0.06851000	0.48525500
C	-3.65261100	1.17078000	0.56612200
C	-3.74075600	-1.23188200	0.19538800
C	-5.02588900	1.24199000	0.35161000
H	-3.07339700	2.05659700	0.80306800
C	-5.10843200	-1.13820800	-0.01711800
H	-3.23133900	-2.18896200	0.14932700
C	-5.76878600	0.09587600	0.05801300
H	-5.67809900	-2.03513700	-0.24184200
H	-5.52727900	2.20269600	0.41733100
C	-7.25640400	0.16848400	-0.15929200
H	-7.53695100	-0.32378400	-1.09428200
H	-7.78672800	-0.34247000	0.64991400
H	-7.60309300	1.20258400	-0.19391100
O	3.14707100	-1.43481700	-1.32832700
H	3.39615600	-1.44321300	-2.26472900
H	3.79934100	-0.88118000	-0.86254400
H	4.31056000	1.92281800	-0.59141600
C	0.24564000	3.11205200	-1.33594800
H	0.23938600	3.98875500	-0.68994100
H	0.45357400	3.40335600	-2.36639600
H	-0.73377700	2.62370100	-1.31116700



APCOTF (**7a**)

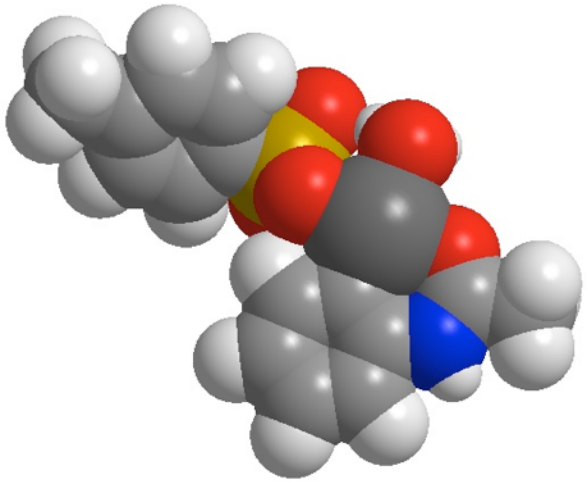
Zero-point correction=	0.307752 (Hartree/Particle)
Thermal correction to Energy=	0.330777
Thermal correction to Enthalpy=	0.331721
Thermal correction to Gibbs Free Energy=	0.251646
Sum of electronic and zero-point Energies=	-1537.986483
Sum of electronic and thermal Energies=	-1537.963457
Sum of electronic and thermal Enthalpies=	-1537.962513
Sum of electronic and thermal Free Energies=	-1538.042589

rm062x

APCOTF

0 1

H	4.58949700	3.19823900	-0.13871900
C	3.54597800	2.89806100	-0.09250100
C	3.21843400	1.53698000	-0.15496600
C	2.55322800	3.85604600	0.03598600
C	1.22095500	3.45650000	0.10733000
H	2.82146000	4.90582700	0.08465800
N	4.32737700	0.65908800	-0.27331700
H	5.22642400	1.11307500	-0.37117200
C	4.35281000	-0.67185200	-0.21249700
O	3.32902800	-1.37919700	-0.08508600
Pd	1.36701500	-0.75942000	-0.18660200
H	0.43233300	4.19406200	0.21486800
C	1.88145300	1.11586600	-0.09930000
O	-0.71206500	-0.33249100	-0.39339500
O	0.77017300	-2.92480900	-0.25982700
H	-0.12566400	-2.92574400	0.14439100
H	1.33455300	-3.46803000	0.30428700
C	0.89736900	2.10456700	0.04038000
H	-0.14111700	1.79988500	0.09290200
S	-1.59967800	-0.79034300	0.75361800
O	-1.63300500	-2.27098800	0.81724400
O	-1.25971300	-0.12106900	2.01309200
C	-3.21942700	-0.25521100	0.27208800
C	-3.68206600	0.97858800	0.71639700
C	-3.99082400	-1.05908400	-0.56428100
C	-4.94143800	1.41165000	0.31288800
H	-3.06629900	1.58088200	1.37602400
C	-5.24538200	-0.61052200	-0.95746400
H	-3.61463100	-2.02355000	-0.88888400
C	-5.73819200	0.62673200	-0.52505200
H	-5.85671100	-1.23038700	-1.60716900
H	-5.31275300	2.37198300	0.65809900
C	-7.11253100	1.08273000	-0.93844100
H	-7.28628400	0.89082600	-2.00014700
H	-7.88121900	0.54088600	-0.37838800
H	-7.24975300	2.14931400	-0.75084600
C	5.68864900	-1.35100300	-0.29289400
H	6.50750000	-0.65198200	-0.45818600
H	5.85596600	-1.89287100	0.64027900
H	5.65779400	-2.07906500	-1.10523700



APTOTF (*trans*-isomer of product, **7b**)

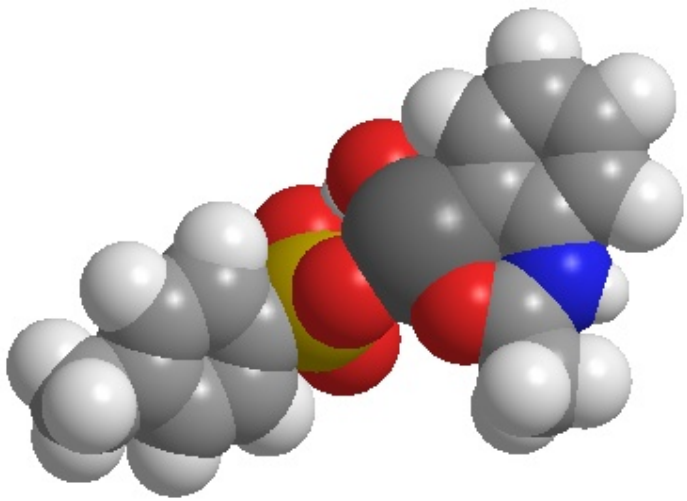
Zero-point correction=	0.307681 (Hartree/Particle)
Thermal correction to Energy=	0.330354
Thermal correction to Enthalpy=	0.331299
Thermal correction to Gibbs Free Energy=	0.252430
Sum of electronic and zero-point Energies=	-1537.984558
Sum of electronic and thermal Energies=	-1537.961885
Sum of electronic and thermal Enthalpies=	-1537.960940
Sum of electronic and thermal Free Energies=	-1538.039809

rm062x

APTOTF

0 1

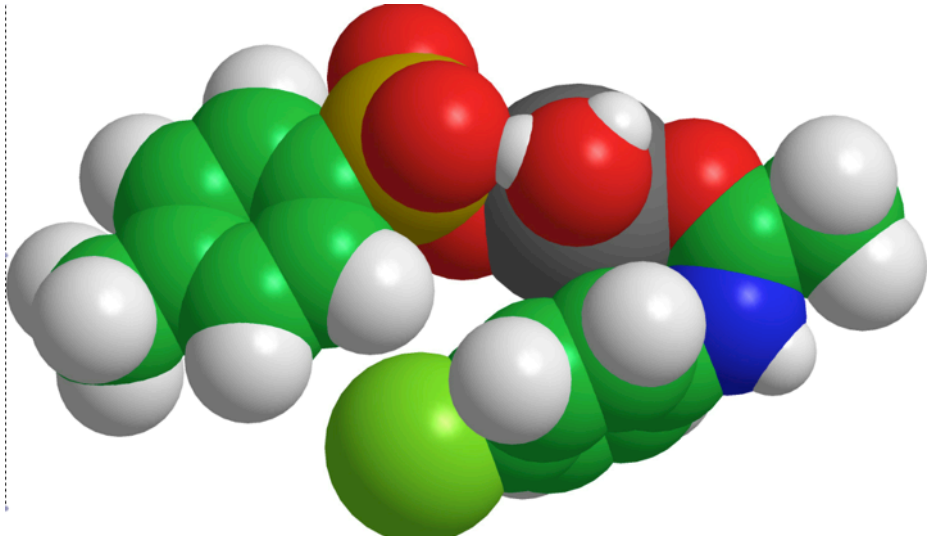
H	6.15473400	0.95088300	0.01976300
C	5.43290900	0.14697700	-0.09607600
C	4.06477800	0.44411700	-0.09303400
C	5.86698700	-1.16013700	-0.26030300
C	4.93416900	-2.17886900	-0.43769700
H	6.92958700	-1.37684300	-0.26196100
N	3.72960400	1.81661100	0.03855300
H	4.49982100	2.43362100	0.26220300
C	2.56210700	2.40397200	-0.23603900
O	1.52701900	1.77445700	-0.54601200
Pd	1.20015800	-0.23004700	-0.16480500
H	5.26056300	-3.20289100	-0.58618900
C	3.11111100	-0.57403400	-0.22728400
O	-0.99446300	0.16498500	-0.21626600
O	0.74390900	-2.25716300	0.38225400
H	-0.19064900	-2.18923000	0.73752900
H	1.30033800	-2.55524800	1.11413900
C	3.57406400	-1.88050400	-0.42304900
H	2.85592900	-2.68089700	-0.57132700
S	-1.86994800	-0.26376300	0.93095300
O	-1.65892800	-1.71287400	1.21948400
O	-1.74878800	0.60784700	2.10330100
C	-3.52649700	-0.12059200	0.31374100
C	-4.34774000	0.89755400	0.78109200
C	-3.97219400	-1.02241400	-0.65167600
C	-5.63705200	1.01575900	0.26728000
H	-3.97933700	1.57737800	1.54151500
C	-5.25932800	-0.88957100	-1.15388400
H	-3.32251800	-1.82307800	-0.99116300
C	-6.10741100	0.13206800	-0.70615100
H	-5.61860200	-1.59073300	-1.90182300
H	-6.28781500	1.80546400	0.63121300
C	-7.49181000	0.27677600	-1.28109500
H	-7.44884800	0.74874200	-2.26797700
H	-7.96959900	-0.69806200	-1.40550700
H	-8.12409800	0.89537700	-0.64134000
C	2.49943700	3.90216100	-0.17748600
H	3.44794000	4.35576800	0.10700600
H	2.19983800	4.27082900	-1.16052400
H	1.72623800	4.18741700	0.53823600



ARCOTF4Cl **5b**

- Zero-point correction= 0.336133 (Hartree/Particle)
- Thermal correction to Energy= 0.363699
- Thermal correction to Enthalpy= 0.364643
- Thermal correction to Gibbs Free Energy= 0.275116
- Sum of electronic and zero-point Energies= -2074.351615
- Sum of electronic and thermal Energies= -2074.324049
- Sum of electronic and thermal Enthalpies= -2074.323105
- Sum of electronic and thermal Free Energies= -2074.412633
- rm062x
- ARCOTF4Cl

- 1 1
- H 2.48626200 1.41021100 -2.24382900
- C 2.08143600 1.78728000 -1.31073500
- C 2.83561100 1.70169700 -0.14211400
- C 0.80101500 2.33050600 -1.26472100
- C 0.30659800 2.78813900 -0.04663600
- N 4.14380600 1.11362400 -0.18498000
- H 4.93588900 1.73692700 -0.28737800
- C 4.40630600 -0.18615600 -0.09000200
- O 3.53429200 -1.08413800 0.05251200
- Pd 1.49454200 -0.98117600 0.21411700
- C 2.34054500 2.18040600 1.06919900
- O -0.52152600 -0.85301400 0.47445300
- O 1.35367900 -1.31796900 -1.82381100
- H 0.40568400 -1.61945300 -1.96135600
- H 1.94560200 -2.03016100 -2.10763900
- C 1.06248500 2.72597900 1.12106100
- H 0.65835600 3.09933600 2.05481100
- S -1.49476500 -1.82959400 -0.21244800
- O -1.13325700 -1.93488600 -1.64915800
- O -1.60064100 -3.09743900 0.49998600
- C -3.02642300 -0.96170300 -0.09754200
- C -4.10487800 -1.56710100 0.53342200
- C -3.12112700 0.31531600 -0.65179500
- C -5.30955400 -0.87214900 0.60976800
- H -3.99769300 -2.55984600 0.95632500
- C -4.32690400 0.99252400 -0.55905900
- H -2.26351000 0.77067300 -1.13790300
- C -5.43691400 0.40921600 0.06990000
- H -4.41325000 1.99082100 -0.97880500
- H -6.16134300 -1.33398100 1.09936500
- C -6.73878100 1.16045500 0.14831800
- H -6.59060700 2.14824100 0.59305400
- H -7.15559800 1.31269800 -0.85169300
- H -7.47415000 0.61885800 0.74559500
- O 1.60312900 -0.62213500 2.27593600
- H 1.95173800 -1.38226500 2.76668200
- H 0.70142800 -0.46973100 2.60330200
- H 2.94623300 2.10965400 1.96609600
- C 5.83749600 -0.62552600 -0.16232700
- H 6.52922100 0.21214800 -0.23742300
- H 6.06244600 -1.21148100 0.73028800
- H 5.95194100 -1.27631400 -1.03149200
- H 0.19623300 2.39558600 -2.16195700
- Cl -1.29888800 3.46433300 0.01934300



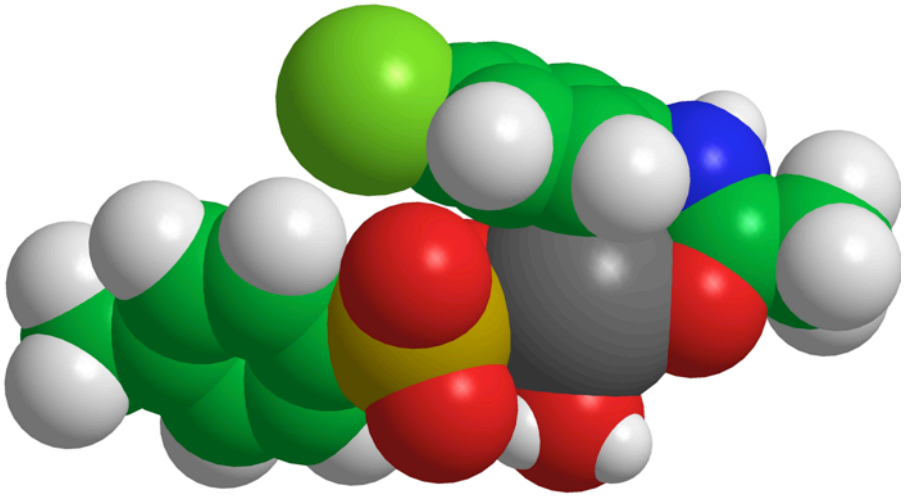
AWCOTS4Cl (4-chloro analogue of **6a**)

- Zero-point correction= 0.309684 (Hartree/Particle)
- Thermal correction to Energy= 0.334706
- Thermal correction to Enthalpy= 0.335650
- Thermal correction to Gibbs Free Energy= 0.252741
- Sum of electronic and zero-point Energies= -1997.956131
- Sum of electronic and thermal Energies= -1997.931108
- Sum of electronic and thermal Enthalpies= -1997.930164
- Sum of electronic and thermal Free Energies= -1998.013073
- rm062x

- AWCOTS4Cl

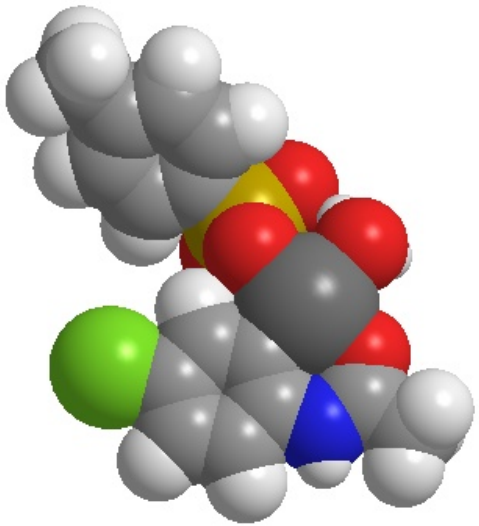
- 1 1

H	2.23145000	1.84093200	-2.52495300
C	1.85460300	1.88589000	-1.50924100
C	2.62963400	1.36118100	-0.45746400
C	0.62842800	2.45727200	-1.22768900
C	0.17519200	2.51718300	0.09790100
H	0.01302400	2.85432900	-2.02649300
N	3.98050300	0.94416900	-0.71451800
H	4.63006500	1.64901400	-1.04552700
C	4.43509500	-0.28018500	-0.46517900
O	3.65763000	-1.20251200	-0.08823000
Pd	1.67341700	-0.79800500	-0.02018300
C	2.17173400	1.44301600	0.87808300
O	-0.30300500	-0.41242700	-0.16356700
O	1.19502400	-2.85257000	-0.17848300
H	0.36273500	-2.93696700	0.35137600
H	1.86665800	-3.42465200	0.22026200
C	0.92821900	2.02759900	1.15049800
H	0.56138800	2.08236200	2.16727200
S	-1.22764600	-0.87548000	0.98933200
O	-1.00254600	-2.32007800	1.22027900
O	-1.10168500	-0.01547700	2.16124500
C	-2.82995100	-0.66884400	0.28242200
C	-3.65492900	0.34633700	0.75245400
C	-3.23445800	-1.53140300	-0.73579800
C	-4.91463600	0.50064500	0.18079800
H	-3.31318900	0.99559000	1.55086100
C	-4.49343400	-1.35938800	-1.29244300
H	-2.57745800	-2.32478300	-1.07797000
C	-5.34939400	-0.34455500	-0.84306200
H	-4.82289600	-2.02262700	-2.08667100
H	-5.56984900	1.28926400	0.53797600
C	-6.72355500	-0.19342300	-1.43817800
H	-6.70877000	-0.38579700	-2.51338100
H	-7.41485000	-0.91143700	-0.98547700
H	-7.12236300	0.80810800	-1.26703300
H	2.82531000	1.14703600	1.69355900
C	5.88537700	-0.58344700	-0.63878700
H	5.98522600	-1.37034100	-1.38871200
H	6.45774800	0.29216700	-0.93942400



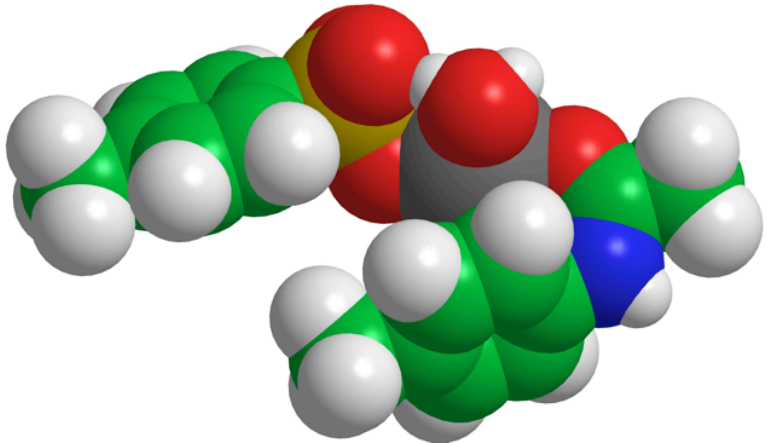
APCOTF4Cl (4-chloro analogue of **7**)

- Zero-point correction= 0.298036 (Hartree/Particle)
- Thermal correction to Energy= 0.321402
- Thermal correction to Enthalpy= 0.322346
- Thermal correction to Gibbs Free Energy= 0.242728
- Sum of electronic and zero-point Energies= -1997.562420
- Sum of electronic and thermal Energies= -1997.539054
- Sum of electronic and thermal Enthalpies= -1997.538109
- Sum of electronic and thermal Free Energies= -1997.617728
- Rm062x
  APCOTF4Cl
- 0 1
- C 3.50946200 2.60863100 -0.10374100
- C 3.20469400 1.24236400 -0.15431700
- C 2.50663900 3.56031700 -0.03039300
- C 1.18728000 3.12416100 -0.00473800
- N 4.32699300 0.37943700 -0.22035400
- H 5.22399000 0.84354000 -0.28220500
- C 4.36589900 -0.95255400 -0.17008500
- O 3.34723100 -1.67292400 -0.09010100
- Pd 1.38042400 -1.08028700 -0.20767700
- C 1.87223600 0.80299800 -0.13831600
- O -0.69579500 -0.66975400 -0.41279500
- O 0.80787500 -3.24285100 -0.26595700
- H -0.08713500 -3.25579400 0.13995100
- H 1.38034100 -3.78245700 0.29366300
- C 0.86676100 1.77450700 -0.05643500
- S -1.57389600 -1.12619400 0.74500900
- O -1.60062200 -2.60626700 0.81306100
- O -1.22234100 -0.45001700 1.99719700
- C -3.19742000 -0.59548400 0.27399600
- C -3.64621000 0.65244300 0.69272800
- C -3.98606900 -1.41791800 -0.52740700
- C -4.91040200 1.08030900 0.29930500
- H -3.01677900 1.26993500 1.32512800
- C -5.24519600 -0.97386700 -0.91097000
- H -3.61913000 -2.39229900 -0.83217700
- C -5.72509100 0.27656500 -0.50311800
- H -5.87007900 -1.60769900 -1.53374400
- H -5.27160900 2.05125500 0.62485100
- C -7.10448100 0.72739300 -0.90498300
- H -7.29101700 0.52270300 -1.96216600
- H -7.86590300 0.19169600 -0.32933600
- H -7.23978800 1.79608900 -0.72859000
- C 5.71221900 -1.61392000 -0.20377200
- H 6.52791300 -0.90341200 -0.33154800
- H 5.84978200 -2.16152100 0.73087700
- H 5.72199800 -2.33526600 -1.02256800
- H 4.54746900 2.92891700 -0.11734000
- H -0.17191900 1.46826300 -0.03877700
- H 2.74514800 4.61639200 0.00917500
- Cl -0.10130000 4.30380800 0.09132600



ARCOTF4Me (4-methyl analogue of **5**)

- Zero-point correction= 0.373403 (Hartree/Particle)
- Thermal correction to Energy= 0.401604
- Thermal correction to Enthalpy= 0.402549
- Thermal correction to Gibbs Free Energy= 0.311419
- Sum of electronic and zero-point Energies= -1654.049624
- Sum of electronic and thermal Energies= -1654.021422
- Sum of electronic and thermal Enthalpies= -1654.020478
- Sum of electronic and thermal Free Energies= -1654.111608
- Rm062x
- ARCOTF4Me
- 1 1
- H 2.60196000 0.96576200 -2.11863900
- C 2.35628900 1.58036300 -1.25768600
- C 3.19642400 1.58103200 -0.14463700
- C 1.19988800 2.35379500 -1.24017400
- C 0.87676800 3.14905700 -0.13483700
- N 4.35168300 0.73706800 -0.12714900
- H 5.26237300 1.18100000 -0.12234900
- C 4.32719500 -0.59296100 -0.08538300
- O 3.28005300 -1.28853400 -0.02718800
- Pd 1.27269400 -0.87529600 0.15649200
- C 2.91744800 2.39175100 0.95372200
- O -0.72267500 -0.52604800 0.36667900
- O 1.04762600 -1.60801800 -1.76965800
- H 0.09510500 -1.90748500 -1.82117000
- H 1.61958900 -2.37420400 -1.92543600
- C 1.75876600 3.16926300 0.95128100
- H 1.53837100 3.79818300 1.80865900
- S -1.74286000 -1.62823900 0.01346900
- O -1.47061400 -2.10579900 -1.36421400
- O -1.80708500 -2.66121800 1.04109600
- C -3.25832800 -0.72471500 -0.01235900
- C -4.18860300 -0.92158900 1.00146300
- C -3.47396100 0.19495000 -1.03770600
- C -5.36294400 -0.17513800 0.98307300
- H -3.99285600 -1.64699600 1.78347100
- C -4.65050900 0.93088600 -1.03590800
- H -2.73521300 0.32709500 -1.82184100
- C -5.60932900 0.75666900 -0.02904200
- H -4.83108800 1.65322200 -1.82627200
- H -6.09901500 -0.31848900 1.76824100
- C -6.89405500 1.54034200 -0.05560400
- H -6.74556000 2.52568000 -0.50235500
- H -7.64667900 1.01589400 -0.65314500
- H -7.29988800 1.66886700 0.94976800
- O 1.46835900 -0.10497200 2.09696100
- H 0.65175800 -0.28691000 2.58877500
- H 1.55916000 0.86368700 2.05487400
- H 3.59467600 2.40384500 1.80268900
- C 5.63645500 -1.32204000 -0.11351000
- H 6.49021000 -0.64706700 -0.14446900
- H 5.69568500 -1.95642700 0.77237500
- H 5.64850500 -1.96811700 -0.99344700
- H 0.53651700 2.33739000 -2.10016500
- C -0.38238700 3.97436100 -0.13402500
- H -0.54788800 4.44365800 0.83709400
- H -0.32460600 4.76337400 -0.88959600
- H -1.25108500 3.35454000 -0.37259600

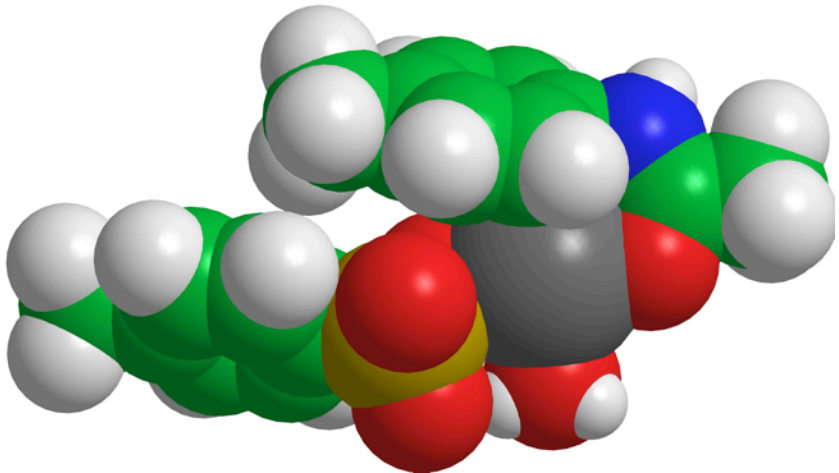


AWCOTS4Me (4-Me analogue of **6a**)

- Zero-point correction= 0.346927 (Hartree/Particle)
- Thermal correction to Energy= 0.371704
- Thermal correction to Enthalpy= 0.372648
- Thermal correction to Gibbs Free Energy= 0.290277
- Sum of electronic and zero-point Energies= -1577.657690
- Sum of electronic and thermal Energies= -1577.632914
- Sum of electronic and thermal Enthalpies= -1577.631969
- Sum of electronic and thermal Free Energies= -1577.714340
- rm062x

- AWCOTS4Me

- 1 1
- H 2.17289100 2.30285600 -2.23582700
- C 1.73611500 2.18743000 -1.24989600
- C 2.48279100 1.56287200 -0.23146700
- C 0.46830100 2.65089500 -0.96204000
- C -0.09611100 2.52378600 0.32528100
- N 3.87270200 1.26723800 -0.45462400
- H 4.48103200 2.04414100 -0.68701500
- C 4.40680700 0.06209000 -0.29141700
- O 3.68390400 -0.94433800 -0.03969100
- Pd 1.67335200 -0.68390900 -0.09267000
- C 1.94399700 1.44138200 1.07086000
- O -0.32338500 -0.41663100 -0.32182700
- O 1.37469700 -2.74669000 -0.50356000
- H 0.46791300 -2.95670500 -0.16527300
- H 2.00793400 -3.31592400 -0.04364000
- C 0.65248400 1.92505100 1.32874300
- H 0.24181800 1.81700600 2.32623400
- S -1.23503300 -1.14806400 0.69149100
- O -1.11049200 -2.60602200 0.46622400
- O -0.99463800 -0.69385400 2.05894800
- C -2.84593300 -0.63780100 0.18748600
- C -3.61034700 0.13422900 1.05499600
- C -3.32122700 -1.02273500 -1.06536900
- C -4.88140000 0.53238400 0.65041100
- H -3.21137400 0.41353800 2.02427000
- C -4.59003200 -0.61356200 -1.44975400
- H -2.70987100 -1.63315300 -1.72229800
- C -5.38674500 0.16542700 -0.59898700
- H -4.97389000 -0.90332300 -2.42338400
- H -5.48928300 1.13672900 1.31685700
- C -6.77371200 0.57340000 -1.01750400
- H -6.80825900 0.81639100 -2.08188000
- H -7.47936600 -0.24509400 -0.84329000
- H -7.11900200 1.43901600 -0.44907200
- H 2.57138500 1.08383500 1.88271400
- C 5.88160000 -0.12106400 -0.42688200
- H 6.07018400 -0.73687000 -1.30912500
- H 6.40778300 0.82746200 -0.51948300
- H 6.24225300 -0.66360800 0.44834300
- H -0.11132900 3.12692500 -1.74725300
- C -1.49277400 3.01310000 0.57965900
- H -2.20711400 2.41681200 0.00204700
- H -1.75579100 2.93227500 1.63569200
- H -1.60405500 4.05485200 0.26723200



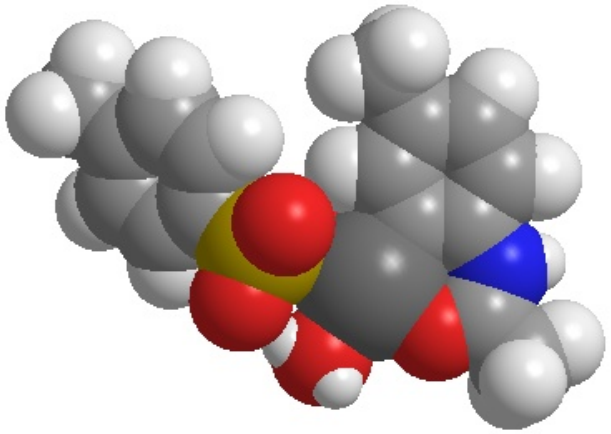
APCOTF4Me (4-Me analogue of **7**)

- Zero-point correction= 0.335344 (Hartree/Particle)
- Thermal correction to Energy= 0.360127
- Thermal correction to Enthalpy= 0.361072
- Thermal correction to Gibbs Free Energy= 0.277553
- Sum of electronic and zero-point Energies= -1577.257625
- Sum of electronic and thermal Energies= -1577.232842
- Sum of electronic and thermal Enthalpies= -1577.231898
- Sum of electronic and thermal Free Energies= -1577.315416

- rm062x

- APCOTF4Me

- 0 1
- C 3.50347700 2.75400700 -0.17523300
- C 3.20006200 1.38601400 -0.20997200
- C 2.49936500 3.69515000 -0.03302000
- C 1.16472800 3.29432800 0.08367100
- N 4.31740300 0.52025400 -0.34177000
- H 5.20596900 0.98214300 -0.48547500
- C 4.36182700 -0.80616000 -0.22950600
- O 3.35048600 -1.51934900 -0.04177200
- Pd 1.37893900 -0.92870000 -0.16482300
- C 1.87179900 0.95305800 -0.11339200
- O -0.70186000 -0.52764400 -0.40176200
- O 0.79996900 -3.10395500 -0.19892300
- H -0.10261200 -3.10487700 0.18914500
- H 1.35833400 -3.62845700 0.38840100
- C 0.87855100 1.93015300 0.04120900
- S -1.59412800 -0.96857900 0.74787100
- O -1.63323900 -2.44803200 0.82887200
- O -1.25475900 -0.28556800 2.00038700
- C -3.20993100 -0.43044300 0.25653000
- C -3.65830800 0.81936500 0.66991500
- C -3.99221700 -1.24772200 -0.55628500
- C -4.91456500 1.25470200 0.25922800
- H -3.03462500 1.43234900 1.31242600
- C -5.24349700 -0.79658300 -0.95711800
- H -3.62663000 -2.22407600 -0.85651300
- C -5.72217900 0.45630900 -0.55547900
- H -5.86321500 -1.42671000 -1.58879000
- H -5.27507500 2.22732400 0.58065100
- C -7.09280300 0.91542400 -0.97770700
- H -7.26201900 0.71823600 -2.03925900
- H -7.86638800 0.37954000 -0.41877100
- H -7.22661900 1.98362200 -0.79711500
- C 5.70272700 -1.47337100 -0.32606900
- H 6.51103600 -0.76937900 -0.52033400
- H 5.89452000 -1.99744100 0.61248000
- H 5.66299300 -2.21596300 -1.12496100
- H 4.53959000 3.07351700 -0.25258200
- H -0.15364700 1.60857200 0.12655100
- H 2.75427100 4.75077500 -0.00608500
- C 0.06719000 4.31434300 0.24559400
- H 0.00717100 4.96685600 -0.63080900
- H -0.90356900 3.83142800 0.37636200
- H 0.25142800 4.95317900 1.11436800



ARCOTF4F (4-F analogue of **5**)

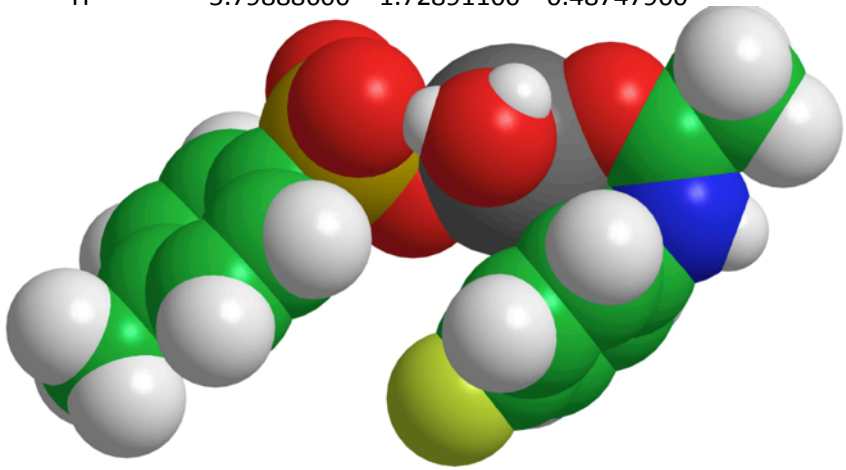
- Zero-point correction= 0.337455 (Hartree/Particle)
- Thermal correction to Energy= 0.364807
- Thermal correction to Enthalpy= 0.365751
- Thermal correction to Gibbs Free Energy= 0.277133
- Sum of electronic and zero-point Energies= -1713.989053
- Sum of electronic and thermal Energies= -1713.961702
- Sum of electronic and thermal Enthalpies= -1713.960757
- Sum of electronic and thermal Free Energies= -1714.049375

- rm062x

- ARCOTF4F

- 1 1

H	2.73204000	1.61740200	-2.10169500
C	2.30470000	1.93583900	-1.15651500
C	2.97963700	1.66860300	0.03418300
C	1.07543400	2.58518600	-1.11976700
C	0.56314900	2.96066700	0.11381800
H	0.51748800	2.79881100	-2.02373400
N	4.21889300	0.94790800	-0.00810000
H	5.07983900	1.47484500	0.07778700
C	4.32551600	-0.36611300	-0.17875100
O	3.34470500	-1.15289800	-0.27360700
Pd	1.34420400	-0.83523100	0.05973600
C	2.46024600	2.07352100	1.26300900
O	-0.63625800	-0.53315100	0.41667000
O	0.97473500	-0.92030700	-1.98353500
H	0.09338700	-1.38073100	-2.02926800
H	1.62734100	-1.46773200	-2.44491100
C	1.23496500	2.72958400	1.30713800
S	-1.63824100	-1.62592200	-0.01700300
O	-1.33133700	-2.02833700	-1.41023300
O	-1.71215000	-2.71130100	0.95445300
C	-3.16723600	-0.74364600	-0.03150200
C	-4.09455600	-0.95734600	0.98188100
C	-3.39950400	0.17140300	-1.05698700
C	-5.28268600	-0.23333800	0.96172700
H	-3.88764700	-1.67999900	1.76366700
C	-4.59026800	0.88400300	-1.05785600
H	-2.66259400	0.31549200	-1.84085800
C	-5.54666800	0.69175600	-0.05240300
H	-4.78410500	1.60117800	-1.84979500
H	-6.01706000	-0.38999600	1.74600700
C	-6.84790100	1.44754300	-0.08325300
H	-6.72041800	2.43316000	-0.53582300
H	-7.58906000	0.90339800	-0.67755600
H	-7.25643200	1.57337400	0.92137300
O	1.67229700	-0.77669700	2.13708100
H	1.79529100	-1.66472000	2.50692700
H	0.89151300	-0.40120600	2.57466700
C	5.69829200	-0.95804100	-0.27817900
H	6.48268400	-0.21208000	-0.15880700
H	5.79888600	-1.72891100	0.48747900



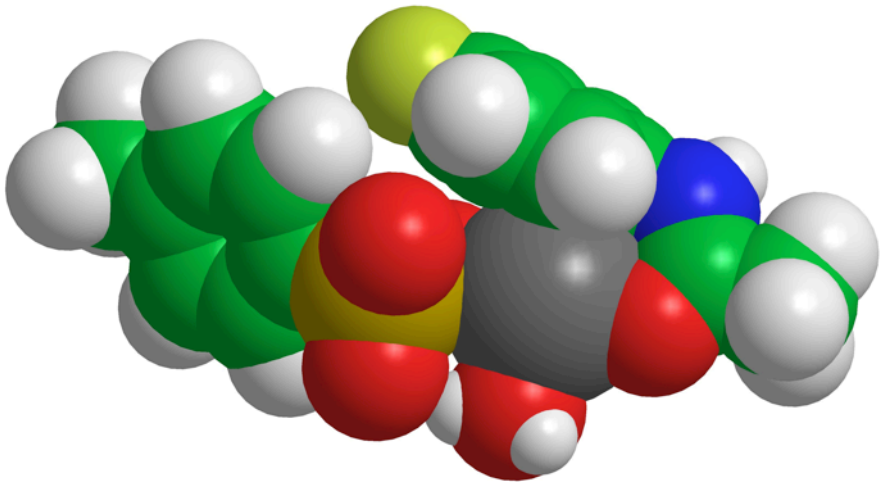
AWCOTF4F (4-F analogue of **6a**)

- Zero-point correction= 0.311244 (Hartree/Particle)
- Thermal correction to Energy= 0.334992
- Thermal correction to Enthalpy= 0.335937
- Thermal correction to Gibbs Free Energy= 0.256650
- Sum of electronic and zero-point Energies= -1637.595134
- Sum of electronic and thermal Energies= -1637.571386
- Sum of electronic and thermal Enthalpies= -1637.570442
- Sum of electronic and thermal Free Energies= -1637.649729

- rm062x

- AWCOTF4F

- 1 1
- H 2.12592800 2.17064600 -2.26367300
- C 1.67806500 2.09987400 -1.27869400
- C 2.42425100 1.53911200 -0.21719800
- C 0.40075900 2.56253400 -1.03899600
- C -0.12223300 2.47642300 0.25563100
- H -0.20416100 2.99024300 -1.82957000
- N 3.82890800 1.28672200 -0.40417200
- H 4.42420800 2.08782900 -0.58333800
- C 4.38763900 0.08851500 -0.27143100
- O 3.68104400 -0.94013600 -0.06918500
- Pd 1.67001500 -0.69526100 -0.12261000
- C 1.87810400 1.48266800 1.08925000
- O -0.32283200 -0.43659300 -0.34294000
- O 1.37301700 -2.76462200 -0.49026300
- H 0.46914700 -2.97649900 -0.14954700
- H 2.00908500 -3.32680500 -0.02531900
- C 0.58278100 1.95208000 1.32122300
- S -1.22683000 -1.14661300 0.69842000
- O -1.12131600 -2.60716000 0.49536600
- O -0.94406200 -0.66245800 2.04770000
- C -2.84255000 -0.62938300 0.22138200
- C -3.39520500 0.49140600 0.83439800
- C -3.52315100 -1.33653200 -0.76711100
- C -4.66214000 0.90747500 0.44232400Cl
- H -2.84624100 1.01815600 1.60713900
- C -4.78773300 -0.90306600 -1.14347300
- H -3.07288800 -2.21369300 -1.21958900
- C -5.37415800 0.21868000 -0.54496300
- H -5.33210600 -1.44497800 -1.91097200
- H -5.10815100 1.77780300 0.91398500
- C -6.76117000 0.65368900 -0.93482600
- H -6.94857800 0.47017000 -1.99492200
- H -7.50850900 0.09172800 -0.36535900
- H -6.91563900 1.71468100 -0.72940000
- H 2.49855600 1.15522000 1.91823900
- C 5.86849000 -0.05780400 -0.37666100
- H 6.09107600 -0.65194500 -1.26565500
- H 6.37399800 0.90423600 -0.43945800
- H 6.22160300 -0.60862100 0.49654000
- F -1.36038500 2.91926800 0.46214800
- H 0.13507900 1.90289500 2.30557300



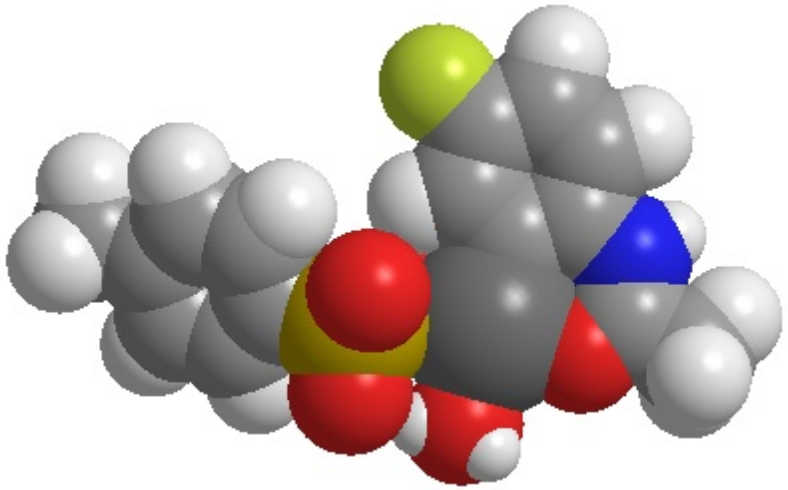
APCOTF4F (4-F analogue of **7**)

- Zero-point correction= 0.299587 (Hartree/Particle)
- Thermal correction to Energy= 0.323389
- Thermal correction to Enthalpy= 0.324334
- Thermal correction to Gibbs Free Energy= 0.243353
- Sum of electronic and zero-point Energies= -1637.198774
- Sum of electronic and thermal Energies= -1637.174971
- Sum of electronic and thermal Enthalpies= -1637.174027
- Sum of electronic and thermal Free Energies= -1637.255008

- rm062x

- APCOTF4F

- 0 1
- H 4.57753200 3.03539000 -0.15690100
- C 3.53529500 2.73125800 -0.11951600
- C 3.20985900 1.36962200 -0.16882300
- C 2.54826600 3.69762300 -0.01579600
- C 1.23095300 3.27092400 0.04140300
- H 2.78674200 4.75351300 0.02459100
- N 4.31889800 0.48879000 -0.26450300
- H 5.22025700 0.93943700 -0.35552300
- C 4.34008200 -0.84128400 -0.19719100
- O 3.31292400 -1.54649900 -0.07930000
- Pd 1.35400700 -0.92637900 -0.19250400
- C 1.87133000 0.94852600 -0.12304300
- O -0.71763000 -0.48378600 -0.39775700
- O 0.75420100 -3.08369200 -0.25097300
- H -0.14072600 -3.08207300 0.15547000
- H 1.31935900 -3.62799100 0.31147000
- C 0.88214700 1.93251400 -0.00951900
- S -1.60594100 -0.93258700 0.75427000
- O -1.64303800 -2.41244600 0.82571900
- O -1.25971900 -0.25632800 2.00798800
- C -3.22380700 -0.39403300 0.27180800
- C -3.67777800 0.84760000 0.70312600
- C -4.00298300 -1.20436700 -0.55103900
- C -4.93675400 1.28203800 0.30001800
- H -3.05616100 1.45498000 1.35256700
- C -5.25702400 -0.75417600 -0.94386600
- H -3.63312200 -2.17469400 -0.86520300
- C -5.74143200 0.49078600 -0.52440400
- H -5.87449800 -1.37882800 -1.58307600
- H -5.30153600 2.24843400 0.63503500
- C -7.11527300 0.94865100 -0.93725600
- H -7.29177500 0.75153200 -1.99757000
- H -7.88429800 0.41193100 -0.37277700
- H -7.24892900 2.01662400 -0.75517700
- C 5.67489400 -1.52428400 -0.25682600
- H 6.49652900 -0.82946100 -0.42600300
- H 5.83359000 -2.05216300 0.68586400
- H 5.64881900 -2.26444800 -1.05825500
- H -0.16468000 1.65777800 0.03439000
- F 0.25453200 4.18966000 0.14995600



AWOOTF (**6d**)

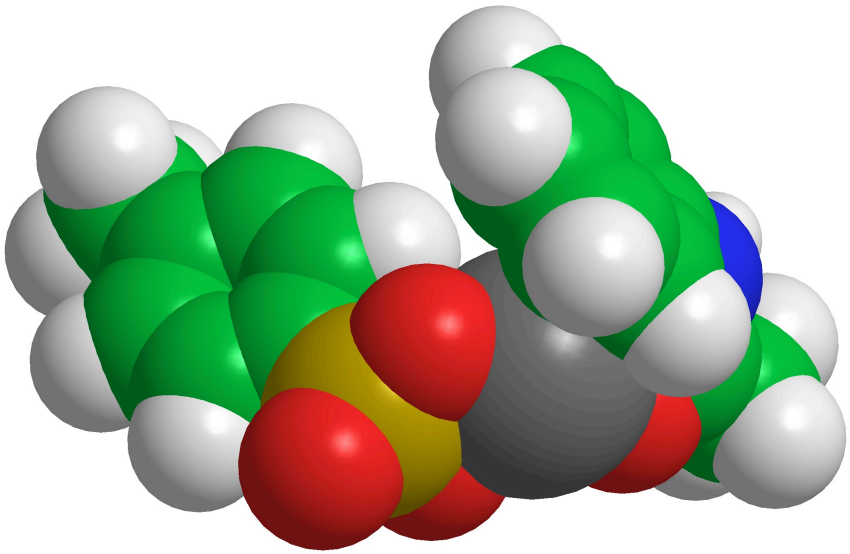
- Zero-point correction= 0.293625 (Hartree/Particle)
- Thermal correction to Energy= 0.315104
- Thermal correction to Enthalpy= 0.316048
- Thermal correction to Gibbs Free Energy= 0.241397
- Sum of electronic and zero-point Energies= -1461.985357
- Sum of electronic and thermal Energies= -1461.963879
- Sum of electronic and thermal Enthalpies= -1461.962935
- Sum of electronic and thermal Free Energies= -1462.037586

- rm062x

- AWOOTF1

- 1 1

H	1.65373100	3.23920500	-0.31708100
C	1.81800000	2.49483500	0.45411100
C	2.60692100	1.37705900	0.18314400
C	1.25576700	2.63076300	1.71960300
C	1.45682600	1.66113200	2.70866400
H	0.64243600	3.49878500	1.93551200
N	3.24054300	1.24358500	-1.08805300
H	3.77790500	2.03075600	-1.43276300
C	3.17136900	0.14194500	-1.83586400
O	2.43717100	-0.83323900	-1.52367400
Pd	1.15061100	-0.78836700	0.05497500
H	1.00294800	1.78243300	3.68511700
C	2.84137900	0.39512300	1.17396700
O	-0.48538900	-1.93778100	-0.70443000
C	2.25051800	0.55536600	2.44377600
H	2.43545000	-0.19110600	3.20802600
O	-0.38046400	-0.89609800	1.42511100
H	3.60247200	-0.36492600	1.01401500
C	3.98603700	0.05477600	-3.08436200
H	4.49031300	0.99140100	-3.31602700
H	4.72943000	-0.73412000	-2.94744800
H	3.33146400	-0.23490100	-3.90716000
S	-1.36356400	-1.64056600	0.50571500
O	-1.99770400	-2.79771700	1.09787900
C	-2.58757700	-0.46493300	0.03981900
C	-2.22576700	0.87302600	-0.12620300
C	-3.88528400	-0.90959100	-0.19065700
C	-3.19486400	1.77426700	-0.54024400
H	-1.21179300	1.20288200	0.08183500
C	-4.83979700	0.01311400	-0.60489000
H	-4.14117000	-1.95309500	-0.04232300
C	-4.51094300	1.35918200	-0.78578700
H	-2.93193100	2.81974000	-0.67030800
H	-5.85661400	-0.31943400	-0.78847900
C	-5.55162200	2.35896400	-1.21006600
H	-5.85667100	2.97321400	-0.35714500
H	-5.15721200	3.03282100	-1.97436300
H	-6.44034400	1.86369900	-1.60448600

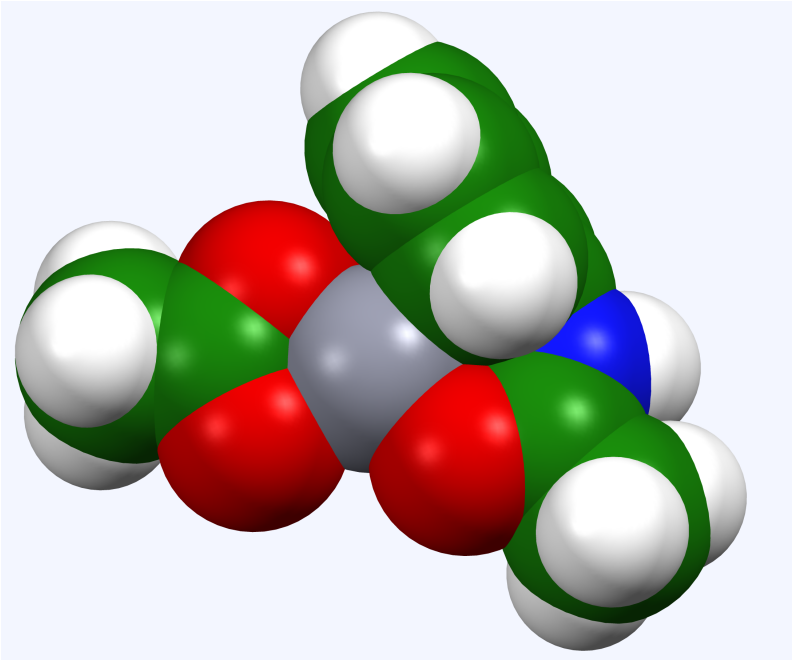


- Structures and free energies of species shown in Scheme 5

Ground state for CMD (**3a**)Pd(OAc)$^+$ M06-2x (Scheme 3)

- Zero-point correction= 0.211332 (Hartree/Particle)
- Thermal correction to Energy= 0.226034
- Thermal correction to Enthalpy= 0.226978
- Thermal correction to Gibbs Free Energy= 0.168307
- Sum of electronic and zero-point Energies= -795.921236
- Sum of electronic and thermal Energies= -795.906535
- Sum of electronic and thermal Enthalpies= -795.905591
- Sum of electronic and thermal Free Energies= -795.964262
-
- ASCGS01

- 1 1
- C 1.06990700 1.87429800 -1.25799600
- C 1.49260000 1.07480700 -0.18312800
- C 0.97570700 1.28035300 1.11623000
- C 0.01802300 2.29092600 1.31861600
- C -0.39949600 3.07262200 0.25438300
- C 0.12908600 2.86595000 -1.02844500
- N 2.56724400 0.14423500 -0.37117200
- C 2.47118700 -1.15544200 -0.09148200
- C 3.68308300 -2.02114900 -0.19915000
- Pd -0.31743500 -0.51932000 0.18502400
- O -2.14242200 0.32268900 -0.01881800
- C -2.70426000 -0.81779700 -0.20834500
- C -4.17267300 -0.92581900 -0.42516700
- O 1.37584200 -1.67297100 0.25527300
- O -1.94660000 -1.83402400 -0.17894900
- H 4.57092400 -1.45841400 -0.48196400
- H 3.48486500 -2.80055200 -0.93721100
- H 3.45429400 0.51243800 -0.69505500
- H 1.40791700 0.74823400 1.95917900
- H -0.37156000 2.45617100 2.31651700
- H -1.13297300 3.85468400 0.41329100
- H -0.19948600 3.48756900 -1.85370100
- H 3.84371400 -2.50288300 0.76716600
- H -4.57814200 0.03434400 -0.74160600
- H -4.37500400 -1.69837000 -1.16762900
- H -4.64009000 -1.22247700 0.51774300
- H 1.49330800 1.71031400 -2.24277200

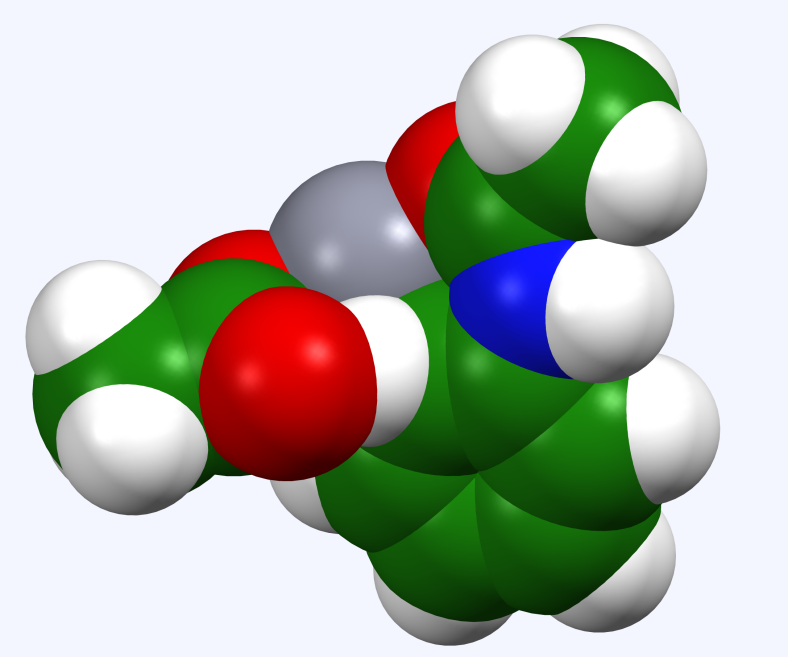


Transition state for CMD (**3a**)Pd(OAc)$^{+}$ M06-2x (Scheme 3)

- Zero-point correction= 0.206154 (Hartree/Particle)
- Thermal correction to Energy= 0.221189
- Thermal correction to Enthalpy= 0.222133
- Thermal correction to Gibbs Free Energy= 0.162747
- Sum of electronic and zero-point Energies= -795.891805
- Sum of electronic and thermal Energies= -795.876769
- Sum of electronic and thermal Enthalpies= -795.875825
- Sum of electronic and thermal Free Energies= -795.935211

- ASCTS01

- 1 1
- C -0.16251700 0.90507400 0.09577100
- C -1.53437600 1.04432900 0.42354700
- C -2.16296000 2.28126000 0.31893000
- C -1.46411700 3.36706300 -0.19916900
- C -0.13815000 3.23842000 -0.62090900
- C 0.50049600 2.02084100 -0.47391400
- N -2.31137700 -0.04575100 0.86688700
- C -2.32716100 -1.26905700 0.31265900
- C -3.35114200 -2.24632800 0.79795000
- Pd 0.40946400 -0.95965700 -0.65979500
- O 2.36023000 -0.46964300 -0.49696700
- C 2.73540600 -0.13685500 0.69144000
- C 4.22419900 -0.11707600 0.91845400
- O -1.53524300 -1.61313400 -0.59578400
- O 1.94201000 0.15337800 1.60993300
- H -4.09416900 -1.79004400 1.45001600
- H -2.83176300 -3.04206900 1.33744800
- H -3.06267400 0.16731600 1.51329700
- H -3.20524700 2.38491700 0.60071300
- H -1.97099900 4.32138500 -0.29548600
- H 0.38759700 4.08752600 -1.04129400
- H 1.54497500 1.91438400 -0.74987300
- H -3.83964000 -2.69081600 -0.07005000
- H 4.71396000 0.40038700 0.09267000
- H 4.45508700 0.36385100 1.86652100
- H 4.58611300 -1.14810400 0.92973200
- H 0.60701600 0.40490600 0.92264000



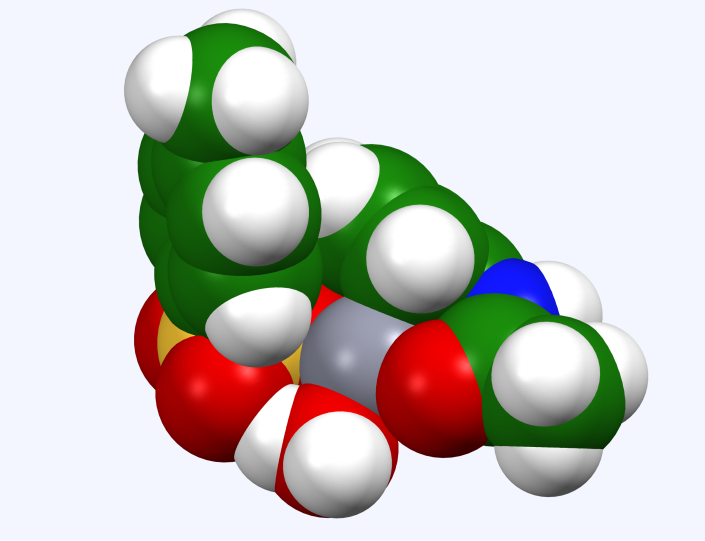
AWCOTSI, **6a** conformer

- Zero-point correction= 0.319664 (Hartree/Particle)
- Thermal correction to Energy= 0.343154
- Thermal correction to Enthalpy= 0.344098
- Thermal correction to Gibbs Free Energy= 0.266386
- Sum of electronic and zero-point Energies= -1538.386376
- Sum of electronic and thermal Energies= -1538.362885
- Sum of electronic and thermal Enthalpies= -1538.361941
- Sum of electronic and thermal Free Energies= -1538.439653

- AWCOTSI

- 1 1

H	2.80013200	-0.93338900	2.84938600
C	1.89467600	-1.16206900	2.29820600
C	1.97010900	-1.42036200	0.91985500
C	0.66017100	-1.22046600	2.92386900
C	-0.49943500	-1.54146400	2.20219400
H	0.59459200	-1.01989700	3.98735200
N	3.25506100	-1.55500600	0.29370100
H	3.89657500	-2.23310000	0.68917500
C	3.59907300	-0.92300000	-0.82453200
O	2.86100600	-0.02499300	-1.32131300
Pd	1.27517400	0.60647100	-0.22650600
H	-1.45455200	-1.59501100	2.71377000
C	0.80573900	-1.73487700	0.17951000
O	-0.16586900	1.31467300	1.00350300
O	1.45006900	2.54408500	-1.05163900
H	0.51771000	2.88292300	-1.06051200
H	1.78442500	2.53871200	-1.96008000
C	-0.43150900	-1.79611100	0.84375300
H	-1.32124700	-2.05833800	0.28009500
S	-1.46240000	1.95625100	0.45810400
O	-2.17964500	2.56051600	1.56965500
O	-1.13275500	2.83272300	-0.68593800
C	-2.41663500	0.60512700	-0.16872800
C	-2.17835500	0.13213200	-1.45629600
C	-3.32535900	-0.02019500	0.68027400
C	-2.86216400	-0.99836000	-1.89236100
H	-1.46984500	0.63998000	-2.10436200
C	-3.99993900	-1.14799400	0.22693200
H	-3.49579100	0.37427400	1.67658800
C	-3.77846800	-1.65263500	-1.06064500
H	-4.71058400	-1.64553500	0.88022700
H	-2.68646300	-1.37761100	-2.89463300
C	-4.53770700	-2.85706500	-1.54813300
H	-4.69844900	-3.57449100	-0.74047800
H	-5.52117800	-2.55751100	-1.92400300
H	-4.00818000	-3.35719200	-2.36120800
H	0.89263100	-2.06560100	-0.85204600
C	4.87342300	-1.27687000	-1.51451000
H	5.43451100	-0.36048900	-1.70145400
H	5.47466300	-1.97623000	-0.93577000
H	4.62186000	-1.72493500	-2.47883900



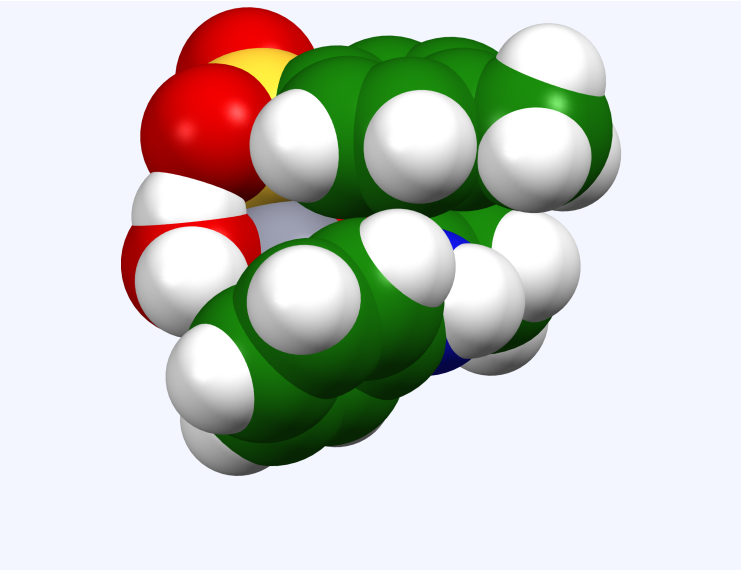
AWTOTFI conformer of 6b

- Zero-point correction= 0.320889 (Hartree/Particle)
- Thermal correction to Energy= 0.343808
- Thermal correction to Enthalpy= 0.344752
- Thermal correction to Gibbs Free Energy= 0.269206
- Sum of electronic and zero-point Energies= -1538.382944
- Sum of electronic and thermal Energies= -1538.360026
- Sum of electronic and thermal Enthalpies= -1538.359082
- Sum of electronic and thermal Free Energies= -1538.434628

- AWTOTFI

- 1 1

H	0.47772300	2.57115800	1.95018200
C	1.32758500	2.14824100	1.42643100
C	1.27260900	1.96885900	0.04680000
C	2.47872300	1.77089500	2.11308200
C	3.57142200	1.20804700	1.44440800
H	2.52035100	1.90931200	3.18788300
N	0.11264900	2.36500500	-0.67373100
H	-0.30813000	3.25639300	-0.43607400
C	-0.44104000	1.64605100	-1.65593200
O	-0.06508600	0.47590600	-1.92967000
Pd	1.19028500	-0.57653500	-0.72293600
H	4.45860800	0.92235600	1.99786300
C	2.37740100	1.43080800	-0.65701800
O	-0.06305800	-2.19757200	-0.96820700
O	2.29680400	-1.77677100	0.56355900
H	1.60322600	-2.30081200	1.04325500
H	2.80750200	-1.28387900	1.22464400
C	3.52773400	1.05231500	0.06474900
H	4.38013200	0.65630600	-0.47713600
S	-0.92964200	-2.53145800	0.26404000
O	-1.87835900	-3.57789500	-0.08436100
O	-0.04085300	-2.78443000	1.41966400
C	-1.80710600	-1.02257500	0.59143600
C	-1.43254900	-0.21926000	1.66448500
C	-2.79946000	-0.62119900	-0.30215100
C	-2.06223600	1.01124100	1.83742200
H	-0.66105700	-0.55403000	2.35060200
C	-3.41186200	0.61197900	-0.11580600
H	-3.08124000	-1.26068100	-1.13295300
C	-3.04935800	1.44757400	0.94991000
H	-4.18480400	0.93565400	-0.80738900
H	-1.78464800	1.63875900	2.67959200
C	-3.73143300	2.77558100	1.14216700
H	-3.92245800	3.26201200	0.18247800
H	-4.69769900	2.63985100	1.63791500
H	-3.12835400	3.44352200	1.76015600
H	2.41602300	1.49494200	-1.74218000
C	-1.52416700	2.26060500	-2.47975500
H	-2.27033800	1.49856100	-2.70174800
H	-1.98595000	3.11150800	-1.97967500
H	-1.07943200	2.59908300	-3.42012300



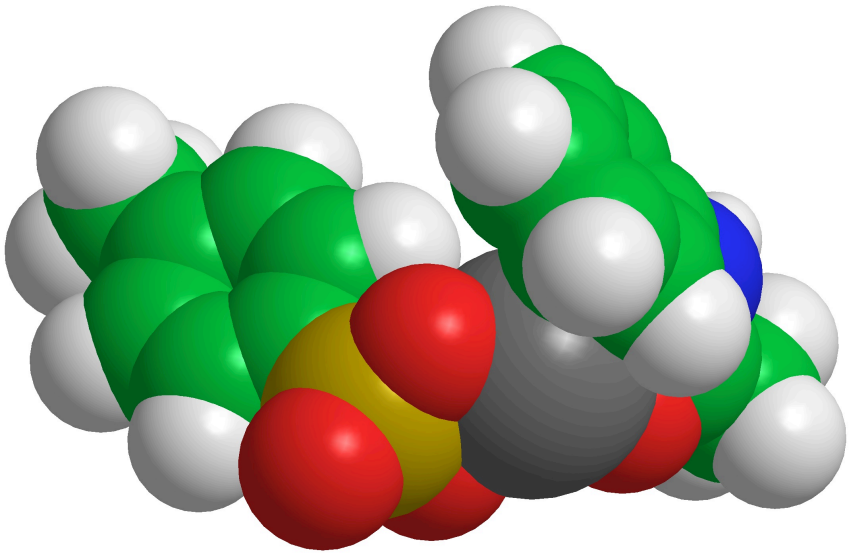
AWOOTF

- Zero-point correction= 0.293625 (Hartree/Particle)
- Thermal correction to Energy= 0.315104
- Thermal correction to Enthalpy= 0.316048
- Thermal correction to Gibbs Free Energy= 0.241397
- Sum of electronic and zero-point Energies= -1461.985357
- Sum of electronic and thermal Energies= -1461.963879
- Sum of electronic and thermal Enthalpies= -1461.962935
- Sum of electronic and thermal Free Energies= -1462.037586

- rm062x

- AWOOTF1

- 1 1
- H 1.65373100 3.23920500 -0.31708100
- C 1.81800000 2.49483500 0.45411100
- C 2.60692100 1.37705900 0.18314400
- C 1.25576700 2.63076300 1.71960300
- C 1.45682600 1.66113200 2.70866400
- H 0.64243600 3.49878500 1.93551200
- N 3.24054300 1.24358500 -1.08805300
- H 3.77790500 2.03075600 -1.43276300
- C 3.17136900 0.14194500 -1.83586400
- O 2.43717100 -0.83323900 -1.52367400
- Pd 1.15061100 -0.78836700 0.05497500
- H 1.00294800 1.78243300 3.68511700
- C 2.84137900 0.39512300 1.17396700
- O -0.48538900 -1.93778100 -0.70443000
- C 2.25051800 0.55536600 2.44377600
- H 2.43545000 -0.19110600 3.20802600
- O -0.38046400 -0.89609800 1.42511100
- H 3.60247200 -0.36492600 1.01401500
- C 3.98603700 0.05477600 -3.08436200
- H 4.49031300 0.99140100 -3.31602700
- H 4.72943000 -0.73412000 -2.94744800
- H 3.33146400 -0.23490100 -3.90716000
- S -1.36356400 -1.64056600 0.50571500
- O -1.99770400 -2.79771700 1.09787900
- C -2.58757700 -0.46493300 0.03981900
- C -2.22576700 0.87302600 -0.12620300
- C -3.88528400 -0.90959100 -0.19065700
- C -3.19486400 1.77426700 -0.54024400
- H -1.21179300 1.20288200 0.08183500
- C -4.83979700 0.01311400 -0.60489000
- H -4.14117000 -1.95309500 -0.04232300
- C -4.51094300 1.35918200 -0.78578700
- H -2.93193100 2.81974000 -0.67030800
- H -5.85661400 -0.31943400 -0.78847900
- C -5.55162200 2.35896400 -1.21006600
- H -5.85667100 2.97321400 -0.35714500
- H -5.15721200 3.03282100 -1.97436300
- H -6.44034400 1.86369900 -1.60448600



AWOOTF **6d**

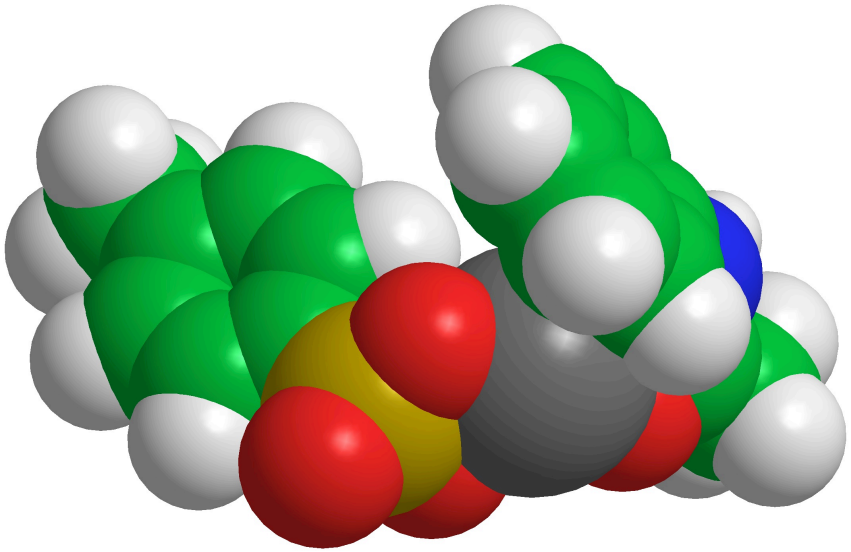
- Zero-point correction= 0.293625 (Hartree/Particle)
- Thermal correction to Energy= 0.315104
- Thermal correction to Enthalpy= 0.316048
- Thermal correction to Gibbs Free Energy= 0.241397
- Sum of electronic and zero-point Energies= -1461.985357
- Sum of electronic and thermal Energies= -1461.963879
- Sum of electronic and thermal Enthalpies= -1461.962935
- Sum of electronic and thermal Free Energies= -1462.037586

- rm062x

- AWOOTF1

- 1 1

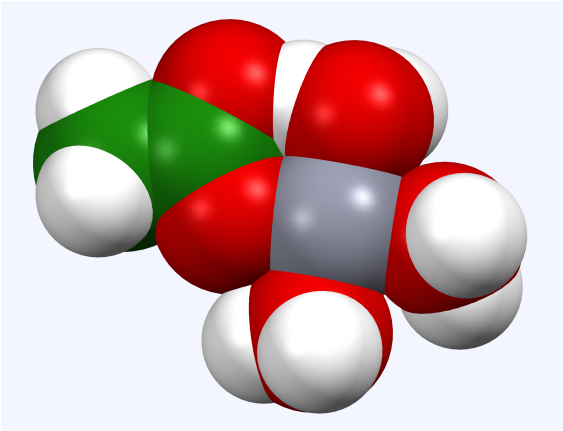
H	1.65373100	3.23920500	-0.31708100
C	1.81800000	2.49483500	0.45411100
C	2.60692100	1.37705900	0.18314400
C	1.25576700	2.63076300	1.71960300
C	1.45682600	1.66113200	2.70866400
H	0.64243600	3.49878500	1.93551200
N	3.24054300	1.24358500	-1.08805300
H	3.77790500	2.03075600	-1.43276300
C	3.17136900	0.14194500	-1.83586400
O	2.43717100	-0.83323900	-1.52367400
Pd	1.15061100	-0.78836700	0.05497500
H	1.00294800	1.78243300	3.68511700
C	2.84137900	0.39512300	1.17396700
O	-0.48538900	-1.93778100	-0.70443000
C	2.25051800	0.55536600	2.44377600
H	2.43545000	-0.19110600	3.20802600
O	-0.38046400	-0.89609800	1.42511100
H	3.60247200	-0.36492600	1.01401500
C	3.98603700	0.05477600	-3.08436200
H	4.49031300	0.99140100	-3.31602700
H	4.72943000	-0.73412000	-2.94744800
H	3.33146400	-0.23490100	-3.90716000
S	-1.36356400	-1.64056600	0.50571500
O	-1.99770400	-2.79771700	1.09787900
C	-2.58757700	-0.46493300	0.03981900
C	-2.22576700	0.87302600	-0.12620300
C	-3.88528400	-0.90959100	-0.19065700
C	-3.19486400	1.77426700	-0.54024400
H	-1.21179300	1.20288200	0.08183500
C	-4.83979700	0.01311400	-0.60489000
H	-4.14117000	-1.95309500	-0.04232300
C	-4.51094300	1.35918200	-0.78578700
H	-2.93193100	2.81974000	-0.67030800
H	-5.85661400	-0.31943400	-0.78847900
C	-5.55162200	2.35896400	-1.21006600
H	-5.85667100	2.97321400	-0.35714500
H	-5.15721200	3.03282100	-1.97436300
H	-6.44034400	1.86369900	-1.60448600



- Structures and energies of intermediates on the reaction pathway of Scheme 5

Precursor to acetate TS in Scheme 5a

- Zero-point correction= 0.130176 (Hartree/Particle)\
- Thermal correction to Energy= 0.142491\
- Thermal correction to Enthalpy= 0.143435\
- Thermal correction to Gibbs Free Energy= 0.091009\
- Sum of electronic and zero-point Energies= -585.139878\
- Sum of electronic and thermal Energies= -585.127563\
- Sum of electronic and thermal Enthalpies= -585.126619\
- Sum of electronic and thermal Free Energies= -585.179045\
- \
- AUPREA\
- \
- 1 1\
- O 2.70658800 -0.61038100 0.15540000\
- Pd 0.70014700 0.03118600 -0.01906500\
- O -1.17432400 0.72117300 -0.07562000\
- O 0.14901900 -1.93389900 -0.12812000\
- H -0.89318600 -1.81439400 -0.04805900\
- H 0.47952400 -2.42768700 0.63608200\
- O 1.24249800 2.06414700 0.05665300\
- H 0.44057800 2.59034400 0.20464200\
- H 1.63222500 2.38212800 -0.77160000\
- H 3.13452200 -0.80333500 -0.69181300\
- H 3.28648200 0.00020800 0.63319300\
- C -2.22437500 -0.02774300 -0.00661500\
- O -2.20691300 -1.27157000 0.00831200\
- C -3.52754700 0.71981300 0.07986900\
- H -4.35958000 0.03437400 -0.06892100\
- H -3.60141800 1.17498400 1.07090700\
- H -3.54931000 1.52062500 -0.65997500}



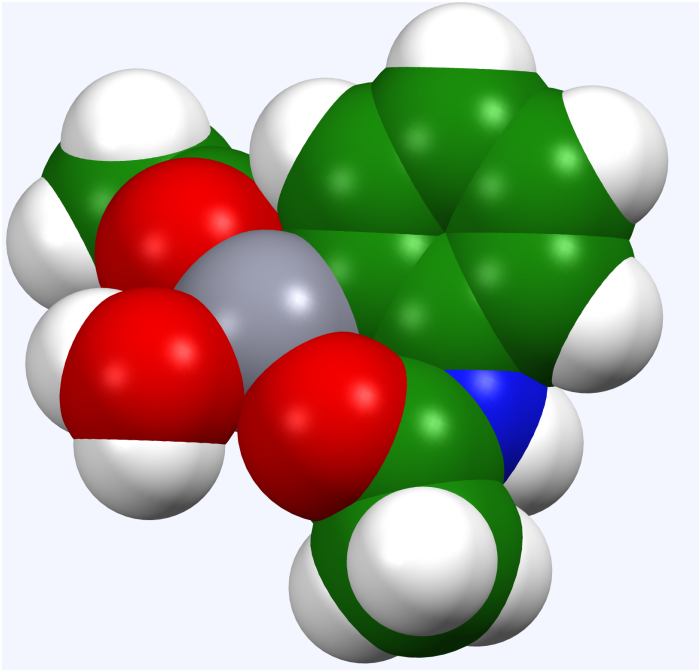
Scheme 5 a) CMD with acetate

Zero-point correction= 0.231895 (Hartree/Particle)
Thermal correction to Energy= 0.249677
Thermal correction to Enthalpy= 0.250621
Thermal correction to Gibbs Free Energy= 0.185448
Sum of electronic and zero-point Energies= -872.293907
Sum of electronic and thermal Energies= -872.276125
Sum of electronic and thermal Enthalpies= -872.275181
Sum of electronic and thermal Free Energies= -872.340354

ASCTS02

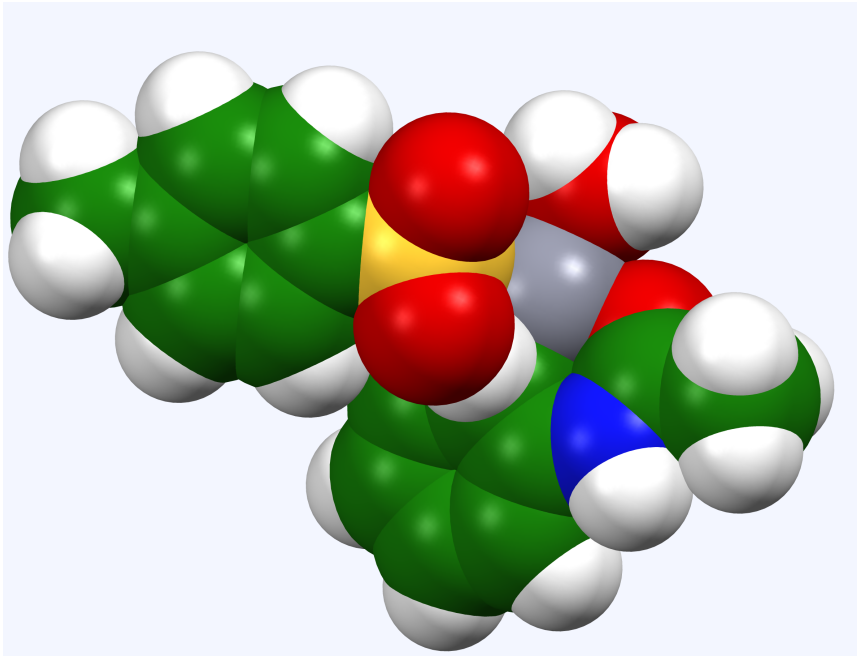
1 1

C	-0.46171000	1.04785800	0.05838000
C	-1.83928900	0.91763400	0.33718800
C	-2.72488300	1.95438100	0.05417300
C	-2.25796600	3.10941600	-0.56429700
C	-0.91356500	3.24023800	-0.91624400
C	-0.03221700	2.21775100	-0.60622400
N	-2.38434400	-0.26249400	0.89901700
C	-2.12945100	-1.51163800	0.48584600
C	-2.97113200	-2.62233200	1.03214400
Pd	0.53189800	-0.75016100	-0.44963700
O	2.36658300	0.10507400	-0.30546000
C	2.58433700	0.69456700	0.81719500
C	4.00990900	1.09804500	1.08302700
O	-1.24207500	-1.78285000	-0.35867300
O	1.68448800	0.94394000	1.64978500
H	-3.71944500	-2.27513900	1.74280400
H	-2.31265800	-3.34832100	1.51275300
H	-3.18474800	-0.14246600	1.50905400
H	-3.77937400	1.84417200	0.28476400
H	-2.95820200	3.90691100	-0.78916500
H	-0.56161100	4.13828500	-1.41046300
H	1.02457900	2.32490900	-0.83397700
H	-3.46287500	-3.11833200	0.19285200
H	4.34753100	1.75743100	0.28089300
H	4.08832900	1.60213500	2.04370600
H	4.64098800	0.20736000	1.07030800
H	0.40745500	0.79448900	0.92945300
O	1.49864300	-2.55961700	-1.12953900
H	2.45695100	-2.51630600	-1.00019800
H	1.19087000	-3.35817700	-0.67863900



Scheme 5 b) CMD with sulfonate

- Zero-point correction= 0.313066 (Hartree/Particle)\
- Thermal correction to Energy= 0.335980\
- Thermal correction to Enthalpy= 0.336924\
- Thermal correction to Gibbs Free Energy= 0.259566\
- Sum of electronic and zero-point Energies= -1538.357939\
- Sum of electronic and thermal Energies= -1538.335025\
- Sum of electronic and thermal Enthalpies= -1538.334081\
- Sum of electronic and thermal Free Energies= -1538.411439\
- \
- rm062x\
- \
- ASCTS03\
- \
- 1 1\
- C -1.34158400 1.13090400 -0.14243600\
- C -2.50966900 1.73144900 0.39679100\
- C -2.69442900 3.11016400 0.33352200\
- C -1.76850700 3.89547500 -0.34341200\
- C -0.65316800 3.32734400 -0.96852100\
- C -0.45168700 1.96370600 -0.87266900\
- N -3.51755500 0.97290500 1.01852200\
- C -3.97341000 -0.22378100 0.60901700\
- C -5.17351000 -0.79288900 1.29705500\
- Pd -1.43330400 -0.85071800 -0.67230200\
- O 0.65882700 -0.91521100 -0.76654000\
- O -3.45139900 -0.86569200 -0.33168600\
- O 1.26434400 -2.29119600 1.21716600\
- H -4.85536800 -1.67340600 1.86068100\
- H -5.88199900 -1.11899400 0.53447100\
- H -4.07620600 1.45334500 1.71506600\
- H -3.57791300 3.55957200 0.77407500\
- H -1.93168900 4.96652800 -0.40086400\
- H 0.04919800 3.95202200 -1.50751800\
- H 0.43188300 1.50596000 -1.30888900\
- H -5.65102300 -0.08335700 1.97053800\
- H -0.58360900 0.59803700 0.72602600\
- O -1.53645500 -2.94961700 -1.25918300\
- H -0.70132000 -3.40313200 -1.07502200\
- H -2.22726400 -3.44222600 -0.79453300\
- C 2.91082500 -0.37711400 0.43594100\
- C 3.15488500 0.99326200 0.36033100\
- C 3.93077600 -1.31265900 0.30785000\
- C 4.45591700 1.42408100 0.14495300\
- H 2.34560600 1.70556300 0.48627300\
- C 5.22792800 -0.85777900 0.09055600\
- H 3.71367900 -2.37250100 0.38585700\
- C 5.50715400 0.50812200 0.00238900\
- H 4.66416400 2.48858700 0.09125200\
- H 6.03469600 -1.57710200 -0.00925800\
- C 6.90763300 1.00093000 -0.24388300\
- H 7.62762700 0.18141700 -0.21758500\
- H 6.97642000 1.48550500 -1.22243000\
- H 7.19657600 1.74107200 0.50714200\
- S 1.25622300 -0.95354900 0.64123600\
- O 0.53054900 0.08238000 1.46227800}



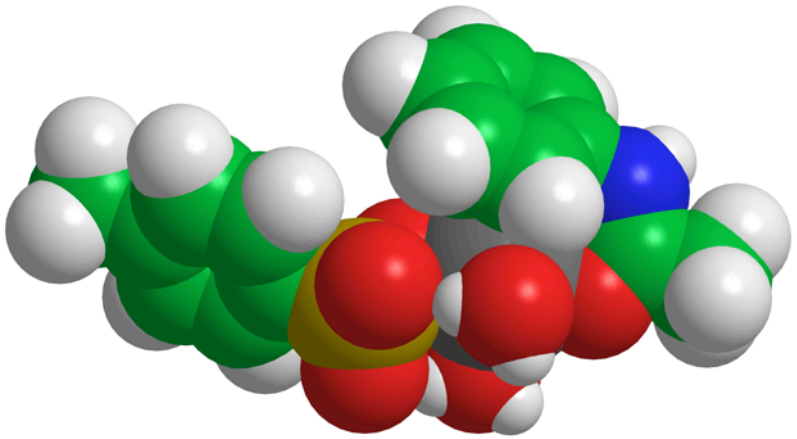
- Structures and energies of intermediates on the general base promoted reaction pathway of Scheme 6, Fig. 3

AWGBR1 (**8a**)

- Zero-point correction= 0.344855 (Hartree/Particle)
- Thermal correction to Energy= 0.371672
- Thermal correction to Enthalpy= 0.372617
- Thermal correction to Gibbs Free Energy= 0.286304
- Sum of electronic and zero-point Energies= -1614.767400
- Sum of electronic and thermal Energies= -1614.740582
- Sum of electronic and thermal Enthalpies= -1614.739638
- Sum of electronic and thermal Free Energies= -1614.825951
- rm062x
- AWGBR

1 1

H	2.89237400	3.17489600	-1.70355200
C	2.28287900	2.83563400	-0.87345400
C	2.74064100	1.81114600	-0.04986800
C	1.03956200	3.40473800	-0.61231800
C	0.24540700	2.95140100	0.44440700
H	0.68029000	4.20339400	-1.25210700
N	4.03887000	1.26086800	-0.26524700
H	4.80969400	1.91028900	-0.37168100
C	4.30195700	-0.04252000	-0.33813600
O	3.39565800	-0.91911900	-0.33105900
Pd	1.40523200	-0.52311300	-0.28340400
H	-0.72606900	3.39798700	0.62242800
C	1.96675700	1.35171800	1.03957400
O	-0.58890200	-0.15994400	-0.41118200
O	1.03396600	-2.32171500	-1.39634100
H	0.15357400	-2.63516000	-1.08875100
H	1.67974300	-3.01203900	-1.18796900
C	0.70561300	1.93541800	1.26915100
H	0.10470800	1.57603900	2.09835700
S	-1.49088800	-1.10585400	0.40832200
O	-1.40536000	-2.46746300	-0.15435600
O	-1.19693600	-0.99159700	1.84412800
C	-3.10339800	-0.45982600	0.11385600
C	-3.61296800	0.49045300	0.99410800
C	-3.81664300	-0.88344100	-1.00488600
C	-4.87146500	1.02353800	0.74276000
H	-3.03695800	0.79409400	1.86176100
C	-5.07168300	-0.33585400	-1.23772600
H	-3.39839100	-1.63153100	-1.66995600
C	-5.61586300	0.61939900	-0.37047400
H	-5.64207800	-0.65511000	-2.10481200
H	-5.28396900	1.76185300	1.42351600
C	-6.99216000	1.17494600	-0.61923700
H	-7.17810900	1.30057400	-1.68823000
H	-7.75285600	0.49026800	-0.23081200
H	-7.12605000	2.13877700	-0.12476800
H	2.39982600	0.68058200	1.77821500
C	5.72326200	-0.49200600	-0.43957000
H	5.82036000	-1.14187500	-1.31037200
H	6.41769300	0.34292000	-0.51559900
H	5.95674900	-1.07974200	0.45100100
O	1.54955400	-1.52251800	2.26137400
H	1.75496500	-2.46192400	2.19107900
H	0.58070300	-1.47313100	2.33276300



AWGBTS4F(**8a,9a** TS)

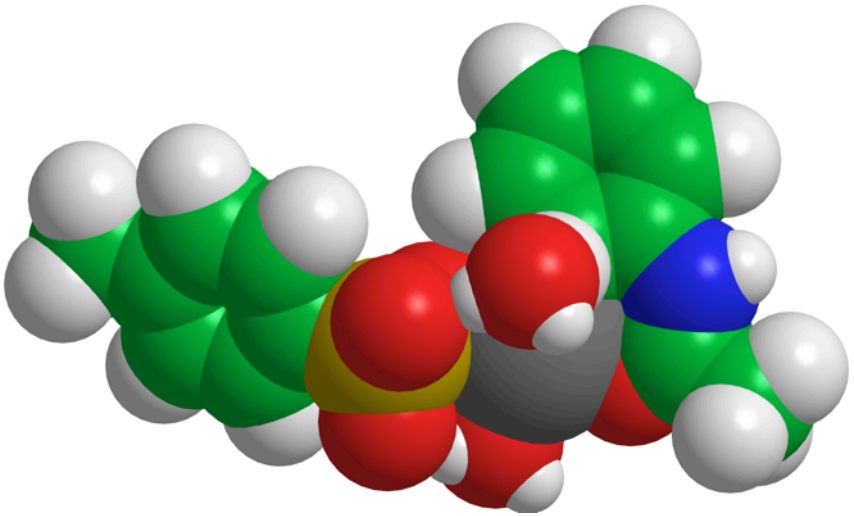
- Zero-point correction= 0.340204 (Hartree/Particle)
- Thermal correction to Energy= 0.365978
- Thermal correction to Enthalpy= 0.366922
- Thermal correction to Gibbs Free Energy= 0.282969
- Sum of electronic and zero-point Energies= -1614.754876
- Sum of electronic and thermal Energies= -1614.729101
- Sum of electronic and thermal Enthalpies= -1614.728157
- Sum of electronic and thermal Free Energies= -1614.812110

- rm062x

- AWGBTS4F

- 1 1

H	4.89390900	2.81405500	-0.41792700
C	3.82161400	2.65911200	-0.35981400
C	3.31482100	1.39652000	-0.06071400
C	2.94462300	3.70626700	-0.61478800
C	1.56066800	3.51500400	-0.56914400
H	3.34865900	4.68232800	-0.86250100
N	4.25568400	0.37512100	0.17937700
H	5.16916100	0.68123400	0.49458600
C	4.13980800	-0.92459800	-0.12572600
O	3.10751700	-1.42224600	-0.63208100
Pd	1.20687700	-0.71149300	-0.45681000
H	0.88813900	4.33940300	-0.77530800
C	1.91878600	1.17556500	0.04413000
O	-0.77264000	-0.09023600	-0.26436700
O	0.49127600	-2.63236900	-1.13331800
H	-0.31877300	-2.79432900	-0.60265000
H	1.11260500	-3.34937600	-0.94641300
C	1.06132100	2.26590600	-0.24760200
H	-0.00972500	2.10411400	-0.18022100
S	-1.66851300	-0.80806900	0.74748400
O	-1.60666400	-2.26902800	0.55572000
O	-1.37255800	-0.34540800	2.11770700
C	-3.28876500	-0.25481100	0.32224800
C	-3.73289500	0.97545200	0.79704900
C	-4.06980100	-1.04001800	-0.52251100
C	-4.98951600	1.42561100	0.40733500
H	-3.11131900	1.56162100	1.46598300
C	-5.32256800	-0.57267000	-0.89704600
H	-3.70254300	-2.00068300	-0.86655100
C	-5.79641200	0.66470200	-0.44450300
H	-5.94571600	-1.17761400	-1.54913300
H	-5.35132500	2.38153400	0.77308800
C	-7.14847800	1.16184000	-0.88089200
H	-7.44620500	2.04806400	-0.31801700
H	-7.13487200	1.42250600	-1.94360800
H	-7.91027200	0.39015700	-0.74410300
H	1.59232200	0.69557600	1.18292800
C	5.31301600	-1.81716900	0.13422600
H	5.51546600	-2.38988900	-0.77184400
H	6.20375900	-1.26638600	0.43180800
H	5.03714200	-2.51998300	0.92401600
O	1.18657600	0.44913700	2.51193300
H	1.69083500	-0.28224700	2.89643200
H	0.24344400	0.15276200	2.46909500



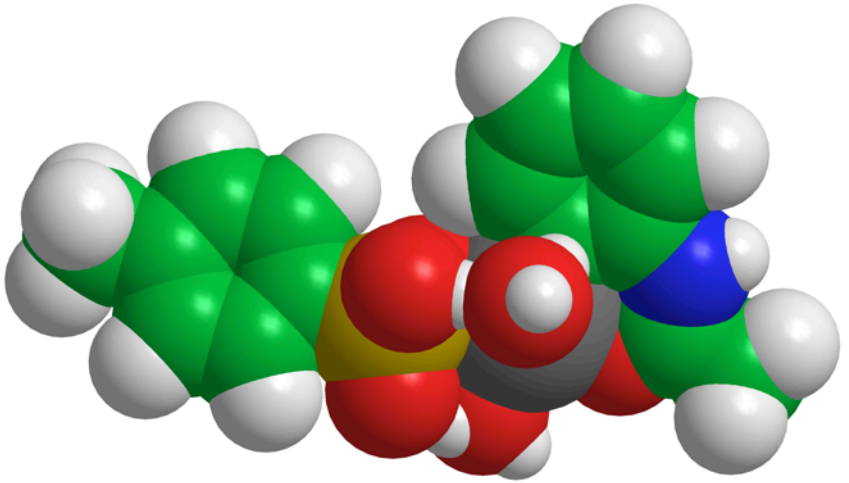
AWGBP2 (**9a**)

- Zero-point correction= 0.343838 (Hartree/Particle)
- Thermal correction to Energy= 0.370538
- Thermal correction to Enthalpy= 0.371482
- Thermal correction to Gibbs Free Energy= 0.285123
- Sum of electronic and zero-point Energies= -1614.785554
- Sum of electronic and thermal Energies= -1614.758854
- Sum of electronic and thermal Enthalpies= -1614.757910
- Sum of electronic and thermal Free Energies= -1614.844268

- AWGBP

- 1 1

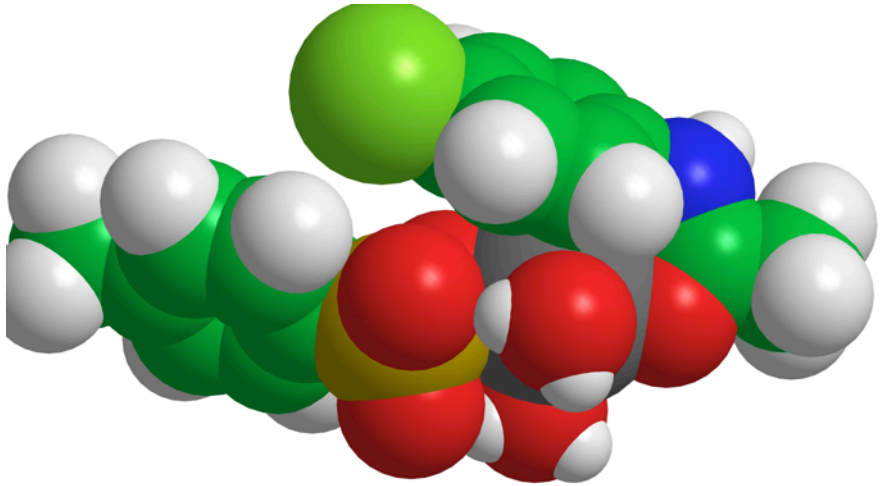
H	4.82383300	2.81306700	0.29174000
C	3.77652000	2.62512600	0.07279900
C	3.33491100	1.30491700	-0.09072700
C	2.89282600	3.68508900	-0.05259400
C	1.55443800	3.43617500	-0.34767000
H	3.25191700	4.70004700	0.07604300
N	4.33386600	0.30846300	0.03839400
H	5.25334500	0.64963600	0.28932400
C	4.24123300	-1.00149000	-0.19469200
O	3.17586800	-1.57285000	-0.51867600
Pd	1.28732800	-0.76938000	-0.53255200
H	0.85252500	4.25592100	-0.45639800
C	1.98569000	1.03584200	-0.36899900
O	-0.80593100	-0.15605100	-0.55523800
O	0.48719000	-2.86010100	-0.65409300
H	-0.23330800	-2.91720900	-0.00363600
C	1.11320600	2.12527500	-0.50288300
H	0.06985700	1.93852200	-0.73140700
S	-1.64800600	-0.49412600	0.62985600
O	-1.50904500	-1.86677600	1.10833700
O	-1.36043600	0.53528800	1.75430400
C	-3.30968700	-0.14261700	0.19876400
C	-3.59298300	1.02771500	-0.50465900
C	-4.29973400	-1.04323000	0.57451900
C	-4.91401600	1.29327100	-0.83134300
H	-2.79816500	1.70591100	-0.79770600
C	-5.61676100	-0.75389200	0.23333300
H	-4.04205200	-1.94836800	1.11317300
C	-5.94090800	0.41160900	-0.46650400
H	-6.40347900	-1.44754100	0.51276800
H	-5.15615100	2.19560800	-1.38407500
C	-7.37009000	0.73101700	-0.81094000
H	-7.99233200	-0.16526100	-0.79185300
H	-7.78236300	1.44283800	-0.08886400
H	-7.44248300	1.18777600	-1.80050500
C	5.48487600	-1.82933100	-0.06612000
H	6.35699200	-1.24114700	0.21538100
H	5.30807200	-2.60506300	0.68115300
H	5.66894300	-2.31940600	-1.02415400
H	-0.35922400	0.51073500	2.11973800
O	0.96494900	0.49806000	2.59014700
H	1.07881500	0.85619900	3.48170000
H	1.55573100	0.99404000	2.00109900
H	1.14558700	-3.52144100	-0.40455800



AWGBRCl

- Zero-point correction= 0.334895 (Hartree/Particle)
- Thermal correction to Energy= 0.362923
- Thermal correction to Enthalpy= 0.363867
- Thermal correction to Gibbs Free Energy= 0.274565
- Sum of electronic and zero-point Energies= -2074.340052
- Sum of electronic and thermal Energies= -2074.312024
- Sum of electronic and thermal Enthalpies= -2074.311080
- Sum of electronic and thermal Free Energies= -2074.400382
- rm062x
- AWGBRCl

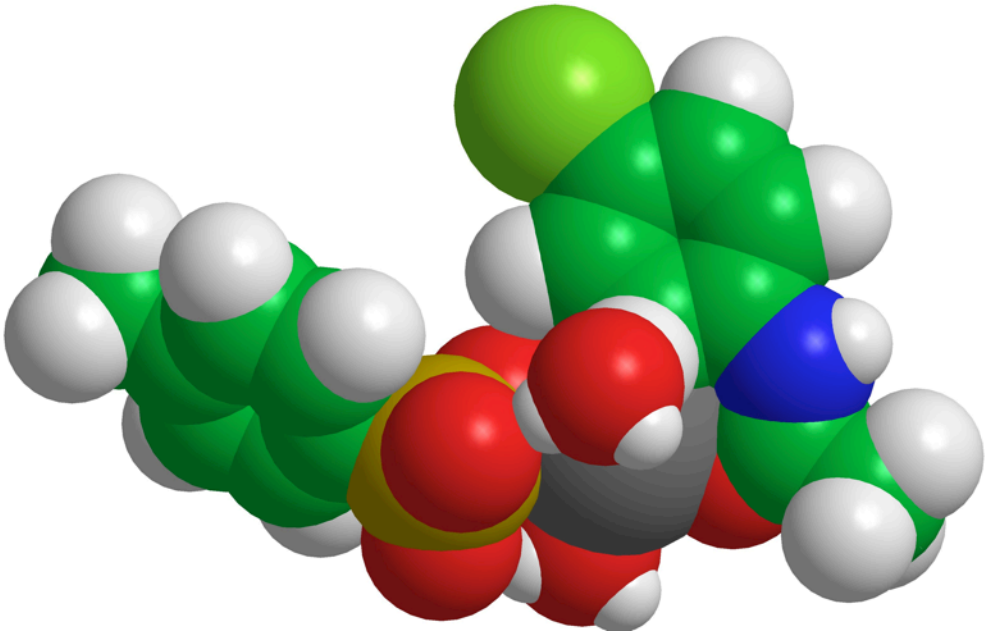
- 1 1
- H 2.11486500 2.33689300 -2.43266200
- C 1.73989300 2.22264900 -1.42176200
- C 2.53340100 1.58882000 -0.45160500
- C 0.48622400 2.69011700 -1.06990200
- C 0.02535500 2.53107700 0.24376300
- H -0.14640100 3.16799000 -1.80884900
- N 3.88367700 1.21940600 -0.76614500
- H 4.51038800 1.95621600 -1.06951700
- C 4.37687000 -0.00475000 -0.59928300
- O 3.63816600 -0.97911500 -0.27949200
- Pd 1.63565100 -0.69943500 -0.20016600
- C 2.07310900 1.45083200 0.87603300
- O -0.36283600 -0.38874800 -0.31984500
- O 1.28215800 -2.70664400 -0.87918400
- H 0.43650300 -2.95686100 -0.43890500
- H 1.96559900 -3.32260200 -0.57826800
- C 0.80011400 1.92906500 1.21890300
- H 0.43050700 1.81540500 2.23110700
- S -1.26123600 -1.15409100 0.67644400
- O -1.03312300 -2.60364200 0.51125000
- O -1.09652700 -0.64087900 2.04208200
- C -2.88495700 -0.75862200 0.12002000
- C -3.66576200 0.10783900 0.87763700
- C -3.34870000 -1.31922800 -1.06888900
- C -4.94316900 0.41985500 0.42578400
- H -3.27546700 0.52067700 1.80103000
- C -4.62605200 -0.99207700 -1.50218400
- H -2.72458800 -2.00118900 -1.63761300
- C -5.43955800 -0.12339300 -0.76295400
- H -5.00293300 -1.41836700 -2.42689700
- H -5.56517800 1.09340100 1.00747500
- C -6.83641400 0.19196800 -1.22517800
- H -6.90849800 0.16185400 -2.31432400
- H -7.54209200 -0.54380400 -0.82624600
- H -7.15435800 1.17738700 -0.87899200
- H 2.73095200 1.05996600 1.64644500
- C 5.83696000 -0.24382700 -0.79570700
- H 5.96204400 -1.02512200 -1.54703700
- H 6.36611400 0.65735300 -1.10115000
- H 6.24987500 -0.60997500 0.14673200
- O 1.65660800 -1.10815500 2.48650400
- H 1.84708000 -2.03094300 2.69219500
- H 0.69880700 -1.00658900 2.61960200
- Cl -1.56932600 3.07926200 0.64616600



AWGBTSCl (**8b,9b** TS)

- Zero-point correction= 0.331054 (Hartree/Particle)
- Thermal correction to Energy= 0.357737
- Thermal correction to Enthalpy= 0.358681
- Thermal correction to Gibbs Free Energy= 0.272886
- Sum of electronic and zero-point Energies= -2074.326003
- Sum of electronic and thermal Energies= -2074.299320
- Sum of electronic and thermal Enthalpies= -2074.298376
- Sum of electronic and thermal Free Energies= -2074.384171
- rm062x
- AWGBTSCl

- 1 1
- H 4.70201600 2.70970100 -0.03881000
- C 3.64061200 2.48667200 -0.01972500
- C 3.20069900 1.17738900 0.17646300
- C 2.71866800 3.50245500 -0.22194000
- C 1.35097200 3.21520200 -0.22503500
- H 3.05946500 4.51836300 -0.38919000
- N 4.18879800 0.19171500 0.36797800
- H 5.07065900 0.51592000 0.74954600
- C 4.15843700 -1.08147400 -0.05250500
- O 3.17812200 -1.58794200 -0.64710000
- Pd 1.23329900 -1.00631600 -0.48779800
- C 1.82064100 0.87701600 0.22291900
- O -0.76411600 -0.48114600 -0.30604000
- O 0.66326900 -2.87802200 -1.38139900
- H -0.20868900 -3.10927800 -0.99060100
- H 1.27975800 -3.59420400 -1.17588300
- C 0.90258800 1.92709700 -0.00782600
- H -0.16046000 1.71082800 0.01815800
- S -1.68407800 -1.38844900 0.51956100
- O -1.68417900 -2.75737400 -0.02716600
- O -1.35560800 -1.28796200 1.95468400
- C -3.27709200 -0.67770500 0.26713500
- C -3.70031100 0.34562400 1.11107200
- C -4.04974600 -1.10918900 -0.80733600
- C -4.92692300 0.94905000 0.86283400
- H -3.08232100 0.65521200 1.94719200
- C -5.27352900 -0.49191400 -1.03693000
- H -3.69926900 -1.91453300 -1.44392500
- C -5.72700100 0.54219500 -0.21081400
- H -5.88689700 -0.81662300 -1.87193100
- H -5.26951300 1.74916000 1.51200700
- C -7.06471900 1.18687300 -0.45616200
- H -7.84865900 0.65914500 0.09636800
- H -7.06802600 2.22696300 -0.12385600
- H -7.32876400 1.15669100 -1.51527900
- H 1.47824200 0.23362900 1.26803900
- C 5.36555700 -1.93225600 0.18818200
- H 5.59626200 -2.46887300 -0.73258900
- H 6.23090100 -1.35579800 0.51095100
- H 5.11303300 -2.66866100 0.95548900
- O 1.05101300 -0.19645700 2.54902400
- H 1.63916700 -0.88153200 2.89772500
- H 0.16292000 -0.61496700 2.43142900
- Cl 0.21005800 4.49774000 -0.49605800

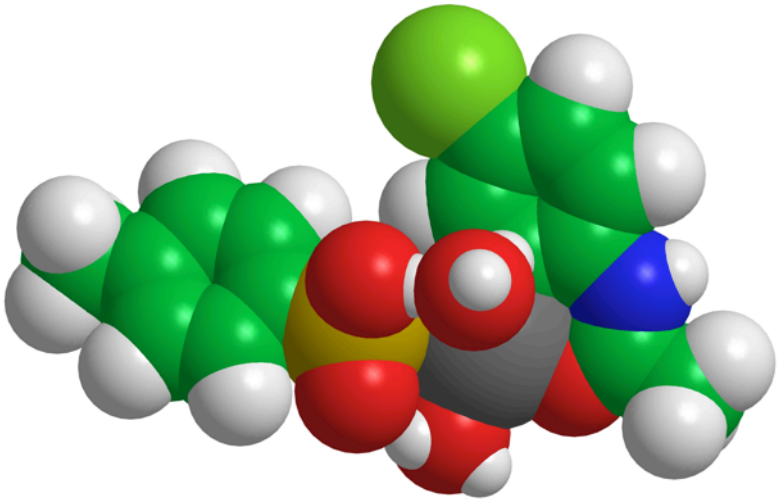


AWGBPCl (**9b**)

- Zero-point correction= 0.333626 (Hartree/Particle)
- Thermal correction to Energy= 0.361867
- Thermal correction to Enthalpy= 0.362811
- Thermal correction to Gibbs Free Energy= 0.270663
- Sum of electronic and zero-point Energies= -2074.360213
- Sum of electronic and thermal Energies= -2074.331972
- Sum of electronic and thermal Enthalpies= -2074.331028
- Sum of electronic and thermal Free Energies= -2074.423176

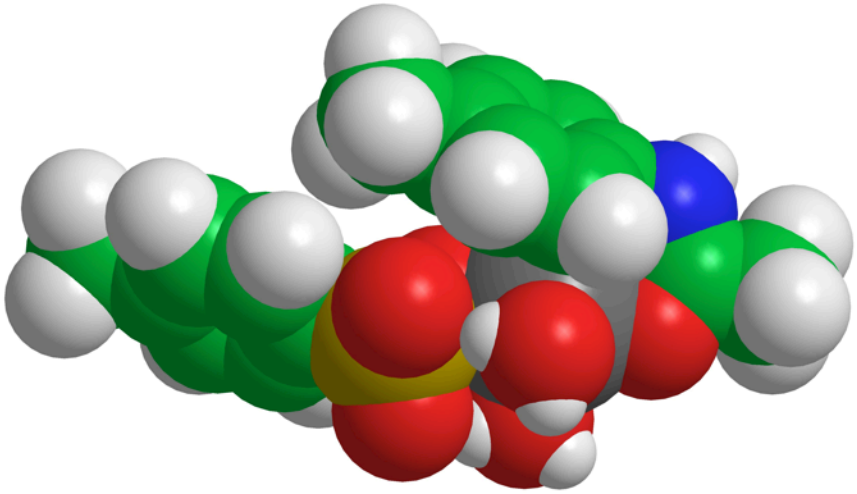
rm062x
AWGBPCl

- 1 1
- H 4.82100100 2.44365900 0.39062100
- C 3.76994900 2.26482700 0.18442800
- C 3.32010900 0.95579900 -0.03330700
- C 2.89632800 3.33797100 0.13476300
- C 1.55653200 3.09029400 -0.14264300
- H 3.25075100 4.34750800 0.30528400
- N 4.31517300 -0.04892400 0.03011100
- H 5.24302700 0.27700200 0.27026300
- C 4.20499800 -1.35148600 -0.23821500
- O 3.12640200 -1.90480400 -0.54814400
- Pd 1.24830000 -1.08439400 -0.53782100
- C 1.96459900 0.70595600 -0.29871100
- O -0.82953700 -0.43926700 -0.54943000
- O 0.43190300 -3.14818400 -0.74752700
- H -0.30205300 -3.22855100 -0.11481100
- C 1.09126500 1.79942400 -0.35814400
- H 0.04105600 1.64211100 -0.57311300
- S -1.68435800 -0.81403400 0.61714900
- O -1.57117400 -2.20836600 1.03450700
- O -1.37899200 0.16050300 1.78560400
- C -3.33668200 -0.41217000 0.19725100
- C -3.60071600 0.80576300 -0.42921700
- C -4.33973900 -1.32324200 0.50717400
- C -4.91608700 1.10863400 -0.74491500
- H -2.79654200 1.49364200 -0.66973600
- C -5.65102700 -0.99525500 0.17838700
- H -4.09714700 -2.26514100 0.98666500
- C -5.95623600 0.21754100 -0.44448100
- H -6.44777900 -1.69611100 0.40628700
- H -5.14328800 2.04910900 -1.23732300
- C -7.37817900 0.57872100 -0.77686400
- H -8.02370400 -0.30096000 -0.76786800
- H -7.76812300 1.29208100 -0.04411700
- H -7.44206100 1.05105300 -1.75987400
- C 5.44395000 -2.19309000 -0.16943200
- H 6.32831400 -1.62311400 0.11114600
- H 5.27736400 -2.99295700 0.55435900
- H 5.59963500 -2.65057900 -1.14835800
- H -0.38568200 0.08575100 2.15893500
- O 0.93911900 -0.00275000 2.63456100
- H 1.04269600 0.19546500 3.57584900
- H 1.54327900 0.57933500 2.14892800
- H 1.07776800 -3.82932800 -0.51902400
- Cl 0.43218100 4.42258600 -0.21720700



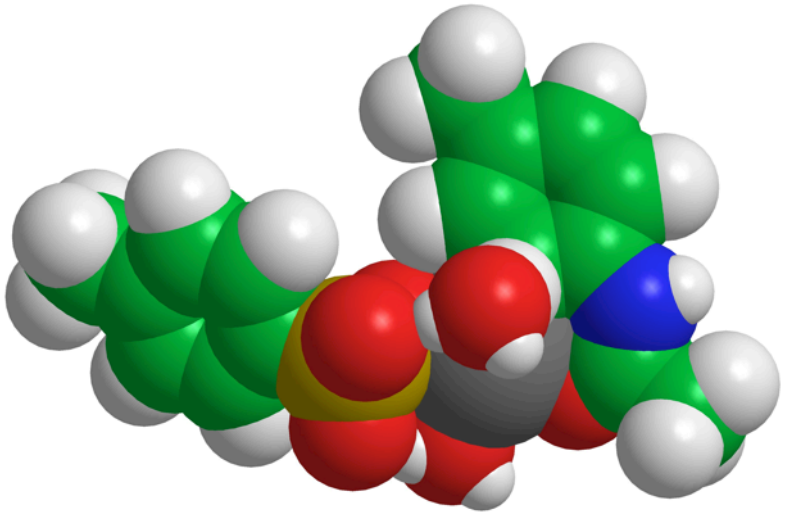
AWGBRMe (**9c**)

Zero-point correction=	0.371843 (Hartree/Particle)		
Thermal correction to Energy=	0.398910		
Thermal correction to Enthalpy=	0.399854		
Thermal correction to Gibbs Free Energy=	0.313836		
Sum of electronic and zero-point Energies=	-1654.041880		
Sum of electronic and thermal Energies=	-1654.014813		
Sum of electronic and thermal Enthalpies=	-1654.013869		
Sum of electronic and thermal Free Energies=	-1654.099886		
Rm062x			
AWGBRMe			
1 1			
H	2.00979500	2.54257200	-2.25381100
C	1.66977700	2.36092700	-1.23997300
C	2.48541800	1.63216500	-0.35555000
C	0.44980000	2.82957700	-0.79128500
C	0.00443300	2.60145800	0.52694500
H	-0.18871900	3.38097300	-1.47507900
N	3.82322100	1.27841600	-0.74338100
H	4.44616900	2.03179600	-1.01164000
C	4.31135800	0.04552600	-0.65849200
O	3.56915300	-0.93694700	-0.36963100
Pd	1.57719900	-0.61197200	-0.24062100
C	2.07386500	1.41685200	0.97917900
O	-0.42438200	-0.25704600	-0.32415800
O	1.16527300	-2.62067400	-0.87282500
H	0.30906400	-2.84015700	-0.43569900
H	1.83031600	-3.24816100	-0.55552200
C	0.82875900	1.90787700	1.40114900
H	0.51146000	1.72635700	2.42257400
S	-1.33324900	-1.00271100	0.67161900
O	-1.14638100	-2.45842100	0.50018100
O	-1.15601800	-0.50619600	2.04176200
C	-2.94827400	-0.56367300	0.11772700
C	-3.75080600	0.23545900	0.92458000
C	-3.38470100	-1.02831800	-1.12263600
C	-5.01933900	0.58212200	0.46893500
H	-3.38447100	0.57535100	1.88725100
C	-4.65248600	-0.67040000	-1.55735800
H	-2.74520700	-1.65978100	-1.73122300
C	-5.48582500	0.13683500	-0.77049400
H	-5.00675800	-1.02266400	-2.52143200
H	-5.65585300	1.20731400	1.08750200
C	-6.86902500	0.49047100	-1.24622000
H	-6.87910000	0.67411100	-2.32292900
H	-7.56134100	-0.33360700	-1.04654800
H	-7.24857600	1.37748800	-0.73576200
H	2.75518800	0.96278200	1.69279900
C	5.76405200	-0.19493800	-0.90244000
H	5.86669900	-1.01795800	-1.61039800
H	6.26900700	0.69209900	-1.28196200
H	6.22129400	-0.49817400	0.04256700
O	1.56681300	-1.30204200	2.36924200
H	1.65689500	-2.24104300	2.56986300
H	0.63831300	-1.08645400	2.55846700
C	-1.35731100	3.07094100	0.95015000
H	-2.12538900	2.49605400	0.42131800
H	-1.50799300	2.93469500	2.02227800
H	-1.50632800	4.12489400	0.70182800



AWGBTSMe (**8c,9c TS**)

- Zero-point correction= 0.367804 (Hartree/Particle)
- Thermal correction to Energy= 0.394458
- Thermal correction to Enthalpy= 0.395402
- Thermal correction to Gibbs Free Energy= 0.309820
- Sum of electronic and zero-point Energies= -1654.026840
- Sum of electronic and thermal Energies= -1654.000185
- Sum of electronic and thermal Enthalpies= -1653.999241
- Sum of electronic and thermal Free Energies= -1654.084824
- rm062x
- AWGBTSMe
- 1 1
- H 4.90478000 2.61615900 -0.20658100
- C 3.83114700 2.46340100 -0.16401700
- C 3.31546200 1.18549700 0.04516700
- C 2.96449600 3.53014200 -0.35002600
- C 1.56944700 3.36999600 -0.32757900
- H 3.38194500 4.51757300 -0.52781700
- N 4.24684900 0.14197200 0.21618300
- H 5.16284500 0.41852400 0.55025900
- C 4.11572300 -1.13515700 -0.16566000
- O 3.07441600 -1.59104400 -0.69301200
- Pd 1.18297000 -0.86333000 -0.48158100
- C 1.91798400 0.97864200 0.12880000
- O -0.79422300 -0.23044700 -0.26818800
- O 0.43926000 -2.75145600 -1.22700900
- H -0.37046500 -2.92111100 -0.69872500
- H 1.05158900 -3.48249200 -1.06703400
- C 1.07460000 2.09696200 -0.09053200
- H 0.00113900 1.93800800 -0.03684900
- S -1.69649300 -0.96931100 0.72126700
- O -1.64979900 -2.42466300 0.48635300
- O -1.39673100 -0.55154100 2.10563700
- C -3.31263500 -0.38711500 0.31879300
- C -3.72429700 0.85778600 0.79192400
- C -4.12628000 -1.16576400 -0.49665000
- C -4.97970600 1.32480600 0.42839600
- H -3.07734100 1.43920500 1.44085900
- C -5.38178700 -0.67974000 -0.84671700
- H -3.78426900 -2.13648000 -0.83832600
- C -5.82192200 0.56815900 -0.39727900
- H -6.02991800 -1.28142500 -1.47644600
- H -5.31776000 2.29020900 0.79311400
- C -7.16849700 1.10533000 -0.80159200
- H -7.67126100 1.58061800 0.04401800
- H -7.05629300 1.86276300 -1.58380900
- H -7.81142000 0.31355100 -1.19005900
- H 1.58990800 0.42840000 1.23807100
- C 5.27993300 -2.05566500 0.03029400
- H 5.45889500 -2.58439700 -0.90682400
- H 6.18402400 -1.53396600 0.34035300
- H 5.00648000 -2.79383000 0.78819800
- O 1.18984400 0.07696100 2.54395100
- H 1.65446500 -0.71601200 2.84804100
- H 0.23082500 -0.16285700 2.48311700
- C 0.66177000 4.54951300 -0.54681200
- H 0.84036400 5.32168900 0.20633900
- H 0.84299700 4.99817000 -1.52744800
- H -0.38697300 4.25279800 -0.49417900



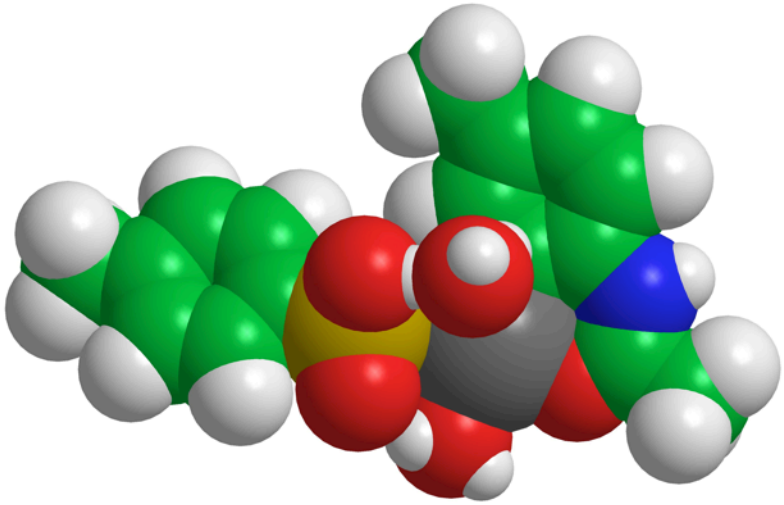
AWGBPMe (**9c**)

- Zero-point correction= 0.370902 (Hartree/Particle)
- Thermal correction to Energy= 0.398811
- Thermal correction to Enthalpy= 0.399755
- Thermal correction to Gibbs Free Energy= 0.309585
- Sum of electronic and zero-point Energies= -1654.057496
- Sum of electronic and thermal Energies= -1654.029587
- Sum of electronic and thermal Enthalpies= -1654.028643
- Sum of electronic and thermal Free Energies= -1654.118813

- rm062x

- AWGBPMe

- 1 1
- H 4.91980200 2.55172700 0.18316600
- C 3.85629600 2.38460300 0.03590100
- C 3.38267100 1.07543000 -0.12520400
- C 2.98662900 3.46048400 0.00790500
- C 1.61623400 3.26325000 -0.18765700
- H 3.37703800 4.46536700 0.13745600
- N 4.36993100 0.05961000 -0.08715300
- H 5.31503700 0.38436000 0.07421700
- C 4.22585200 -1.25190300 -0.27305200
- O 3.12145100 -1.80299000 -0.48254300
- Pd 1.26085200 -0.94078400 -0.47318600
- C 2.01278200 0.84379500 -0.31073200
- O -0.82188100 -0.28267000 -0.51216400
- O 0.41721800 -3.01412000 -0.59994400
- H -0.30672200 -3.06097300 0.04746200
- C 1.15620400 1.95431800 -0.34139300
- H 0.09375000 1.79137700 -0.49311600
- S -1.69631600 -0.61625300 0.64993700
- O -1.57308900 -1.98727100 1.13724900
- O -1.43891100 0.41800200 1.77669600
- C -3.34721900 -0.26327900 0.17948000
- C -3.61596800 0.91598300 -0.51474400
- C -4.34478900 -1.16765100 0.52468600
- C -4.93012000 1.18623700 -0.86422200
- H -2.81524000 1.59852300 -0.78104600
- C -5.65486400 -0.87306400 0.16177600
- H -4.09794100 -2.07878200 1.05829400
- C -5.96462300 0.30130800 -0.52929400
- H -6.44748800 -1.56898000 0.41783900
- H -5.16128400 2.09593900 -1.40961000
- C -7.38683900 0.62820300 -0.89484500
- H -8.01431100 -0.26450900 -0.88439700
- H -7.80540300 1.34293500 -0.17929100
- H -7.44216400 1.08497000 -1.88554600
- C 5.45597600 -2.10931100 -0.23538800
- H 6.35684300 -1.54448000 -0.00015100
- H 5.30829600 -2.89259900 0.50993100
- H 5.57031800 -2.58765100 -1.21028800
- H -0.43988500 0.41264500 2.15199300
- O 0.87774300 0.42616200 2.62642500
- H 0.98506600 0.80201900 3.51143200
- H 1.45768600 0.92301800 2.02698300
- H 1.06552500 -3.68439800 -0.34781000
- C 0.66782200 4.43131800 -0.25011100
- H 0.77384000 4.96293800 -1.20086500
- H -0.36987800 4.10266500 -0.16303300
- H 0.87294900 5.14751300 0.54962700

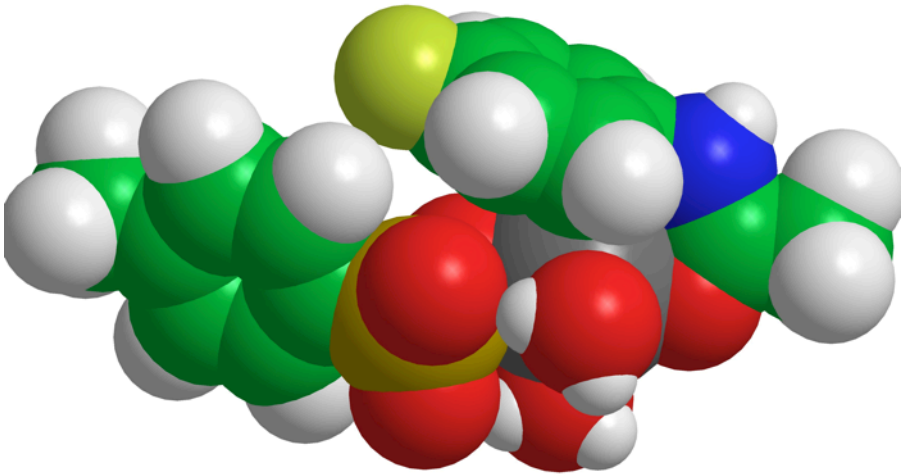


AWGBRF (**8d**)

- Zero-point correction= 0.336147 (Hartree/Particle)
- Thermal correction to Energy= 0.363156
- Thermal correction to Enthalpy= 0.364100
- Thermal correction to Gibbs Free Energy= 0.277007
- Sum of electronic and zero-point Energies= -1713.979784
- Sum of electronic and thermal Energies= -1713.952775
- Sum of electronic and thermal Enthalpies= -1713.951831
- Sum of electronic and thermal Free Energies= -1714.038923
- rm062x

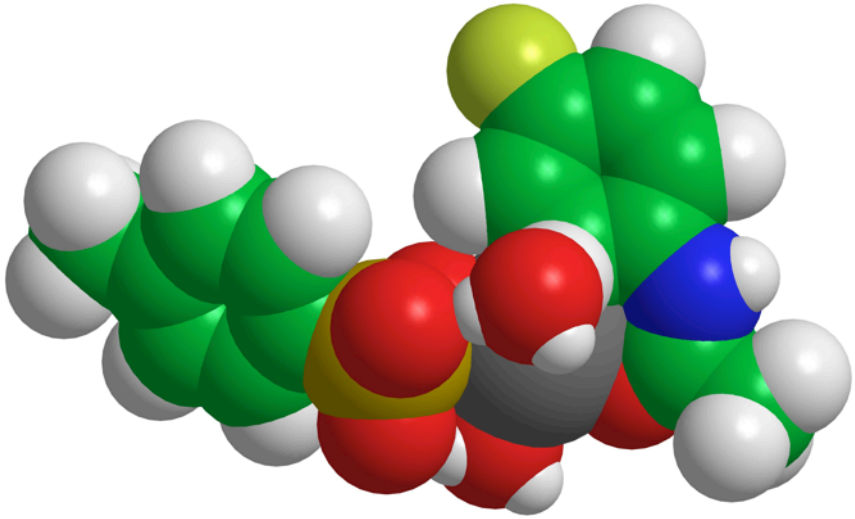
- AWGBRF
- 1 1

H	2.10412200	2.25194000	-2.17738400
C	1.62539600	2.18413700	-1.20633600
C	2.34012800	1.62077100	-0.12149800
C	0.34210300	2.65838900	-1.00651900
C	-0.20405500	2.58802600	0.27424500
H	-0.23789900	3.08583200	-1.81525900
N	3.75625700	1.38465400	-0.26271100
H	4.36845400	2.19000000	-0.19461700
C	4.29860800	0.18532400	-0.42861100
O	3.57817200	-0.85025800	-0.52233700
Pd	1.58789000	-0.59606000	-0.39474900
C	1.76238700	1.58175400	1.17053100
O	-0.42098800	-0.31820200	-0.38383300
O	1.27186300	-2.64934700	-0.93882600
H	0.41021600	-2.90296300	-0.53444500
H	1.95465400	-3.23119100	-0.57596900
C	0.47297300	2.05977000	1.36409800
H	-0.00294100	2.02477300	2.33626700
S	-1.27271400	-1.13628300	0.61068000
O	-1.11957100	-2.57567000	0.32375600
O	-0.99003200	-0.73270700	1.99410200
C	-2.91076400	-0.63839200	0.19674800
C	-3.40719800	0.54564000	0.73772100
C	-3.65189600	-1.40753200	-0.69469900
C	-4.67894000	0.96210300	0.36754900
H	-2.80931200	1.12490600	1.43311200
C	-4.92443500	-0.97323200	-1.04815700
H	-3.24033500	-2.32813200	-1.09396100
C	-5.45307500	0.21166100	-0.52593800
H	-5.51709400	-1.56369000	-1.74017300
H	-5.08013000	1.88378600	0.77819700
C	-6.84082900	0.66217900	-0.89493600
H	-7.14912100	0.24741800	-1.85653900
H	-7.56108700	0.32904900	-0.14088700
H	-6.89945500	1.75149900	-0.94792900
H	2.34351200	1.19471300	2.00112200
C	5.78186200	0.03890500	-0.50023700
H	6.03107900	-0.51381900	-1.40713800
H	6.29224000	1.00054600	-0.49645800
H	6.10559600	-0.55291500	0.35877800
O	1.77620000	-1.33809200	2.18925600
H	1.95905900	-2.26600100	2.37769600
H	0.83752400	-1.20675700	2.40662300
F	-1.44012900	3.04721100	0.45720500



AWGBTSF (**8d,9d** TS)

- Zero-point correction= 0.331885 (Hartree/Particle)
- Thermal correction to Energy= 0.358432
- Thermal correction to Enthalpy= 0.359376
- Thermal correction to Gibbs Free Energy= 0.273387
- Sum of electronic and zero-point Energies= -1713.963679
- Sum of electronic and thermal Energies= -1713.937132
- Sum of electronic and thermal Enthalpies= -1713.936187
- Sum of electronic and thermal Free Energies= -1714.022176
- rm062x
- AWGBTSF
- 1 1
- H 4.89804500 2.61564700 -0.27286500
- C 3.82504300 2.47051800 -0.20600000
- C 3.30319700 1.19990700 0.04163400
- C 2.96770800 3.54359300 -0.39387900
- C 1.59107600 3.34083700 -0.32997000
- H 3.35248000 4.53622800 -0.59938500
- N 4.23277500 0.15377000 0.21820500
- H 5.14826600 0.42883800 0.55507800
- C 4.10087600 -1.12324800 -0.16175200
- O 3.05908900 -1.58085300 -0.68911200
- Pd 1.16905900 -0.85926000 -0.47406600
- C 1.90875300 0.99609100 0.15362900
- O -0.79501600 -0.21719100 -0.25724000
- O 0.42943300 -2.72678000 -1.24235200
- H -0.38434000 -2.90385100 -0.72185400
- H 1.04082600 -3.46109200 -1.09244100
- C 1.05409400 2.10062500 -0.06512200
- H -0.02141100 1.97564600 0.00560000
- S -1.70826700 -0.96673800 0.71893000
- O -1.66682800 -2.41755900 0.45848000
- O -1.40952100 -0.57187100 2.10918100
- C -3.31696400 -0.36681100 0.31536700
- C -3.72392200 0.87093800 0.80723200
- C -4.13028500 -1.12792400 -0.51892800
- C -4.97577300 1.35151200 0.44392700
- H -3.07820700 1.43782000 1.47012600
- C -5.37980800 -0.62959100 -0.86696800
- H -3.79141300 -2.09483900 -0.87423700
- C -5.81609200 0.61449900 -0.39866400
- H -6.02853600 -1.21704400 -1.50969600
- H -5.31012600 2.31225100 0.82341700
- C -7.15694300 1.15853000 -0.81247800
- H -7.07697900 1.66852500 -1.77792400
- H -7.89055100 0.35720200 -0.92341400
- H -7.53365700 1.88025600 -0.08515300
- H 1.57825600 0.40254500 1.23596800
- C 5.26396900 -2.04463800 0.03437500
- H 5.44247700 -2.57252100 -0.90334800
- H 6.16837200 -1.52392700 0.34501900
- H 4.98915000 -2.78328500 0.79128600
- O 1.18738500 0.04120600 2.54862700
- H 1.65346700 -0.75357100 2.84585900
- H 0.22793000 -0.19538100 2.49680200
- F 0.77957600 4.38480700 -0.52302100



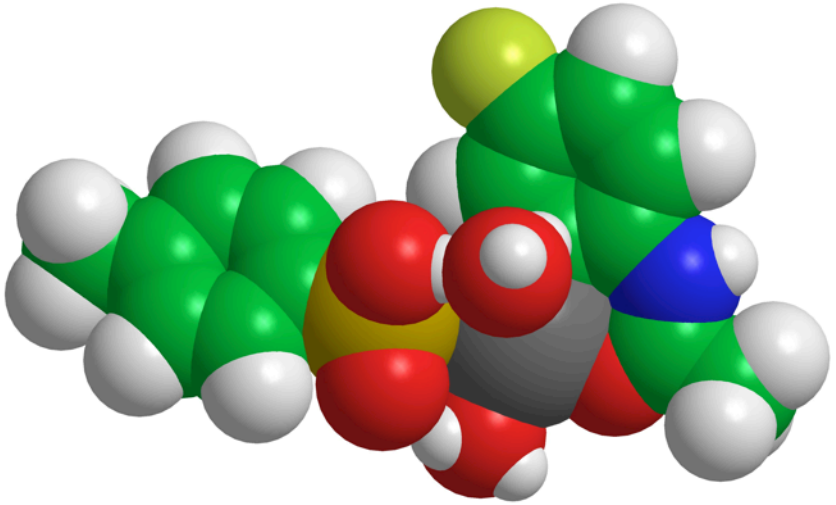
AWGPBF (**9d**)

- Zero-point correction= 0.335186 (Hartree/Particle)
- Thermal correction to Energy= 0.362909
- Thermal correction to Enthalpy= 0.363854
- Thermal correction to Gibbs Free Energy= 0.274621
- Sum of electronic and zero-point Energies= -1713.997111
- Sum of electronic and thermal Energies= -1713.969387
- Sum of electronic and thermal Enthalpies= -1713.968443
- Sum of electronic and thermal Free Energies= -1714.057676

- rm062x

- AWGBPF

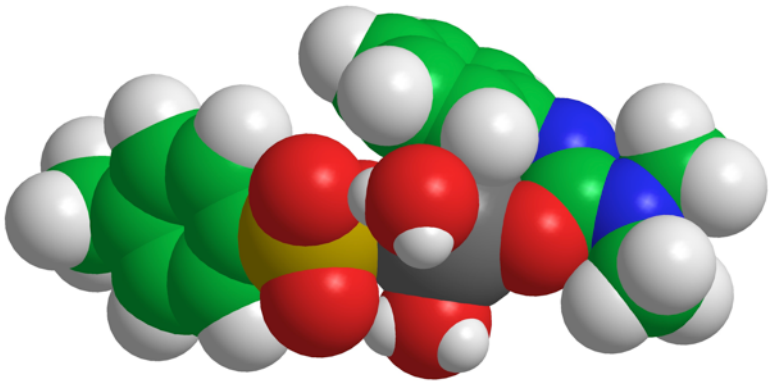
- 1 1
- H 4.82824100 2.59610500 0.37350400
- C 3.77883400 2.42254000 0.15495700
- C 3.32234800 1.11233700 -0.04470900
- C 2.91481800 3.50136500 0.06979900
- C 1.58378000 3.24718100 -0.22421300
- H 3.25830900 4.51722000 0.22240300
- N 4.31099300 0.10079600 0.04972500
- H 5.23533300 0.42359200 0.30677700
- C 4.20023600 -1.20026200 -0.21766900
- O 3.12446000 -1.74996500 -0.54773800
- Pd 1.24830300 -0.92483800 -0.53924700
- C 1.96877200 0.86589200 -0.32554500
- O -0.82662500 -0.27200000 -0.54865800
- O 0.42479000 -2.99238600 -0.71674200
- H -0.29840700 -3.06075100 -0.07040300
- C 1.10329300 1.96301800 -0.41936400
- H 0.05205300 1.82615300 -0.64438800
- S -1.67471600 -0.62916200 0.62793300
- O -1.54979600 -2.01389000 1.07368900
- O -1.37404300 0.37077000 1.77556600
- C -3.33139900 -0.25010400 0.20309400
- C -3.60336000 0.94137000 -0.46868700
- C -4.32940500 -1.15285800 0.55186600
- C -4.92139100 1.22641700 -0.79062600
- H -2.80263700 1.62122400 -0.74086200
- C -5.64322200 -0.84348100 0.21589300
- H -4.08057300 -2.07479100 1.06565200
- C -5.95623600 0.34327400 -0.45223100
- H -6.43612800 -1.53840000 0.47368500
- H -5.15470200 2.14575500 -1.31863300
- C -7.38156300 0.68404000 -0.79181800
- H -8.01514900 -0.20432400 -0.78090100
- H -7.78392300 1.39448800 -0.06288400
- H -7.44873700 1.15124200 -1.77693200
- C 5.43364900 -2.04784300 -0.12430800
- H 6.31597400 -1.48036400 0.16774700
- H 5.25205900 -2.84370800 0.60027600
- H 5.60333100 -2.51049500 -1.09850200
- H -0.37749700 0.31096200 2.14590200
- O 0.94652900 0.23906200 2.61928600
- H 1.06124600 0.51281300 3.54009100
- H 1.55655400 0.76802000 2.08217300
- H 1.07354300 -3.67059700 -0.48778800
- F 0.72891400 4.27660000 -0.31649200



UWGBRFF (**8e**)

- Zero-point correction= 0.390827 (Hartree/Particle)
- Thermal correction to Energy= 0.419779
- Thermal correction to Enthalpy= 0.420723
- Thermal correction to Gibbs Free Energy= 0.329746
- Sum of electronic and zero-point Energies= -1709.354964
- Sum of electronic and thermal Energies= -1709.326011
- Sum of electronic and thermal Enthalpies= -1709.325067
- Sum of electronic and thermal Free Energies= -1709.416045
- M062X

- UWGBRFF1
- 1 1
- H 1.91414900 3.17791500 -1.73586200
- C 1.50871200 2.81077300 -0.79918300
- C 2.19426600 1.81724800 -0.08672900
- C 0.32150100 3.31361200 -0.29049900
- C -0.21966900 2.83516600 0.91288300
- H -0.20245700 4.08463200 -0.84529000
- N 3.44413800 1.36823500 -0.55395400
- H 3.97109600 1.99791100 -1.14511000
- C 3.86901700 0.07416200 -0.43552300
- O 3.05344800 -0.86058500 -0.13647000
- Pd 1.05168100 -0.50493300 -0.11428400
- H -1.15369300 3.23920300 1.28539900
- C 1.66814100 1.32830000 1.13501100
- O -0.93836400 -0.10470600 -0.25704500
- O 0.64157300 -2.36331000 -1.10643900
- H -0.22759600 -2.64034800 -0.73574200
- H 1.28798600 -3.04553700 -0.87553300
- C 0.44914300 1.85624400 1.61937100
- H 0.05449000 1.47482300 2.55468000
- S -1.88689000 -0.96429200 0.59672400
- O -1.71843900 -2.38766500 0.24058500
- O -1.73989900 -0.65132200 2.02507800
- C -3.48040000 -0.43048300 0.06533200
- C -4.01254600 0.73378900 0.61056000
- C -4.16076400 -1.16686800 -0.90123900
- C -5.25721800 1.16807800 0.16849300
- H -3.46744900 1.27921200 1.37406600
- C -5.40399600 -0.71673100 -1.32598600
- H -3.72622000 -2.07826900 -1.29709000
- C -5.96665900 0.45334200 -0.80171100
- H -5.95042000 -1.28299900 -2.07459200
- H -5.68640100 2.07331900 0.58651400
- C -7.31590600 0.91967800 -1.27924200
- H -7.29663700 1.11748400 -2.35475500
- H -8.07411300 0.15144000 -1.10340300
- H -7.62548500 1.83214200 -0.76721000
- H 2.27764800 0.71181600 1.78953300
- O 0.97709800 -1.31295500 2.57667900
- H 1.09736200 -2.26758200 2.63766700
- H 0.01599700 -1.17392700 2.62373700
- N 5.15090700 -0.19452300 -0.64640000
- C 6.15597900 0.85553300 -0.79283600
- H 5.92674300 1.69467800 -0.13511500
- H 7.11935300 0.44152100 -0.49606500
- H 6.22340800 1.19661900 -1.83040100
- C 5.61237500 -1.57675200 -0.75384600
- H 6.18409300 -1.84721800 0.13716400
- H 4.75829700 -2.24131400 -0.85488300
- H 6.25223700 -1.66213400 -1.63400900

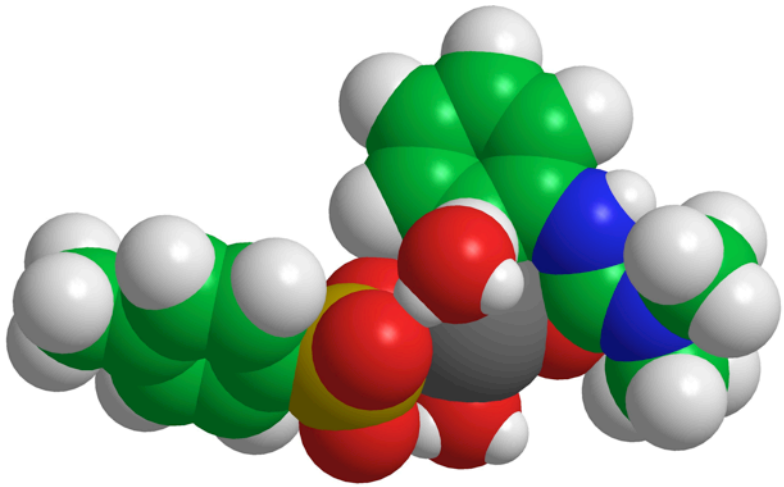


UWGBTSF (**8e,9e** TS)

- Zero-point correction= 0.386273 (Hartree/Particle)
- Thermal correction to Energy= 0.414722
- Thermal correction to Enthalpy= 0.415666
- Thermal correction to Gibbs Free Energy= 0.325741
- Sum of electronic and zero-point Energies= -1709.340596
- Sum of electronic and thermal Energies= -1709.312148
- Sum of electronic and thermal Enthalpies= -1709.311203
- Sum of electronic and thermal Free Energies= -1709.401129
- rm062x
- UWGBTSF

1 1

H	4.09084700	3.47905200	-0.26598900
C	3.05117400	3.17418900	-0.32634700
C	2.69915200	1.84571000	-0.07178200
C	2.07367400	4.08742100	-0.69056500
C	0.73016200	3.70789900	-0.80438300
H	2.36418200	5.11151400	-0.90169700
N	3.72197600	0.97479600	0.30963900
H	4.57130100	1.41967500	0.63350800
C	3.79928400	-0.35451600	-0.01350300
O	2.91847700	-0.91456700	-0.73186300
Pd	0.92324900	-0.51750300	-0.60983900
H	-0.01973500	4.43338900	-1.09735400
C	1.33750000	1.44001400	-0.11782800
O	-1.13457300	-0.15812200	-0.45590400
O	0.52184300	-2.54550800	-1.27827900
H	-0.34221700	-2.80321900	-0.88887500
H	1.18563900	-3.17862400	-0.97409500
C	0.37601400	2.40290100	-0.52762100
H	-0.66275800	2.09270100	-0.57956700
S	-1.94244800	-1.08577100	0.44885400
O	-1.89307400	-2.47383900	-0.04630600
O	-1.53391500	-0.92089300	1.85998000
C	-3.59840600	-0.49900500	0.28813000
C	-4.08027900	0.43429100	1.20235700
C	-4.37925500	-0.95967500	-0.76787500
C	-5.37431600	0.91460800	1.04486600
H	-3.45709300	0.76065700	2.02790200
C	-5.67080200	-0.46509700	-0.90763600
H	-3.98665500	-1.70155000	-1.45519000
C	-6.18320600	0.47817000	-0.01045300
H	-6.29373100	-0.82092000	-1.72264200
H	-5.76676800	1.63542000	1.75593600
C	-7.57335700	1.02930000	-0.18200500
H	-8.05900800	1.17781700	0.78507300
H	-7.53719700	2.00097500	-0.68506500
H	-8.19222800	0.36335300	-0.78612500
H	0.99773300	0.97855700	1.02522900
O	0.58350200	0.65870400	2.32492000
H	1.26366700	0.12391600	2.75918200
H	-0.21687300	0.08038800	2.23323200
N	4.86080300	-1.03326500	0.42170600
C	5.88279700	-0.42062700	1.26594000
H	5.42514200	0.10418500	2.10769600
H	6.50909400	-1.21657300	1.66524000
H	6.51838200	0.26383700	0.69495000
C	5.08023900	-2.41654800	0.00631300
H	6.04647600	-2.49096200	-0.49778300
H	5.08129200	-3.06454000	0.88565200
H	4.29045200	-2.72267500	-0.67375600

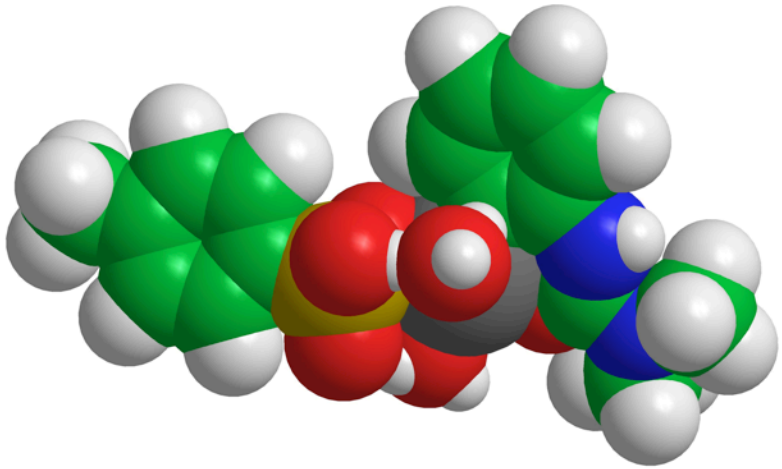


UWGBP (**9e**)

- Zero-point correction= 0.389033 (Hartree/Particle)
- Thermal correction to Energy= 0.418906
- Thermal correction to Enthalpy= 0.419850
- Thermal correction to Gibbs Free Energy= 0.325737
- Sum of electronic and zero-point Energies= -1709.368191
- Sum of electronic and thermal Energies= -1709.338319
- Sum of electronic and thermal Enthalpies= -1709.337374
- Sum of electronic and thermal Free Energies= -1709.431487
- Rm062x

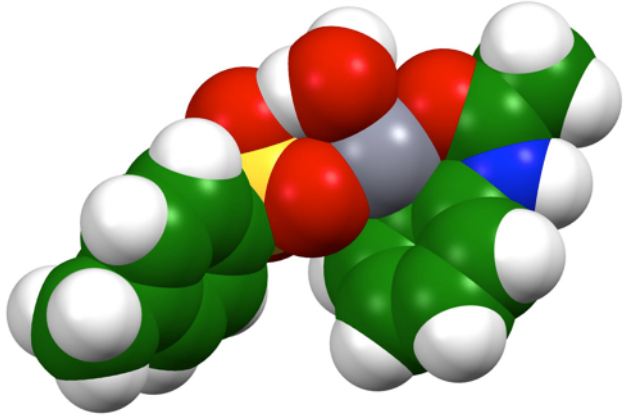
UWGBP

- 1 1
- H 4.18103100 3.22293800 0.43606200
- C 3.17629800 2.98278200 0.09951400
- C 2.80503200 1.63877300 -0.04496000
- C 2.27989100 3.99910400 -0.19828600
- C 1.00106400 3.68742200 -0.65356300
- H 2.58649200 5.03272800 -0.08073800
- N 3.78169300 0.67508000 0.29650100
- H 4.57825600 1.03211300 0.80446700
- C 3.84408000 -0.60272900 -0.16359700
- O 2.88876900 -1.12922400 -0.80289900
- Pd 0.92322000 -0.52532600 -0.63177500
- H 0.29611900 4.47516000 -0.89673100
- C 1.50889100 1.31410300 -0.47561100
- O -1.17967400 -0.00898700 -0.47765600
- O 0.25971800 -2.66727400 -0.78759000
- H -0.41701800 -2.79582100 -0.10140800
- C 0.62573900 2.35350600 -0.79026100
- H -0.37551900 2.10834200 -1.12945700
- S -1.97303400 -0.49753700 0.68694300
- O -1.70673400 -1.87807400 1.08111300
- O -1.77393700 0.48498100 1.86931400
- C -3.66609700 -0.28038800 0.28752300
- C -4.08442000 0.94243300 -0.23856900
- C -4.54133200 -1.33875800 0.49664000
- C -5.42462200 1.09537900 -0.55591800
- H -3.37560000 1.74848900 -0.39878200
- C -5.88186600 -1.15991200 0.16814500
- H -4.17893200 -2.27706100 0.90166000
- C -6.33943400 0.05067800 -0.35699000
- H -6.58129100 -1.97557100 0.32067100
- H -5.77244400 2.03745800 -0.96860300
- C -7.79144400 0.24802200 -0.69739100
- H -8.33903600 -0.69506600 -0.66385700
- H -8.25722800 0.93875200 0.01209000
- H -7.90153100 0.68117200 -1.69466200
- H -0.75147200 0.62049100 2.14321500
- O 0.59385900 0.79897500 2.48920200
- H 0.73582300 1.24126700 3.33776900
- H 1.06742800 1.30992500 1.81202100
- H 0.97840100 -3.28337800 -0.59613000
- N 4.96526000 -1.29871400 0.07421800
- C 6.13462200 -0.69674900 0.70395100
- H 5.95341800 -0.47303700 1.76035200
- H 6.95488200 -1.40994700 0.64268500
- H 6.44134200 0.21110100 0.17727600
- C 5.04927400 -2.71114400 -0.28191900
- H 5.80083800 -2.85489400 -1.06244600
- H 5.33409000 -3.28963700 0.60010700
- H 4.08365800 -3.05279900 -0.64416800



AWGBRB (B3LYP for **3a**)

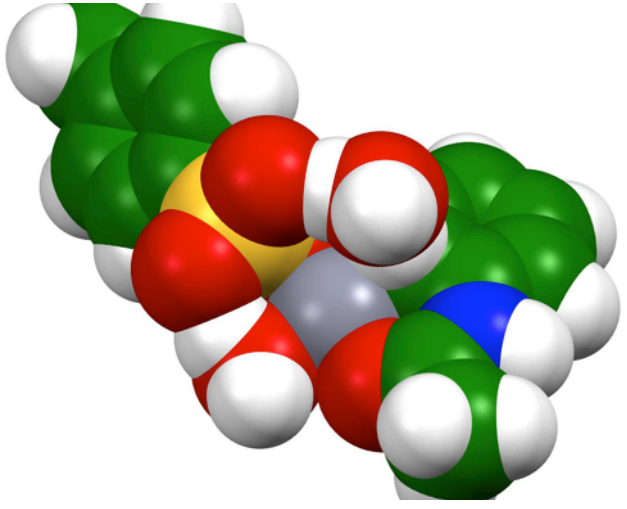
- Zero-point correction= 0.340538 (Hartree/Particle)\
- Thermal correction to Energy= 0.367951\
- Thermal correction to Enthalpy= 0.368896\
- Thermal correction to Gibbs Free Energy= 0.277874\
- Sum of electronic and zero-point Energies= -1615.398218\
- Sum of electronic and thermal Energies= -1615.370805\
- Sum of electronic and thermal Enthalpies= -1615.369861\
- Sum of electronic and thermal Free Energies= -1615.460882\
- \
- AWGBRB\
- \
- B3LYP\
- \
- 1 1\
- H 3.45743500 3.31771000 -1.48342400\
- C 2.74687800 2.94118300 -0.75527700\
- C 2.97512700 1.72791500 -0.11263400\
- C 1.58827100 3.66269600 -0.45503400\
- C 0.64881400 3.18920700 0.47301600\
- H 1.41295300 4.60613100 -0.96220900\
- N 4.18079300 1.02929100 -0.36613100\
- H 5.01056600 1.58838500 -0.52627400\
- C 4.30890800 -0.30348000 -0.45610100\
- O 3.31680800 -1.08668100 -0.45634700\
- Pd 1.35636200 -0.55818800 -0.32158800\
- H -0.24036900 3.77018100 0.68983100\
- C 2.04267300 1.21686600 0.84237200\
- O -0.63676900 -0.10130600 -0.35530600\
- O 0.85766400 -2.39059800 -1.29693100\
- H -0.03143500 -2.62063500 -0.91121800\
- H 1.47834500 -3.08731700 -1.03144400\
- C 0.88092900 1.98927800 1.12477600\
- H 0.18537800 1.61640000 1.86793500\
- S -1.57356700 -1.02762600 0.48406000\
- O -1.48668300 -2.42269100 -0.04018500\
- O -1.32008800 -0.87576100 1.93493900\
- C -3.18846100 -0.38663200 0.11591200\
- C -3.75514500 0.56710500 0.96514100\
- C -3.85881800 -0.83489000 -1.02621800\
- C -5.01528700 1.07503600 0.65835300\
- H -3.22498200 0.89474900 1.85217400\
- C -5.11725200 -0.31380900 -1.31327700\
- H -3.40930600 -1.58444800 -1.66791800\
- C -5.71550900 0.64484000 -0.47928600\
- H -5.64569900 -0.65897700 -2.19717900\
- H -5.46327000 1.81515100 1.31500100\
- C -7.09369900 1.17566100 -0.78434000\
- H -7.26773500 1.23731800 -1.86216800\
- H -7.86213800 0.51288800 -0.36793800\
- H -7.24576600 2.16703600 -0.34969000\
- H 2.36568300 0.50007500 1.60070100\
- O 1.40354400 -1.29279100 2.82312100\
- H 1.63296400 -2.19090800 2.55134700\
- H 0.45895600 -1.20906400 2.59578500\
- C 5.68277900 -0.89007700 -0.56791700\
- H 5.69543900 -1.61945800 -1.38013700\
- H 6.44605700 -0.12993700 -0.73719300\
- H 5.90876200 -1.41840700 0.36379600\



AWGBTS3F1 (B3LYP for **3a** TS)

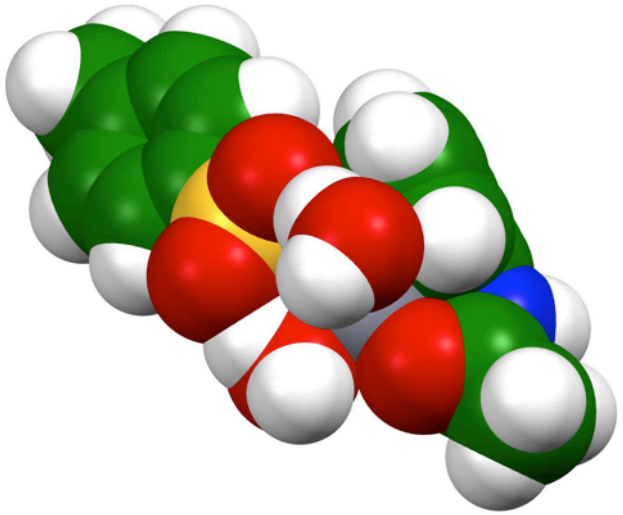
- Zero-point correction= 0.335476 (Hartree/Particle)
- Thermal correction to Energy= 0.360610
- Thermal correction to Enthalpy= 0.361555
- Thermal correction to Gibbs Free Energy= 0.277854
- Sum of electronic and zero-point Energies= -1615.391935
- Sum of electronic and thermal Energies= -1615.366801
- Sum of electronic and thermal Enthalpies= -1615.365857
- Sum of electronic and thermal Free Energies= -1615.449558
-
- AWGBTS3F1
-
- 1 1

H	4.84206900	2.91675600	-0.32559100
C	3.77170300	2.72805300	-0.32315200
C	3.28479600	1.44694500	-0.05765100
C	2.88397400	3.76003500	-0.62457800
C	1.50604400	3.52462400	-0.66596700
H	3.27577800	4.74862600	-0.84290200
N	4.25494900	0.44713400	0.20170000
H	5.17270700	0.79114500	0.45641700
C	4.17811200	-0.87789600	-0.03482900
O	3.13999600	-1.45181000	-0.44833700
Pd	1.23400400	-0.74362300	-0.42072100
H	0.82113100	4.32754300	-0.91683200
C	1.88446000	1.18216400	-0.02080500
O	-0.72572300	-0.13676100	-0.35789000
O	0.58235900	-2.69258500	-1.01298500
H	-0.29059900	-2.80494100	-0.54531800
H	1.17438900	-3.40517400	-0.73430000
C	1.02203000	2.25573800	-0.37904500
H	-0.04515400	2.06388400	-0.38951100
S	-1.65838800	-0.88798700	0.65071300
O	-1.60968600	-2.34964600	0.39096600
O	-1.32633000	-0.47322400	2.04341900
C	-3.27425200	-0.28156000	0.25709700
C	-3.83260800	0.73933400	1.02895700
C	-3.95714800	-0.83366700	-0.83216100
C	-5.09905200	1.21339700	0.69468500
H	-3.29385800	1.13759700	1.88111400
C	-5.21864200	-0.34188400	-1.14734500
H	-3.51612700	-1.63926300	-1.40867000
C	-5.81042700	0.68530100	-0.39265800
H	-5.75810400	-0.76533100	-1.98969700
H	-5.54493100	2.00284400	1.29258400
C	-7.19263400	1.18360000	-0.73058900
H	-7.33466200	1.26204500	-1.81247000
H	-7.95487600	0.49116600	-0.35350600
H	-7.38773100	2.16252600	-0.28589000
H	1.48216800	0.78190000	1.17192800
C	5.41150800	-1.70766400	0.19145100
H	6.26949400	-1.11922000	0.52133500
H	5.19405500	-2.47623500	0.93863800
H	5.66357500	-2.22043100	-0.74115100
O	0.97862700	0.67963900	2.44156800
H	1.48963200	0.10607900	3.03155600
H	0.06530300	0.25897400	2.34775600



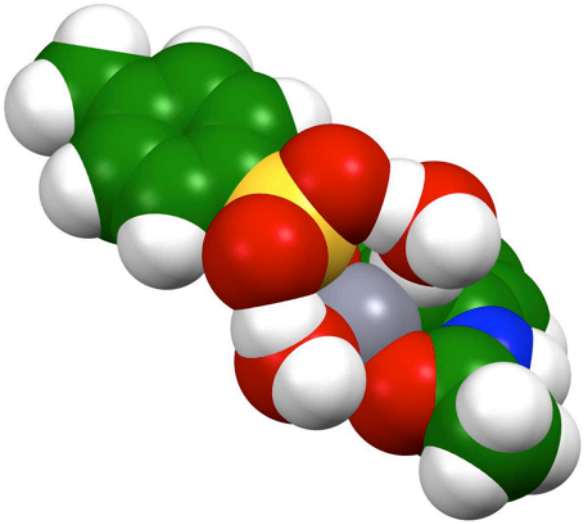
AWGBRW ((ωB97-xD for **3a**)

- Zero-point correction= 0.346049 (Hartree/Particle)
- Thermal correction to Energy= 0.372600
- Thermal correction to Enthalpy= 0.373544
- Thermal correction to Gibbs Free Energy= 0.287949
- Sum of electronic and zero-point Energies= -1615.032967
- Sum of electronic and thermal Energies= -1615.006417
- Sum of electronic and thermal Enthalpies= -1615.005473
- Sum of electronic and thermal Free Energies= -1615.091067
-
- AWGBRW
-
- 1 1
- H 2.06446800 2.97110200 -1.83433400
- C 1.68256700 2.63681400 -0.87665800
- C 2.42275900 1.70588400 -0.12314800
- C 0.49346200 3.11628900 -0.36491500
- C 0.02365000 2.69626300 0.89350900
- H -0.08245700 3.83167400 -0.94097200
- N 3.76656300 1.40216900 -0.52343700
- H 4.39544500 2.18186600 -0.66774600
- C 4.24228400 0.16389800 -0.60116200
- O 3.47095200 -0.83144800 -0.47959400
- Pd 1.49920600 -0.47193500 -0.30562200
- H -0.90277400 3.10450600 1.28076900
- C 1.95499200 1.26063600 1.14103000
- O -0.49291800 -0.12591200 -0.32380800
- O 1.09030000 -2.31580500 -1.26990400
- H 0.21625200 -2.60078100 -0.90873800
- H 1.73946300 -2.98879100 -1.02787700
- C 0.73841100 1.78300200 1.63674100
- H 0.38613200 1.45575600 2.60698300
- S -1.39654400 -1.06520700 0.50657400
- O -1.26854900 -2.44680100 -0.00184100
- O -1.15699000 -0.90246500 1.94567400
- C -3.00627900 -0.45975200 0.11828100
- C -3.48511800 0.66485800 0.78487300
- C -3.75470400 -1.09460300 -0.86987600
- C -4.73933800 1.15856600 0.44815000
- H -2.89220200 1.14034000 1.55842600
- C -5.00709400 -0.58741800 -1.18830000
- H -3.36439100 -1.97353300 -1.37007000
- C -5.51659600 0.54288400 -0.53851400
- H -5.60092500 -1.07793300 -1.95363700
- H -5.12158500 2.03479400 0.96235600
- C -6.88453100 1.06577100 -0.88786400
- H -6.99966700 1.16982000 -1.97033800
- H -7.65791900 0.37197400 -0.54292100
- H -7.07144100 2.03728000 -0.42569500
- H 2.60571300 0.69593000 1.80163100
- C 5.69662600 -0.06928900 -0.82575100
- H 5.81855400 -0.80865700 -1.61825000
- H 6.22503400 0.84765100 -1.08377100
- H 6.12163800 -0.48246000 0.09279700
- O 1.57346900 -1.67920900 2.45055100
- H 1.61187000 -2.60047800 2.17789400
- H 0.62740700 -1.46259300 2.43399000



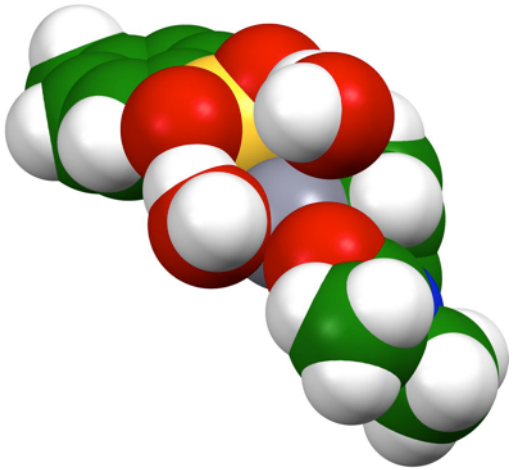
AWGBTS1H(ωB97-xD for **3a** TS)

- Zero-point correction= 0.341498 (Hartree/Particle)
- Thermal correction to Energy= 0.366853
- Thermal correction to Enthalpy= 0.367797
- Thermal correction to Gibbs Free Energy= 0.284986
- Sum of electronic and zero-point Energies= -1615.024869
- Sum of electronic and thermal Energies= -1614.999514
- Sum of electronic and thermal Enthalpies= -1614.998570
- Sum of electronic and thermal Free Energies= -1615.081382
-
- AWGBTS1H
-
- wB97xD
-
- 1 1
- H 4.73608200 2.97876000 -0.33535800
- C 3.67292900 2.76349500 -0.31317200
- C 3.22741400 1.46142500 -0.09487300
- C 2.75010000 3.77715600 -0.53120800
- C 1.37803400 3.51311000 -0.53314800
- H 3.10874500 4.78520900 -0.70969800
- N 4.21494100 0.48351900 0.11755600
- H 5.11908000 0.82967100 0.41274100
- C 4.15009500 -0.82704500 -0.15889300
- O 3.12668800 -1.38832700 -0.61592000
- Pd 1.22211300 -0.74900700 -0.46372200
- C 1.84106100 1.16095300 -0.03599800
- O -0.75873200 -0.19799900 -0.32221400
- O 0.57249600 -2.73982200 -0.97113900
- H -0.24914900 -2.86503400 -0.44754500
- H 1.20188000 -3.41216500 -0.68510500
- C 0.93791200 2.22524000 -0.29792300
- H -0.12404800 2.00907700 -0.26701100
- S -1.63612800 -0.86679800 0.74113000
- O -1.60297500 -2.33418900 0.59717900
- O -1.30200100 -0.36700200 2.08952800
- C -3.25184000 -0.29099300 0.32383500
- C -3.69337000 0.93187200 0.82530500
- C -4.03479300 -1.04341600 -0.54653400
- C -4.94056600 1.40277100 0.43817100
- H -3.07497500 1.49879100 1.51237100
- C -5.28063000 -0.55441600 -0.92161500
- H -3.67869400 -1.99797300 -0.91754000
- C -5.74843000 0.67288200 -0.44234700
- H -5.89983200 -1.13919100 -1.59481500
- H -5.29628900 2.35114700 0.82944000
- C -7.08352300 1.21562000 -0.87820000
- H -7.60035500 1.70418100 -0.04807600
- H -6.95053700 1.96389200 -1.66691700
- H -7.72744800 0.42623900 -1.27193300
- H 1.55270700 0.73029100 1.16056300
- C 5.36528300 -1.66101900 0.09740700
- H 5.22784800 -2.17883900 1.05106900
- H 5.44719100 -2.41214200 -0.68810700
- H 6.28021400 -1.07087400 0.14404500
- O 1.20862300 0.52158500 2.47600200
- H 1.74607000 -0.19464400 2.83794300
- H 0.28001800 0.18064500 2.43148900
- H 0.66692000 4.31162600 -0.70964700



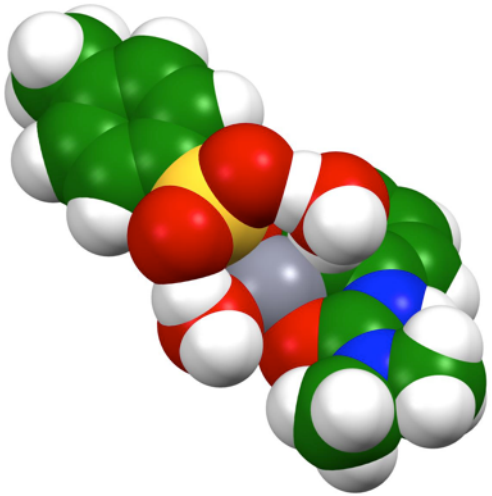
UWGBR97(ωB97-xD for **3e**)

- Zero-point correction= 0.392240 (Hartree/Particle)
- Thermal correction to Energy= 0.421675
- Thermal correction to Enthalpy= 0.422619
- Thermal correction to Gibbs Free Energy= 0.330645
- Sum of electronic and zero-point Energies= -1709.635105
- Sum of electronic and thermal Energies= -1709.605670
- Sum of electronic and thermal Enthalpies= -1709.604726
- Sum of electronic and thermal Free Energies= -1709.696700
-
- UWGBR97
-
- 1 1
- H 1.93540200 3.30735000 -1.59153400
- C 1.51577200 2.87925200 -0.68812600
- C 2.17273100 1.82082800 -0.04453600
- C 0.33794700 3.36936400 -0.15392300
- C -0.22805000 2.82609100 1.01406700
- H -0.16228600 4.19027700 -0.65667400
- N 3.42659300 1.40805600 -0.51245700
- H 3.93905200 2.05591300 -1.09432700
- C 3.85915900 0.11105400 -0.44223200
- O 3.04366600 -0.83599800 -0.19247300
- Pd 1.05548700 -0.47823000 -0.12336400
- H -1.15196500 3.23273400 1.40719900
- C 1.61078500 1.23801800 1.12913400
- O -0.93338100 -0.09506000 -0.22300500
- O 0.66134100 -2.29143600 -1.17548800
- H -0.21652200 -2.57612500 -0.82818300
- H 1.30006200 -2.97622600 -0.94145200
- C 0.40388100 1.78553200 1.64991500
- H -0.00911800 1.34890600 2.55138600
- S -1.88054300 -1.02627800 0.55563700
- O -1.71286100 -2.41717300 0.08417500
- O -1.74387900 -0.83905700 2.00648700
- C -3.46834900 -0.44575700 0.05035000
- C -4.01136800 0.67728000 0.67070000
- C -4.13278000 -1.09665800 -0.98486500
- C -5.24329500 1.15023600 0.23808500
- H -3.48266500 1.16773700 1.48090800
- C -5.36492500 -0.60865700 -1.40168400
- H -3.69445400 -1.97289300 -1.44874000
- C -5.93684600 0.51696800 -0.79998100
- H -5.89039600 -1.11094800 -2.20824700
- H -5.67478600 2.02498000 0.71481400
- C -7.28597100 1.01811300 -1.24201200
- H -7.44956900 0.82953100 -2.30573600
- H -8.08142100 0.50560100 -0.69020700
- H -7.39382200 2.08955600 -1.05790600
- H 2.23646700 0.65067600 1.79638300
- O 0.94423500 -1.63023000 2.61541600
- H 0.98736600 -2.55162000 2.34432700
- H 0.00094500 -1.40674100 2.56500300
- N 5.14314200 -0.14670500 -0.65293300
- C 6.14989200 0.90902600 -0.72707700
- H 5.91392000 1.71125700 -0.02660400
- H 7.11025300 0.48105000 -0.44130200
- H 6.23188100 1.30856600 -1.74253900
- C 5.60004900 -1.52514200 -0.80911300
- H 6.08391000 -1.86805400 0.10901900
- H 4.75463800 -2.17094200 -1.03514400
- H 6.31650500 -1.56265800 -1.63127200



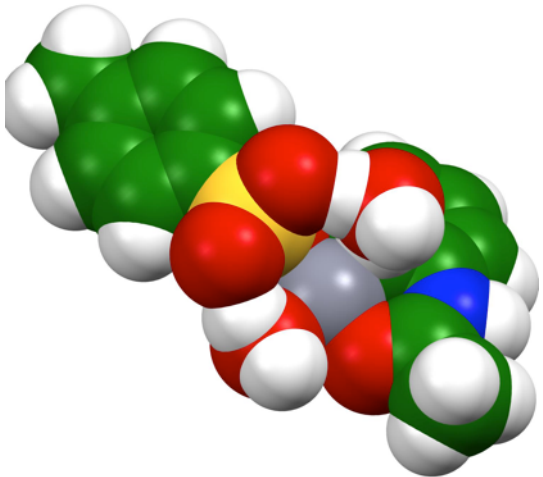
UWGBTS97(ωB97-xD for **3e** TS)

- Zero-point correction= 0.388564 (Hartree/Particle)
- Thermal correction to Energy= 0.416393
- Thermal correction to Enthalpy= 0.417338
- Thermal correction to Gibbs Free Energy= 0.329929
- Sum of electronic and zero-point Energies= -1709.623927
- Sum of electronic and thermal Energies= -1709.596098
- Sum of electronic and thermal Enthalpies= -1709.595154
- Sum of electronic and thermal Free Energies= -1709.682562
-
- UWGBTS97
-
- 1 1
- H 4.15599300 3.39933800 -0.31073200
- C 3.10994500 3.11323700 -0.34821700
- C 2.74211400 1.78161800 -0.13629200
- C 2.13980200 4.06008900 -0.63438800
- C 0.78670300 3.71016600 -0.71537300
- H 2.44273200 5.08752100 -0.80694900
- N 3.76269800 0.88236900 0.17374500
- H 4.63252800 1.30354300 0.46682300
- C 3.78857200 -0.45128100 -0.12896000
- O 2.83094100 -1.01878100 -0.73395000
- Pd 0.88316500 -0.53823000 -0.54947300
- H 0.04036900 4.46057400 -0.94822000
- C 1.37120200 1.40016000 -0.14628800
- O -1.13993900 -0.13293400 -0.38687600
- O 0.36981500 -2.58007100 -1.05345100
- H -0.43329300 -2.75954500 -0.51784100
- H 1.04815100 -3.20345400 -0.76984000
- C 0.41851100 2.40123800 -0.48650700
- H -0.62712900 2.11479300 -0.51671900
- S -1.93509900 -0.86430500 0.69573000
- O -1.80385400 -2.32606700 0.54639500
- O -1.60019200 -0.34891800 2.03928900
- C -3.60574400 -0.41339400 0.34335400
- C -4.13244200 0.74941400 0.89865000
- C -4.35524200 -1.20797100 -0.52131000
- C -5.43437700 1.11573100 0.57849100
- H -3.53727400 1.35254400 1.57518500
- C -5.65381500 -0.82481800 -0.82861700
- H -3.93053100 -2.11396600 -0.93883800
- C -6.21217700 0.33808200 -0.28512500
- H -6.24610900 -1.44029800 -1.49894200
- H -5.85338900 2.01958200 1.00989700
- C -7.63234600 0.72232200 -0.60602600
- H -7.81556500 1.77971600 -0.40277800
- H -7.86570800 0.52474400 -1.65545700
- H -8.33087000 0.13780700 0.00197700
- H 1.09284300 1.03781200 1.08005700
- O 0.77127900 0.83605800 2.38040900
- H 1.38452400 0.19098600 2.75539700
- H -0.11491700 0.39216200 2.34184700
- N 4.88160100 -1.14376600 0.20189800
- C 6.02426000 -0.52337200 0.86531900
- H 5.71668300 -0.00942000 1.78002300
- H 6.71955600 -1.31160600 1.14839300
- H 6.55178500 0.16793200 0.19985800
- C 5.01456100 -2.54676200 -0.18043600
- H 5.83723800 -2.65721100 -0.89172200
- H 5.22327300 -3.14452200 0.70958000
- H 4.09343800 -2.89286300 -0.64056300



AWGBRMe1(ωB97-xD for **3c**)

- Zero-point correction= 0.373983 (Hartree/Particle)
- Thermal correction to Energy= 0.402307
- Thermal correction to Enthalpy= 0.403251
- Thermal correction to Gibbs Free Energy= 0.314404
- Sum of electronic and zero-point Energies= -1654.319850
- Sum of electronic and thermal Energies= -1654.291526
- Sum of electronic and thermal Enthalpies= -1654.290582
- Sum of electronic and thermal Free Energies= -1654.379429
-
- AWGBRMe1
-
- 1 1
- H 2.25295200 2.09360300 -1.91355700
- C 1.55561400 2.02891000 -1.08473100
- C 2.02863500 1.59284400 0.18904100
- C 0.23434000 2.43065100 -1.22808800
- C -0.63130400 2.44539600 -0.13187900
- H -0.12345600 2.74037400 -2.20379800
- N 3.45423800 1.54605400 0.41890100
- H 3.89216900 2.36308400 0.82414100
- C 4.20404700 0.52273900 0.03768600
- O 3.66585500 -0.49924800 -0.48375400
- Pd 1.65919800 -0.46513000 -0.52755700
- C 1.16039600 1.67124400 1.31442700
- O -0.35614900 -0.43429800 -0.57679400
- O 1.58591700 -2.48121000 -1.22490500
- H 0.70155000 -2.84069600 -0.98359200
- H 2.24834400 -3.03655400 -0.79534100
- C -0.14331400 2.07365900 1.13831500
- H -0.81144200 2.10123900 1.99238500
- S -1.10291000 -1.45893900 0.30609500
- O -0.99029200 -2.79368600 -0.31498400
- O -0.68232600 -1.38114700 1.71000500
- C -2.75663300 -0.85874000 0.18332200
- C -3.33158800 -0.22922100 1.28366800
- C -3.42438800 -0.94629000 -1.03597600
- C -4.60080900 0.32100400 1.15298700
- H -2.78978100 -0.16883800 2.22048600
- C -4.69048800 -0.38647400 -1.14654700
- H -2.96336000 -1.43843100 -1.88540900
- C -5.29575600 0.25457000 -0.05888800
- H -5.21639700 -0.44612500 -2.09427200
- H -5.05591500 0.81554300 2.00564100
- C -6.67635900 0.84194800 -0.18154500
- H -6.92883800 1.04926200 -1.22372800
- H -7.42284200 0.14288800 0.21028900
- H -6.76299500 1.76989800 0.38925800
- H 1.54745400 1.39800300 2.28880100
- C 5.68392100 0.55426300 0.21021700
- H 6.15016900 0.44299500 -0.77120500
- H 6.02843700 1.47641900 0.67612800
- H 5.97990400 -0.29988100 0.82269500
- O 2.11020500 -1.20452100 2.34079700
- H 2.47957500 -2.06837800 2.13662100
- H 1.15195300 -1.31797700 2.23682200
- C -2.07229000 2.81787700 -0.31041400
- H -2.63866500 1.92567600 -0.60367600
- H -2.50885200 3.19754600 0.61536300
- H -2.19598500 3.56360600 -1.09874100



AWGBTSMe1(ωB97-xD for **3c** TS)

- Zero-point correction= 0.368975 (Hartree/Particle)
- Thermal correction to Energy= 0.396226
- Thermal correction to Enthalpy= 0.397171
- Thermal correction to Gibbs Free Energy= 0.309462
- Sum of electronic and zero-point Energies= -1654.307759
- Sum of electronic and thermal Energies= -1654.280508
- Sum of electronic and thermal Enthalpies= -1654.279563
- Sum of electronic and thermal Free Energies= -1654.367272
-
- AWGBTSMe1
-
- 1 1
- H 4.57522400 2.98489200 -0.07874800
- C 3.52504400 2.71305100 -0.09948000
- C 3.14302700 1.38204000 0.05568100
- C 2.56015700 3.68601300 -0.30758500
- C 1.19232000 3.37636400 -0.36356800
- H 2.87829300 4.71623300 -0.43860600
- N 4.16857900 0.44223300 0.26645900
- H 5.04291300 0.81413600 0.61521500
- C 4.17321200 -0.85579700 -0.06412100
- O 3.19603800 -1.44163600 -0.58977900
- Pd 1.25878500 -0.89148700 -0.48668900
- C 1.77412800 1.02057100 0.05398000
- O -0.74445400 -0.42340200 -0.38253700
- O 0.71209600 -2.85728500 -1.17239000
- H -0.15173400 -3.05039900 -0.74743200
- H 1.33346000 -3.53509300 -0.88164400
- C 0.82943900 2.05107000 -0.18939900
- H -0.22069200 1.77796100 -0.20023200
- S -1.62964100 -1.22837800 0.57385800
- O -1.64139900 -2.65379800 0.19980200
- O -1.26526900 -0.95860800 1.97982000
- C -3.22838600 -0.53953500 0.28338900
- C -3.56310000 0.66416200 0.90207000
- C -4.09924100 -1.16792700 -0.60009700
- C -4.79316000 1.24119800 0.62263300
- H -2.87363600 1.13642100 1.59343700
- C -5.32901000 -0.57415600 -0.86470600
- H -3.82194800 -2.10559500 -1.06834100
- C -5.69232200 0.63395400 -0.26369500
- H -6.01493400 -1.05895900 -1.55246600
- H -5.06162800 2.17940100 1.09869000
- C -7.02950600 1.26773100 -0.54169000
- H -7.49304200 0.84522400 -1.43579800
- H -7.71265500 1.10656500 0.29872100
- H -6.92982600 2.34756500 -0.68029000
- H 1.46860600 0.49750900 1.21527100
- C 5.41598600 -1.64589200 0.19864100
- H 5.66811500 -2.20821100 -0.70174700
- H 6.26003600 -1.02215800 0.49069200
- H 5.20422500 -2.36327100 0.99565900
- O 1.10747400 0.18380600 2.49443100
- H 1.70355200 -0.49869500 2.82933700
- H 0.21870200 -0.24400700 2.39775800
- C 0.16824100 4.45432500 -0.59877300
- H 0.22932000 5.22541600 0.17468700
- H 0.33424200 4.94274400 -1.56364200
- H -0.84337500 4.04347300 -0.59419400