SUPPORTING INFORMATION

Transition State Analysis of the Arsenolytic Depyrimidination of Thymidine by Human Thymidine Phosphorylase

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1. Experimental Section

A. Kinetic of hTP Arsenolysis

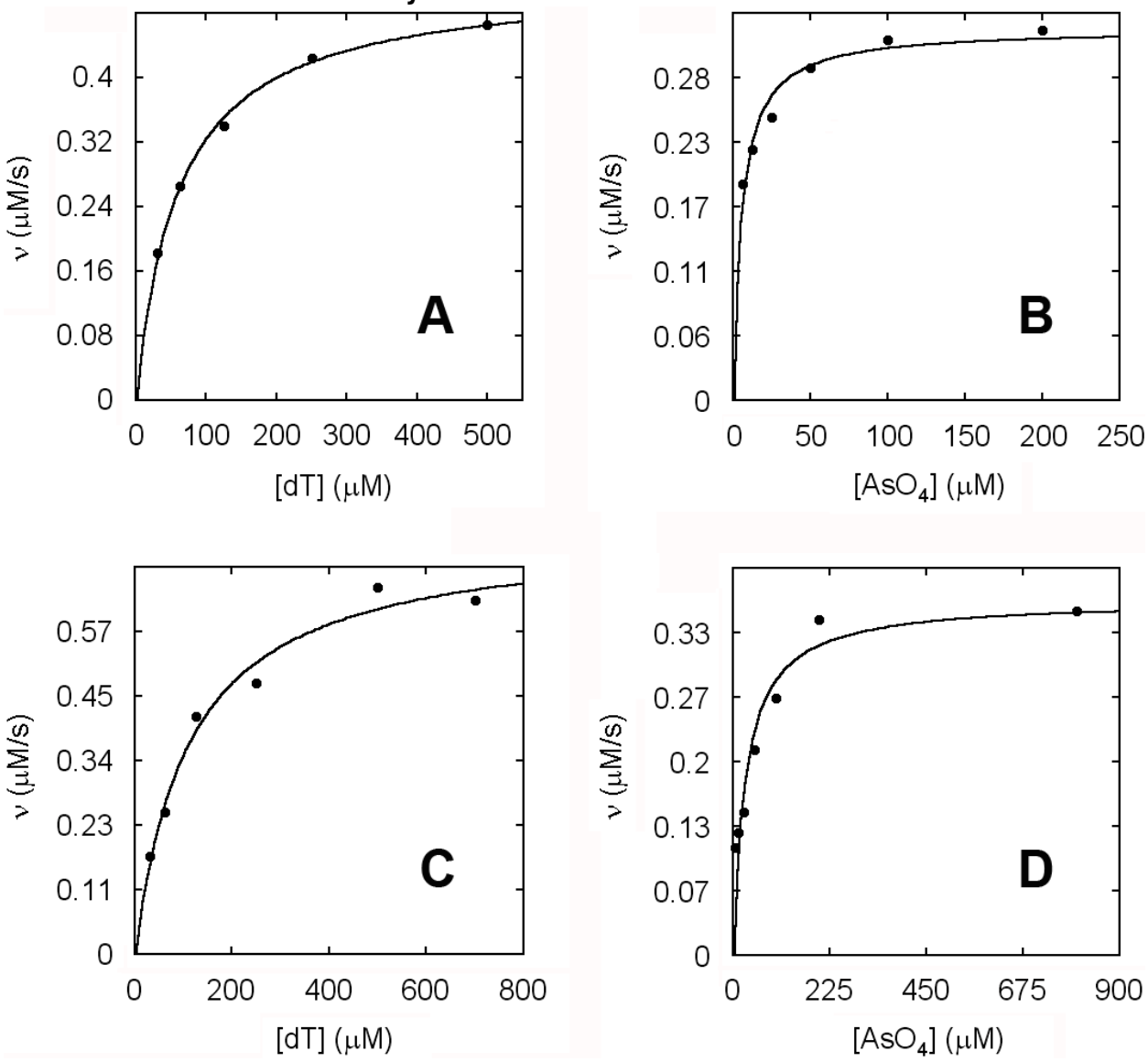
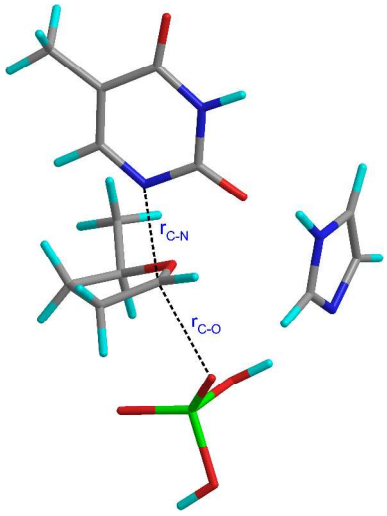


Figure S1. Kinetics of hTP arsenolysis. A model SX-20 stopped-flow spectrometer (Applied Photophysics) outfitted with a mercury-xenon lamp was used to follow the arsenolytic depyrimidination of dT by hTP. In the reaction chamber, 20 mM HEPES pH 7.4, 1 mM DTT, and varying concentrations of dT or sodium arsenate under saturating concentrations of the second substrate were monitored for hTP-catalyzed arsenolysis. The reaction progress was monitored by the decrease in absorbance of dT upon depyrimidination at 290 nm using an extinction coefficient of $\Delta\varepsilon_{290}$ = 1000 M^{-1} cm^{-1}. hTP concentration was maintained at 175 nM (22 ℃) or 90 nM (37 ℃) in the assay. A) 22 ℃, vary dT at 2.5 mM sodium arsenate. B) 22 ℃, vary sodium arsenate at 0.5 mM dT. C) 37 ℃, vary dT at 2.5 mM sodium arsenate. D) 37 ℃, vary sodium arsenate at 0.5 mM dT. Apparent K_Ms and k_{cat} were obtained by fitting data to the Michaelis-Menten equation.

2. Theoretical Section

A. Methodology

A preliminary data set for the analysis of the key isotope effects was generated using a simple model system. The 3′- and 5′- hydroxyl groups were substituted by hydrogen atoms. This was done in order to eliminate calculational artifacts that may arise from interactions between these groups with the nucleophile and/or the leaving group (that might not be representative of catalysis). As discussed in the manuscript, a previous theoretical study on a structurally related enzyme (TP from *E.*coli) proposes a key role for an active site histidine – activation of phosphate and stabilization of thymine anion by hydrogen bonding. Mutation of the analogous residue in hTP makes it catalytically inactive. It was therefore deemed important to include a truncated mimic of this active site residue in our theoretical model in order to better understand the mechanism of catalysis. Therefore, our preliminary model for predicting KIEs for the A_ND_N mechanism consisted of a modified thymidine, arsenate and a histidine mimic (Scheme S1).



Scheme S1. Preliminary model for the prediction of KIEs

Restraining only the distances along the reaction coordinate, a potential energy surface was generated as follows. The breaking C-N bond distance ($r_{C\text{-}N}$) was fixed at 1.7 Å and the forming C-O bond distance ($r_{C\text{-}O}$) was systematically varied between 2.9 and 1.8 Å (at increments of 0.1 Å). Each geometry

was optimized and a frequency calculation was performed to get the imaginary frequency corresponding to motion along the reaction coordinate. Thirteen such grids of optimized geometries were calculated by varying $r_{C\text{-}N}$ between 1.7 and 3.0 (at increments of 0.1 Å) and their energies (E + zpe) were plotted to generate a potential energy surface. The area of the surface indicated in yellow is the chemical saddle point, the transition state of the model system. Isotope effect predictions were made for each of the 143 geometries versus the lowest energy conformation of dT.

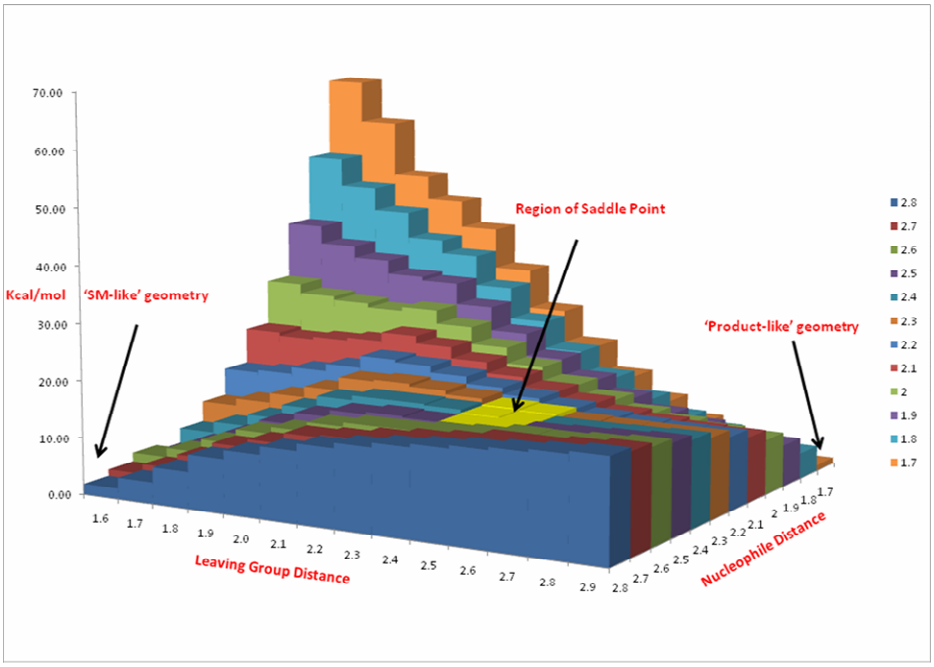


Figure S2. Computed potential energy surface for the preliminary model

It was found that the best match of the key isotope effects (1′- ^{14}C, 1′- ^{3}H and 1′- ^{15}N) were found in the range of $r_{(C\text{-}N)}$ = 2.5 – 2.9 Å and $r_{(C\text{-}N)}$ = 2.9 – 2.5 Å for combinations where the sum of the two distances was 5.4 Å. These geometries correspond to a dissociative transition state with significant oxocarbenium ion character. At this point, the 3′- and 5′- hydroxyl groups were incorporated into the model and these five selected geometries were re-optimized to arrive at the 'most likely' geometry of the transition state structure based on the match with experimental KIEs. The orientation of the arsenate and the leaving group with respect to the 2-deoxyribose ring were tactfully manipulated to locate several minima for each of these geometries. The final transition state that was selected as the best fit model for the experimental KIEs had one imaginary frequency of -76. Apart from the two distances along the

reaction coordinate, the orientation of the nucleophile (arsenate) with respect to the ribose ring was fixed at a dihedral angle of 150˚ defined by As-O-C1-C2.

3. Coordinates of calculated structures

A. Starting Material

Thymidine 2′-endo B3LYP/6-31G*

thymidine-2endo-SM-B3G
E(RB+HF-LYP) = -875.130069089

Zero-point correction= 0.251363 (Hartree/Particle)
Thermal correction to Energy= 0.266935
Thermal correction to Enthalpy= 0.267880
Thermal correction to Gibbs Free Energy= 0.208537
Sum of electronic and zero-point Energies= -874.878707
Sum of electronic and thermal Energies= -874.863134
Sum of electronic and thermal Enthalpies= -874.862189
Sum of electronic and thermal Free Energies= -874.921533

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.505	59.637	124.898

C,0,-2.3087824787,1.0680309401,0.4341890204
C,0,-2.7690109005,1.0201974824,-1.028408447
O,0,-3.1831594353,-0.3105740132,-1.270399439
C,0,-2.5775933909,-1.2018626884,-0.306352973
C,0,-1.6782642293,-0.3136807011,0.5875824656
C,0,-3.6700457079,-1.9615715921,0.4468748051
O,0,-0.3479274121,-0.2151639228,0.0732394212
N,0,-3.8436820278,1.9477075948,-1.4187283268
C,0,-3.6295628498,2.8061924472,-2.489836286
C,0,-4.5402905676,3.6795553083,-2.9731709917
C,0,-5.8593054942,3.7202589022,-2.3444238061
N,0,-6.0044086168,2.8032053631,-1.2868183547
C,0,-5.0854974151,1.9019569687,-0.7873235749
O,0,-5.3706073527,1.1539549858,0.1412596974
O,0,-6.7837015449,4.4506049909,-2.6648194
C,0,-4.2795317853,4.605289209,-4.1260252102
H,0,-4.351089761,-2.4093013176,-0.2947884998
H,0,-6.9102283451,2.7845383912,-0.8307550068
H,0,-2.6397458307,2.7294839827,-2.9267946773
H,0,-1.9269699436,1.2724288016,-1.6844087689
H,0,-1.5854579996,1.8656232463,0.6201522007
H,0,-3.1610952803,1.1668846901,1.1053696747
H,0,-1.9593932173,-1.9219763765,-0.86316077
H,0,-1.6780525787,-0.657567803,1.6289076594
H,0,-3.2655020574,4.478287454,-4.5170898641
H,0,-4.9927270844,4.4255872681,-4.9383738969
H,0,-4.4088981201,5.6503381335,-3.8224341423
H,0,-3.2026325393,-2.7847495092,1.0023392442
O,0,-4.3570791201,-1.1740519124,1.3935585969
H,0,0.0520716119,-1.0983423643,0.1019408426
H,0,-4.821115525,-0.4609619594,0.9122888087

Thymidine 3′-endo B3LYP/6-31G*

thymidine-3endo-SM-B3G
E(RB+HF-LYP) = -875.127071401

Zero-point correction= 0.250918 (Hartree/Particle)
Thermal correction to Energy= 0.266812
Thermal correction to Enthalpy= 0.267756
Thermal correction to Gibbs Free Energy= 0.207519
Sum of electronic and zero-point Energies= -874.876153
Sum of electronic and thermal Energies= -874.860260
Sum of electronic and thermal Enthalpies= -874.859315
Sum of electronic and thermal Free Energies= -874.919552

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.427	60.177	126.779

C,0,-2.8607088612,0.0456624814,-0.5413475501
C,0,-1.4015274633,-0.1274561287,-1.0173979224
O,0,-1.0568919881,1.0090442759,-1.7753042001
C,0,-2.2196704256,1.8220372943,-2.0382506733
C,0,-3.2399073339,1.4773521689,-0.9326543665
N,0,-0.3975972774,-0.3250511185,0.0518738696
C,0,0.3879486927,-1.4678160481,0.0547795007
C,0,1.3472305722,-1.737481971,0.9684635759
C,0,1.5936628781,-0.7547844516,2.0230146909
N,0,0.7727159202,0.3861336369,1.9324361257
C,0,-0.2073282448,0.6716198597,1.0039347983
O,0,-0.8532074785,1.7140641458,1.0400381889
O,0,2.419576198,-0.855811109,2.916322898
C,0,2.1820358107,-2.9854168983,0.9601150355
C,0,-1.7750398221,3.2816006868,-2.089786935
O,0,-4.5847016129,1.5119579229,-1.3982971405
H,0,-0.9056102716,3.3506007985,-2.7637650587
H,0,0.9202294811,1.1020309679,2.6358154525
H,0,0.1711302988,-2.1597446685,-0.7525185414
H,0,-3.510407748,-0.6453333927,-1.0887171175
H,0,-2.9771366418,-0.1514701788,0.52598197
H,0,-2.6484868569,1.5329913699,-3.0100121182
H,0,-3.0997956642,2.1556060161,-0.0884242304
H,0,1.9100086192,-3.6406408412,0.1270182315
H,0,3.2471386423,-2.7408236519,0.8789475522
H,0,2.0598291563,-3.541205479,1.8966826439
H,0,-2.5805192656,3.8783975599,-2.5363104626
O,0,-1.5059470058,3.8443075917,-0.822719324
H,0,-1.0144915511,3.1878702754,-0.2940100037
H,0,-1.3045682137,-1.0263609261,-1.6379873332
H,0,-4.9039975431,2.4222718113,-1.308434556

B. Transition structures discussed in manuscript

A_ND_N mechanism – Best fit transition state geometry

dis295245-AsO4-di-150-fixed
E(RB3LYP) = -3637.27624035

Zero-point correction= 0.355545 (Hartree/Particle)

Thermal correction to Energy= 0.384602
Thermal correction to Enthalpy= 0.385546
Thermal correction to Gibbs Free Energy= 0.291293
Sum of electronic and zero-point Energies= -3636.920696
Sum of electronic and thermal Energies= -3636.891639
Sum of electronic and thermal Enthalpies= -3636.890695
Sum of electronic and thermal Free Energies= -3636.984947

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.341	103.655	198.372

C,0,-0.6800095824,0.2162556531,-2.1357349488
C,0,-0.2919604169,0.4540946622,-0.7207185808
O,0,0.7022052076,1.2507416393,-0.5878775948
C,0,1.2811250304,1.6356752806,-1.9028374415
C,0,0.5163689215,0.7781383773,-2.9561921413
C,0,1.1255072727,3.1291077237,-2.0896529066
O,0,1.828326383,3.8088370309,-1.0633908904
O,0,1.2931058762,-0.1989751463,-3.5674441842
N,0,-2.3178263731,1.5391823874,0.1272749386
C,0,-2.733825965,2.8221719921,0.2479080775
C,0,-3.8050277844,3.2733151731,0.9780820661
C,0,-4.5738939327,2.2919823115,1.7149478192
N,0,-4.0810239059,0.98492758,1.5717805188
C,0,-2.9818302829,0.5762635888,0.8172030014
O,0,-2.6647720919,-0.6328860714,0.8015548527
O,0,-5.5650484806,2.5127082608,2.4163107494
C,0,-4.2221718139,4.7141133421,1.0572399352
N,0,-1.0341810791,-2.8282145748,1.7216928082
C,0,-0.7480156386,-3.4101639146,2.9387368944
C,0,0.4184395655,-4.1085705745,2.7470032536
N,0,0.8576850414,-3.9610970962,1.4481728829
C,0,-0.0418761744,-3.1829970076,0.8657556957
H,0,-4.2129081687,5.0791236869,2.0926114612
H,0,-5.2475091545,4.8582973922,0.6915440089
H,0,-2.1358060599,3.5463430723,-0.3105990255
H,0,-4.5762257935,0.2606876563,2.0784918493
H,0,-1.7571747565,-2.1344531462,1.5170733759
H,0,2.5519089262,0.0007350053,1.2014838208
H,0,-3.5545078682,5.35029003,0.4641316045
H,0,2.3292424856,1.3309250249,-1.8155928808
H,0,1.525598711,3.370750028,-3.0885273198
H,0,0.0527408795,3.3868558027,-2.088978742
H,0,0.147829186,1.4341639066,-3.7552884429
H,0,-1.622538168,0.7337335158,-2.3328388038
H,0,-0.8217341843,-0.8508398621,-2.3187796231
H,0,1.5063948766,-0.8847351964,-2.8600715764
H,0,1.628716603,4.7534317845,-1.1421595449
O,0,1.423985957,-1.8217134785,-1.480240988
O,0,3.3783887848,-2.9776433127,0.1520925913
H,0,2.6303420903,-3.4647863813,0.5781949778
O,0,3.8867000793,-0.4122220394,-0.9459366809
O,0,1.9819621636,-0.7683736784,1.0315180153
H,0,-0.6090730943,-0.1029665644,0.1479462393
As,0,2.7140250257,-1.4633101015,-0.4578492898
H,0,0.0349953866,-2.8182276865,-0.1505478931
H,0,-1.3841704126,-3.278031636,3.8013858254
H,0,0.9677863085,-4.7051628697,3.4636317058

$D_N^{\ddagger *}A_N$ mechanism – transition structures with and without histidine mimic

LG 2.3 with Histidine B3LYP/6-31G*

Dndd23
E(RB3LYP) = -1101.29073074

Zero-point correction= 0.318730 (Hartree/Particle)
Thermal correction to Energy= 0.340113
Thermal correction to Enthalpy= 0.341057
Thermal correction to Gibbs Free Energy= 0.263350
Sum of electronic and zero-point Energies= -1100.972001
Sum of electronic and thermal Energies= -1100.950618
Sum of electronic and thermal Enthalpies= -1100.949674
Sum of electronic and thermal Free Energies= -1101.027381

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.424	77.444	163.548

C,0,0.684670855,0.5689788573,-2.2681495316
C,0,0.8651879597,1.0039484125,-0.8564947946
O,0,1.4345025539,2.1701513448,-0.7660140405
C,0,1.5220053331,2.8081310902,-2.0974786134
C,0,0.6487311088,1.9238642922,-3.0042550122
C,0,1.1250487727,4.2634255118,-2.0024883641
O,0,2.1410257641,4.9454427042,-1.2952149364
O,0,1.2223926531,1.9334302564,-4.2943790388
N,0,-1.3544514614,1.2311749425,-0.2983129038
C,0,-2.0892106971,2.36993111,-0.1419877651
C,0,-3.1876297954,2.500236285,0.6561058168
C,0,-3.5969587187,1.3414771949,1.439726755
N,0,-2.7568630031,0.2214358839,1.2720403633
C,0,-1.6300530344,0.1440625076,0.4715672408
O,0,-0.9110172068,-0.8793489515,0.45920791
O,0,-4.5603177427,1.2869362313,2.1946671972
C,0,-4.0087273358,3.7522562776,0.766245675
N,0,-1.6280426524,-3.2393187569,1.9228982237
C,0,-1.3783423147,-3.4646675108,3.2602136743
C,0,-1.9652212776,-4.6741274204,3.544525703
C,0,-2.340680096,-4.3122221806,1.4731139842
H,0,-4.0522729942,4.1039995557,1.8038905759
H,0,-5.0459299215,3.5749842518,0.4572456207
H,0,-1.7596179692,3.2160468634,-0.7451981434
H,0,-2.9932501922,-0.5956043158,1.8261255841
H,0,-1.3237979754,-2.4284002318,1.3723634324
H,0,-3.5949350495,4.554078985,0.145048058
H,0,2.5711431175,2.7316232983,-2.3992558619
H,0,1.0166319441,4.6292948725,-3.0369247248
H,0,0.1455094419,4.3441427823,-1.5069583856
H,0,-0.3829657261,2.3029104873,-3.0190279063
H,0,-0.1838915568,-0.0751782724,-2.3944239979
H,0,1.5896042389,0.0209881689,-2.5760098538
H,0,0.5862253852,1.5514485125,-4.9182990038
H,0,1.8618321898,5.8639628774,-1.1636969175
H,0,0.9002698712,0.3519478774,0.0086610961
H,0,-2.6702449721,-4.3929062724,0.4453194349
H,0,-0.822121555,-2.7624702309,3.8636015066
H,0,-1.9917573798,-5.1965297992,4.4918899083
N,0,-2.565863971,-5.2001596118,2.4217102956

LG 2.4 with Histidine B3LYP/6-31G*

Dndd24
E(RB3LYP) = -1101.28656569

Zero-point correction= 0.318445
(Hartree/Particle)
Thermal correction to Energy= 0.339928
Thermal correction to Enthalpy= 0.340873
Thermal correction to Gibbs Free Energy= 0.262285
Sum of electronic and zero-point Energies= -1100.968121
Sum of electronic and thermal Energies= -1100.946637
Sum of electronic and thermal Enthalpies= -1100.945693
Sum of electronic and thermal Free Energies= -1101.024280

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.308	77.561	165.401

C,0,0.6735709944,0.5218588933,-2.2098936539
C,0,0.8877885575,0.9801663112,-0.8141480823
O,0,1.4827231143,2.1267639355,-0.7464080362
C,0,1.5675917889,2.7463424431,-2.0911776644
C,0,0.6711630378,1.8612596558,-2.9757638752
C,0,1.1847295923,4.2056046668,-2.0027182938
O,0,2.2174840454,4.8840044966,-1.3171226072
O,0,1.2426858542,1.8282698868,-4.2659353821
N,0,-1.4285839284,1.3110529837,-0.280365535
C,0,-2.1827037451,2.4390157959,-0.1440767452
C,0,-3.2820152742,2.5719004227,0.6543896853
C,0,-3.6766358491,1.423663242,1.4586453961
N,0,-2.8243815348,0.3108179298,1.3062291972
C,0,-1.6984525983,0.2353971486,0.5041933501
O,0,-0.9713813127,-0.7857086847,0.5092077533
O,0,-4.637797834,1.3696599328,2.2174347196
C,0,-4.1178149453,3.8160175953,0.7416142415
N,0,-1.5987543467,-3.2061066916,1.9036160682
C,0,-1.2483842794,-3.5192814035,3.1995950879
C,0,-1.7900271106,-4.7596304789,3.4372683688
C,0,-2.3214315537,-4.261298057,1.4295788684
H,0,-4.1591680338,4.1917199998,1.7710833943
H,0,-5.1548639892,3.6194580491,0.4438665714
H,0,-1.8697855918,3.2791546513,-0.7655105856
H,0,-3.0503699806,-0.4998611157,1.873426112
H,0,-1.346996164,-2.3538435819,1.3895802456
H,0,-3.7178459233,4.6083159816,0.0993465805
H,0,2.6134060633,2.6528023706,-2.3984412705
H,0,1.0633559942,4.5635042459,-3.0386029782
H,0,0.2134371461,4.2965157153,-1.4931642074
H,0,-0.3512145193,2.2634432063,-2.995415518
H,0,-0.2166010227,-0.0971990112,-2.3069295462
H,0,1.5568204804,-0.0628231689,-2.5150426541
H,0,0.5922359437,1.4596847177,-4.8831498997
H,0,1.938114547,5.799296792,-1.1651269377
H,0,0.8470361272,0.361552171,0.0760979982
H,0,-2.7231200616,-4.2772274988,0.4246142951
H,0,-0.6645969184,-2.8475703836,3.8115825189
H,0,-1.7378790427,-5.3479101885,4.3441220906
N,0,-2.460721137,-5.2194050965,2.3250991895

LG 2.5 with Histidine B3LYP/6-31G*

Dndd25
E(RB3LYP) = -1101.28292573

Zero-point correction= 0.318254
(Hartree/Particle)
Thermal correction to Energy= 0.339778
Thermal correction to Enthalpy= 0.340722
Thermal correction to Gibbs Free Energy= 0.262158
Sum of electronic and zero-point Energies= -1100.964671
Sum of electronic and thermal Energies= -1100.943148
Sum of electronic and thermal Enthalpies= -1100.942204
Sum of electronic and thermal Free Energies= -1101.020768

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.214	77.636	165.353

C,0,0.6777410123,0.4912764085,-2.1863257072
C,0,0.9387535295,0.9522196436,-0.8028957317
O,0,1.544119533,2.0869662814,-0.7480125911
C,0,1.6091107454,2.7056733244,-2.0993146629
C,0,0.6853717688,1.8263813701,-2.9617776057
C,0,1.2365500373,4.1663458401,-1.9965549044
O,0,2.2889043691,4.8358969291,-1.3331062645
O,0,1.235666567,1.7754213209,-4.2602973269
N,0,-1.469783956,1.3652834368,-0.2753299517
C,0,-2.2529082077,2.4729517672,-0.1391071988
C,0,-3.3493678263,2.5879776422,0.667578782
C,0,-3.7139386916,1.4367006512,1.4789962421
N,0,-2.8405741185,0.3407323792,1.3208146107
C,0,-1.7194270476,0.2885611231,0.5115982435
O,0,-0.9738664022,-0.7233683362,0.5164765346
O,0,-4.667663504,1.3638808729,2.2463228822
C,0,-4.2101920599,3.8149793533,0.7544239898
N,0,-1.5791879193,-3.1589557213,1.8781267628
C,0,-1.2068269177,-3.4958912914,3.1618952278
C,0,-1.7337259476,-4.7459048133,3.3816735778
C,0,-2.2999541213,-4.2104230486,1.3932838554
H,0,-4.2525649071,4.1952392472,1.7822747564
H,0,-5.2451776144,3.5962355934,0.4647205723
H,0,-1.9670582886,3.317614285,-0.7683699841
H,0,-3.0452507241,-0.4727400456,1.8919264373
H,0,-1.3392342794,-2.2949521991,1.3764624
H,0,-3.8308980845,4.6122645612,0.1056904778
H,0,2.648441376,2.6033580654,-2.4242968526
H,0,1.0931281244,4.5279717488,-3.0284570692
H,0,0.277518709,4.259307459,-1.4649189795
H,0,-0.3313261118,2.2420357189,-2.9656843841
H,0,-0.2320749527,-0.1040934627,-2.2485080741
H,0,1.5363573013,-0.1192636613,-2.5109752977
H,0,0.565172752,1.4261848365,-4.867233728
H,0,2.0140276783,5.7486739968,-1.1593490424
H,0,0.8476074997,0.3564504186,0.1007326919
H,0,-2.7170273155,-4.2089574543,0.394464351
H,0,-0.620353644,-2.8315276801,3.7793404981
H,0,-1.6629387009,-5.3522943038,4.2752585262
N,0,-2.4165330705,-5.1888343771,2.2700521969

LG 2.6 with Histidine B3LYP/6-31G*

Dndd26
E(RB3LYP) = -1101.27973655

Zero-point correction= 0.318039
(Hartree/Particle)
Thermal correction to Energy= 0.339668
Thermal correction to Enthalpy= 0.340612
Thermal correction to Gibbs Free Energy= 0.261163
Sum of electronic and zero-point Energies= -1100.961698
Sum of electronic and thermal Energies= -1100.940069

Sum of electronic and thermal Enthalpies= -1100.939124
Sum of electronic and thermal Free Energies= -1101.018574

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.145	77.789	167.216

C,0,0.6210793908,0.4381415548,-2.1503781722
C,0,0.9566500374,0.8829677969,-0.7806177598
O,0,1.6003479442,1.9914878166,-0.7415272658
C,0,1.6370819291,2.6198655033,-2.0921504697
C,0,0.6624296569,1.7711409522,-2.9301201742
C,0,1.3010586232,4.0868633495,-1.9575836776
O,0,2.392108666,4.7240081085,-1.3257162582
O,0,1.1832511913,1.6953300443,-4.2392643609
N,0,-1.5172520601,1.4640970742,-0.2309774095
C,0,-2.3224751215,2.5588086929,-0.1256543534
C,0,-3.436164021,2.6712519587,0.6586063908
C,0,-3.8022422909,1.5265131842,1.4759402138
N,0,-2.9117065352,0.4410235625,1.3469238323
C,0,-1.7764131113,0.392464811,0.5565823786
O,0,-1.0274991979,-0.6174536941,0.5904063495
O,0,-4.7693516725,1.4488498409,2.2269016711
C,0,-4.3122909815,3.8893417756,0.7137095305
N,0,-1.5201077429,-3.1261293376,1.8594078807
C,0,-1.1366510384,-3.4952356422,3.1306584812
C,0,-1.5666257173,-4.7917592765,3.2828627593
C,0,-2.1508745955,-4.2051160066,1.3144028686
H,0,-4.3737427368,4.2866876126,1.7342388858
H,0,-5.3405789882,3.6537550695,0.4134288336
H,0,-2.0368419701,3.3997962528,-0.7605400335
H,0,-3.1200640221,-0.3698931875,1.9198923453
H,0,-1.3446043099,-2.2223579316,1.4036848322
H,0,-3.9331983756,4.6802532025,0.0569643836
H,0,2.6629214615,2.4952155096,-2.449802131
H,0,1.1274629842,4.4655827118,-2.9787554712
H,0,0.3646734256,4.1914018474,-1.3893296448
H,0,-0.3385408459,2.2222374322,-2.9133764847
H,0,-0.3153510174,-0.1149472301,-2.1753048261
H,0,1.4367113398,-0.2143401911,-2.5046230542
H,0,0.4844040049,1.3809020381,-4.8331388001
H,0,2.1376887814,5.6341417763,-1.1116647226
H,0,0.831872146,0.3047743195,0.1295351917
H,0,-2.5564555022,-4.1870189593,0.3110129721
H,0,-0.6108523253,-2.8182143234,3.7877987486
H,0,-1.4582324108,-5.4336870324,4.1474159594
N,0,-2.2010084022,-5.2313731061,2.1417488207

LG 2.7 with Histidine B3LYP/6-31G*

Dndd27
E(RB3LYP) = -1101.27705566

Zero-point correction= 0.317931 (Hartree/Particle)
Thermal correction to Energy= 0.340496
Thermal correction to Enthalpy= 0.341440
Thermal correction to Gibbs Free Energy= 0.257045
Sum of electronic and zero-point Energies= -1100.959124
Sum of electronic and thermal Energies= -1100.936560
Sum of electronic and thermal Enthalpies= -1100.935616
Sum of electronic and thermal Free Energies= -1101.020011

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.664	79.810	177.624

C,0,0.5060112286,0.4213436843,-2.2693824907
C,0,0.9590513779,0.7186332285,-0.8948466417
O,0,1.6694364544,1.7761907404,-0.7994007058
C,0,1.6695245227,2.5262288351,-2.0901954144
C,0,0.6061326523,1.8089425414,-2.9433939468
C,0,1.414087873,3.9863422199,-1.7970700521
O,0,2.569442628,4.5114638102,-1.1767706312
O,0,1.0654131611,1.8044322994,-4.2773589695
N,0,-1.5185344173,1.5476387662,-0.2134399462
C,0,-2.3527419048,2.6200300185,-0.1034847639
C,0,-3.5049802016,2.6815513781,0.630604768
C,0,-3.8893410504,1.4976482287,1.3794816364
N,0,-2.977686214,0.4307662259,1.2399842068
C,0,-1.8128867241,0.4338225931,0.493167729
O,0,-1.0705921798,-0.5882126938,0.4872388847
O,0,-4.8874609948,1.3708977857,2.0825269228
C,0,-4.3990909925,3.8857913402,0.7025068661
N,0,-1.4585407902,-3.0498227567,1.8715695944
C,0,-1.0975766907,-3.3320132314,3.1713381402
C,0,-1.4373621019,-4.6487817931,3.3701274395
C,0,-1.9878545771,-4.1962575344,1.3570667823
H,0,-4.510811223,4.2354093239,1.7361771997
H,0,-5.410140121,3.6525970817,0.346621461
H,0,-2.0489596929,3.4958514444,-0.6806885964
H,0,-3.2033182063,-0.4108347888,1.7595231495
H,0,-1.3308172409,-2.1569777756,1.3791982611
H,0,-4.0024835228,4.7105367598,0.0998202939
H,0,2.6679507474,2.3872475431,-2.5133914306
H,0,1.2012452794,4.4690489271,-2.7656403582
H,0,0.5176514668,4.0733613802,-1.1654780098
H,0,-0.3604094808,2.3187742526,-2.8425778483
H,0,-0.474125735,-0.0534819959,-2.2716648269
H,0,1.2408833341,-0.2616388969,-2.7277709744
H,0,0.3195027646,1.5989288944,-4.8615464801
H,0,2.3645220462,5.3958871835,-0.83821395
H,0,0.799676504,0.0966575953,-0.0148802186
H,0,-2.3556462847,-4.2534553274,0.3406600825
H,0,-0.6487765411,-2.5886253478,3.8136675154
H,0,-1.3155752482,-5.2412736039,4.2675497124
N,0,-1.9942033146,-5.1852704558,2.2299638697

LG 2.2 without Histidine B3LYP/6-31G*

22
E(RB3LYP) = -875.068013945

C,0,-1.7359265922,-1.0219967427,-1.4264130307
C,0,-0.3133197421,-0.6021964058,-1.5754005029
O,0,-0.205573858,0.6531738658,-1.9691853292
C,0,-1.4760759255,1.3605363181,-1.7480019339
C,0,-2.4407565033,0.3093506211,-1.1355210611
N,0,0.3965728658,-0.5768602317,0.400810644
C,0,1.314568521,0.376734607,0.7193319836
C,0,2.049557842,0.3946643589,1.8676390492
C,0,1.8612645864,-0.7034783497,2.8088861917
N,0,0.9297303732,-1.6659448536,2.3793558952
C,0,0.2059227303,-1.6843549838,1.1883646732
O,0,-0.5439437788,-2.6214416415,0.9083681228
O,0,2.4366099105,-0.830994282,3.8849945631
C,0,3.0399236353,1.4673249489,2.2195300662
C,0,-1.2432179067,2.5815355981,-0.8812582655
O,0,-3.7212995992,0.3195530039,-1.7409204491
H,0,-2.2319244208,3.032425502,-0.6815691368
H,0,0.7922393765,-2.4605142704,2.9940331483
H,0,1.4221314289,1.1655811708,-0.0253553509
H,0,-2.0845636716,-1.3987000835,-2.4001080316
H,0,-1.8553549492,-1.796386146,-0.6690001037

H,0,-1.8247963303,1.6616880365,-2.7399669176
H,0,-2.5144442231,0.4568763111,-0.0501197115
H,0,3.1026387151,2.2231761731,1.4291038197
H,0,2.7688000237,1.9670659621,3.1576651111
H,0,4.0402435659,1.0455049977,2.3741694148
H,0,-0.8196877708,2.2660913675,0.0830588591
O,0,-0.3887639368,3.469597414,-1.5757178365
H,0,-0.17856156,4.2115497331,-0.9888081382
H,0,0.4790228268,-1.2564108829,-1.9236798364
H,0,-4.2692617631,0.9844761842,-1.2978660564

LG 2.3 without Histidine B3LYP/6-31G*

E(RB3LYP) = -875.064849458

C,0,-1.5901380803,-1.0326012853,-1.5568034255
C,0,-0.2231192947,-0.4536169811,-1.6163516141
O,0,-0.2170543056,0.8072780735,-1.9675509449
C,0,-1.5630296034,1.3840503127,-1.7740556053
C,0,-2.4518887061,0.2092165555,-1.2835891489
N,0,0.320414495,-0.355075973,0.5131696231
C,0,1.422476774,0.4113619212,0.7580479158
C,0,2.2077077047,0.3338941633,1.8700139526
C,0,1.8674618417,-0.6734861566,2.8678495556
N,0,0.7481405613,-1.4512286481,2.5245934521
C,0,-0.03186802,-1.3654870134,1.3731316076
O,0,-0.9748216329,-2.1421741641,1.1898012614
O,0,2.4652401137,-0.8717682636,3.9210951924
C,0,3.3892892743,1.2226692562,2.1325059067
C,0,-1.4688093387,2.5529615973,-0.8161954515
O,0,-3.6745283487,0.1266946174,-1.9957035469
H,0,-2.5022945338,2.8716102858,-0.5908013422
H,0,0.4857694846,-2.1754726272,3.1838408695
H,0,1.6351069368,1.1508172954,-0.0150708501
H,0,-1.8400602702,-1.4340110631,-2.55092587
H,0,-1.6743579286,-1.8103991439,-0.7953258935
H,0,-1.8844968161,1.7213461983,-2.7628488837
H,0,-2.6237890431,0.291267142,-0.2036337472
H,0,3.553973632,1.9178623926,1.3021328692
H,0,3.2529108059,1.8065920784,3.0511589123
H,0,4.3021858475,0.6323946801,2.276628285
H,0,-1.0097399589,2.2091521332,0.1212705584
O,0,-0.7244806433,3.5833619335,-1.4384418138
H,0,-0.5282066276,4.2605204962,-0.7738603693
H,0,0.680661976,-0.9998440742,-1.8599209242
H,0,-4.3569024253,0.5997415609,-1.4977406806

LG 2.4 without Histidine B3LYP/6-31G*

E(RB3LYP) = -875.060391938

C,0,-1.3936608412,-0.9562416629,-1.6357058844
C,0,-0.1285391531,-0.185106082,-1.6986936458
O,0,-0.3049162976,1.0643271629,-2.0077517051
C,0,-1.7260586476,1.4377926728,-1.8088769186
C,0,-2.4094762976,0.1554026739,-1.2970681846
N,0,0.4150784341,-0.0802873883,0.5336799645
C,0,1.6689629769,0.3991081784,0.780941734
C,0,2.3981393758,0.1795509959,1.91319966
C,0,1.8078123166,-0.6649722605,2.9432122411
N,0,0.5316096983,-1.1482871722,2.6075888943
C,0,-0.1881264224,-0.9116278402,1.4393427077
O,0,-1.3058554381,-1.4242120739,1.2785391764
O,0,2.3248539734,-0.9618719903,4.0163234712
C,0,3.7577251116,0.7637276177,2.1684572822
C,0,-1.7964073915,2.6178551516,-0.8655978595
O,0,-3.6627972345,0.0394911578,-1.9457444191
H,0,-2.8578613085,2.7456762321,-0.5948062294
H,0,0.0836640467,-1.7466490051,3.2925634569
H,0,2.0744641217,1.0336443348,-0.0082820148
H,0,-1.5968206156,-1.3577057749,-2.6411910555
H,0,-1.3726913484,-1.7555030006,-0.8939998956
H,0,-2.1020748975,1.7122599654,-2.7980801333
H,0,-2.51630841,0.1823515827,-0.2067420035
H,0,4.0942616982,1.3696814957,1.3202134012
H,0,3.7578190716,1.3948093049,3.0656767588
H,0,4.4988287395,-0.0247140003,2.3474187896
H,0,-1.2344280902,2.3741652862,0.0469902381
O,0,-1.2785181933,3.7528871267,-1.5363984974
H,0,-1.1984123193,4.4734259971,-0.8937894882
H,0,0.8599215587,-0.5788129344,-1.9063851449
H,0,-4.2084343467,-0.5725384509,-1.4286148463

LG 2.5 without Histidine B3LYP/6-31G*

E(RB3LYP) = -875.056508687

C,0,-1.3847398868,-0.9518907222,-1.6257814573
C,0,-0.1405674809,-0.160844828,-1.7449197307
O,0,-0.3374056897,1.0783302737,-2.057636254
C,0,-1.7635281922,1.4354794913,-1.8418546993
C,0,-2.4202684862,0.1488683794,-1.3067884387
N,0,0.4046528509,0.0197080081,0.5853450691
C,0,1.6723481193,0.458700435,0.8360262624
C,0,2.4192583726,0.1711831775,1.9425248424
C,0,1.8328846794,-0.7109144213,2.9420695836
N,0,0.5432723062,-1.1551901197,2.6063751059
C,0,-0.1886815166,-0.8477650987,1.4624235788
O,0,-1.3161060803,-1.3416744433,1.2951667877
O,0,2.3636548906,-1.0685383456,3.9902189139
C,0,3.7927413113,0.7205726536,2.1999098783
C,0,-1.8271204343,2.6222517105,-0.9066813125
O,0,-3.6719353887,-0.0025817197,-1.9506646858
H,0,-2.8844653505,2.7416368614,-0.6165315362
H,0,0.0968849022,-1.780508001,3.2678438859
H,0,2.0792239421,1.1240841715,0.0727606706
H,0,-1.5984736943,-1.4036201101,-2.6078890785
H,0,-1.3326752602,-1.7178401799,-0.8495145036
H,0,-2.1549772006,1.6965104054,-2.8285425894
H,0,-2.5226996563,0.1905800733,-0.2167420268
H,0,4.1261937798,1.3569872958,1.3729297914
H,0,3.8190288197,1.3123118639,3.1232898523
H,0,4.52273566,-0.0872639551,2.332397556
H,0,-1.2450624628,2.389170081,-0.0043184382
O,0,-1.3343657327,3.7569953974,-1.596724438
H,0,-1.2080857569,4.4707280472,-0.9540776155
H,0,0.8613516022,-0.535766135,-1.9214540946
H,0,-4.2113190963,-0.6020729463,-1.4127410291

LG 2.6 without Histidine B3LYP/6-31G*

E(RB3LYP) = -875.053130378

C,0,-1.3897909875,-0.9540426956,-1.6194820067
C,0,-0.1602659088,-0.1581821963,-1.800761845
O,0,-0.3661236582,1.0753215529,-2.1106316483
C,0,-1.7904126456,1.4316534781,-1.8652400797
C,0,-2.4352274828,0.1438088965,-1.3184820801
N,0,0.398329071,0.0955319362,0.6227889447
C,0,1.6720903199,0.5117904997,0.8792295414
C,0,2.4307609104,0.1759307981,1.9652534607
C,0,1.8497864631,-0.7388590774,2.9373469649
N,0,0.5542576936,-1.1615238755,2.5982341854
C,0,-0.1854081323,-0.8018352928,1.4747316434
O,0,-1.3177538361,-1.2866815504,1.2999730584
O,0,2.3893796707,-1.1398632482,3.9655889485
C,0,3.8106935521,0.706368167,2.227168623
C,0,-1.8276896912,2.6143945381,-0.9234664241

O,0,-3.6830259053,-0.0276077415,-1.9654001845
H,0,-2.8783664002,2.7380215972,-0.6114988474
H,0,0.1103517912,-1.809422194,3.2392858719
H,0,2.0783055137,1.2036470544,0.1391457848
H,0,-1.6202728362,-1.4573557811,-2.5724198233
H,0,-1.3089740821,-1.6824304872,-0.8079288546
H,0,-2.1992167288,1.6959937394,-2.8437369131
H,0,-2.5407418488,0.1963900257,-0.2293757032
H,0,4.1392549319,1.3707035755,1.4203526829
H,0,3.851786948,1.2635498086,3.1713517149
H,0,4.5368252599,-0.110375027,2.3215594293
H,0,-1.2284500651,2.3714706719,-0.0352797783
O,0,-1.3432220554,3.7494671767,-1.6187873156
H,0,-1.1793375202,4.4525274583,-0.9729471554
H,0,0.8474908156,-0.5246027147,-1.9637616536
H,0,-4.2232792866,-0.6161617927,-1.4163906912

$D_N^*A_N^‡$ mechanism– transition structures with and without histidine mimic

Nuc 2.2 with Histidine B3LYP/6-31G*

E(RB3LYP) = -3183.65102565

Zero-point correction= 0.252453
(Hartree/Particle)
Thermal correction to Energy= 0.272121
Thermal correction to Enthalpy= 0.273065
Thermal correction to Gibbs Free Energy= 0.201443
Sum of electronic and zero-point Energies= -3183.398573
Sum of electronic and thermal Energies= -3183.378905
Sum of electronic and thermal Enthalpies= -3183.377961
Sum of electronic and thermal Free Energies= -3183.449583

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.758	70.620	150.742

C,0,-0.513198098,0.8514886378,-1.7499195603
C,0,0.2717552348,0.9879867651,-0.4952385225
O,0,1.3260368757,1.7153262126,-0.6480515587
C,0,1.6962919886,1.7849973768,-2.0935183739
C,0,0.6109194273,0.9377345527,-2.8206575001
C,0,1.7436394061,3.2399027319,-2.5131758829
O,0,2.6867240637,3.917206082,-1.7076500175
O,0,1.0574425232,-0.32000153,-3.2302322003
N,0,-1.428457982,-4.2191055687,1.397481196
C,0,-0.9824960782,-5.1544184947,2.312480189
C,0,0.3652785981,-4.9349677993,2.4225130181
N,0,0.742502705,-3.8942422063,1.602069403
C,0,-0.3558492486,-3.4832381075,0.9980309336
H,0,-2.3789221467,-4.1065904223,1.0768893439
H,0,2.8950486532,0.4423354797,1.777358456
H,0,2.6789128799,1.307940474,-2.121959696
H,0,2.0219610558,3.2513168712,-3.579495685
H,0,0.7371055435,3.6868669962,-2.4297664646
H,0,0.2608367014,1.457432076,-3.7183816594
H,0,-1.2029458867,1.7074695091,-1.8121891186
H,0,-1.0855325023,-0.0730576166,-1.8140839494
H,0,1.2381542351,-0.8283319199,-2.402762942
H,0,2.7668436378,4.8260417832,-2.0341733972
O,0,0.9745874657,-1.0944729545,-0.5921334163
O,0,2.9899798869,-2.6377422092,0.5811472922
H,0,2.2275083528,-3.1074668659,1.031601705
O,0,3.7123817457,-0.2244357332,-0.6830383528
O,0,2.15970053,-0.1837974345,1.6623454691
H,0,-0.0582929525,0.8509344367,0.5274769693
As,0,2.5352381371,-1.026411898,0.1308201959
H,0,-0.3917258359,-2.6711606315,0.2826388637
H,0,-1.6471143144,-5.8638525622,2.7810513123
H,0,1.0843995677,-5.4574004709,3.0370952306

Nuc 2.3 with Histidine B3LYP/6-31G*

Anhisdis2.3
E(RB3LYP) = -3183.64737417

Zero-point correction= 0.252268
(Hartree/Particle)
Thermal correction to Energy= 0.271963
Thermal correction to Enthalpy= 0.272908
Thermal correction to Gibbs Free Energy= 0.201219
Sum of electronic and zero-point Energies= -3183.395106
Sum of electronic and thermal Energies= -3183.375411
Sum of electronic and thermal Enthalpies= -3183.374467
Sum of electronic and thermal Free Energies= -3183.446155

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.660	70.686	150.880

C,0,-0.5266783598,0.9034292664,-1.7312419306
C,0,0.2561545202,1.0714107874,-0.4824764915
O,0,1.3305340471,1.7526963318,-0.6494801808
C,0,1.7006244558,1.787834196,-2.1008224109
C,0,0.5978170576,0.9446665462,-2.8070311111
C,0,1.7725091945,3.2329003108,-2.5484507991
O,0,2.7192523072,3.9126754448,-1.7501011833
O,0,1.0169434925,-0.3270676902,-3.1923784115
N,0,-1.4114780373,-4.2650030373,1.3764323178
C,0,-0.9670893132,-5.1975449032,2.2951031887
C,0,0.3764999121,-4.9627875115,2.4234772401
N,0,0.7528216497,-3.9159206932,1.6104575992
C,0,-0.3420652562,-3.5159030137,0.9926930169
H,0,-2.3586792729,-4.162769731,1.0430864623
H,0,2.8606503966,0.4369055983,1.8004433713
H,0,2.6739422562,1.2907605924,-2.1114560268
H,0,2.0581753031,3.2164830882,-3.6127201987
H,0,0.7720694367,3.6965179185,-2.4829054867
H,0,0.2539203205,1.4556675796,-3.712387503
H,0,-1.2085842253,1.7637998613,-1.8199379257
H,0,-1.1088547913,-0.0166793323,-1.7637033606
H,0,1.1860898511,-0.8285018654,-2.3544609621
H,0,2.8252372126,4.8092753561,-2.1021270088
O,0,0.9530911141,-1.1181151973,-0.5837464516
O,0,2.9969972828,-2.6164604419,0.6181910109
H,0,2.2380012406,-3.1007682168,1.0571499299
O,0,3.6763719313,-0.2042695819,-0.6668772469
O,0,2.1097397554,-0.1659259694,1.6642137451
H,0,-0.0562681272,0.9250135136,0.5450556532
As,0,2.5044146437,-1.0221287641,0.1417925702
H,0,-0.3769818462,-2.7016912597,0.2791000829
H,0,-1.6297013945,-5.915707804,2.7531483011
H,0,1.0932374125,-5.4785058186,3.0465314801

Nuc 2.4 with Histidine B3LYP/6-31G*

Anhisdis2.4
E(RB3LYP) = -3183.64415745

Zero-point correction= 0.252087
(Hartree/Particle)

Thermal correction to Energy= 0.271814
Thermal correction to Enthalpy= 0.272758
Thermal correction to Gibbs Free Energy= 0.200950
Sum of electronic and zero-point Energies= -3183.392070
Sum of electronic and thermal Energies= -3183.372344
Sum of electronic and thermal Enthalpies= -3183.371399
Sum of electronic and thermal Free Energies= -3183.443207

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.566	70.740	151.133

C,0,-0.5417504329,0.9643228755,-1.7082234612
C,0,0.2422506882,1.1661882372,-0.468094669
O,0,1.3384493509,1.795367122,-0.6533057177
C,0,1.7053462879,1.7866594391,-2.1102107226
C,0,0.5801810614,0.9508959451,-2.7898789858
C,0,1.8075853048,3.218332829,-2.5925976059
O,0,2.7630895849,3.899632917,-1.8067472909
O,0,0.9655309315,-0.3369135878,-3.1471298328
N,0,-1.3928519898,-4.3191537343,1.3534313285
C,0,-0.9449793571,-5.2584142746,2.2636184804
C,0,0.3924553095,-5.0025647131,2.414265632
N,0,0.7621607406,-3.9381792094,1.6211746764
C,0,-0.3309937922,-3.5471056256,0.994538196
H,0,-2.3369558499,-4.2278837588,1.0084033391
H,0,2.8233404152,0.4443347302,1.8308880798
H,0,2.6668378775,1.2663335728,-2.1028329785
H,0,2.0977673109,3.167593923,-3.6545439274
H,0,0.816257068,3.7034925875,-2.5454635009
H,0,0.2429010975,1.4508390641,-3.7041445093
H,0,-1.2132785614,1.829603111,-1.8262521328
H,0,-1.1368762347,0.051762359,-1.7037693339
H,0,1.126026539,-0.8287563954,-2.2979032182
H,0,2.8976194165,4.7804574397,-2.1876841741
O,0,0.9251681613,-1.132665244,-0.5624167741
O,0,2.9969859555,-2.5837098657,0.6677419337
H,0,2.2423989498,-3.0860737106,1.092253424
O,0,3.6358425639,-0.1802787016,-0.645669787
O,0,2.0578202841,-0.1344438852,1.6738467955
H,0,-0.0575861762,1.0256669711,0.5647300355
As,0,2.4688898643,-1.008330271,0.1628827641
H,0,-0.3688106219,-2.7228980878,0.2921442862
H,0,-1.6013739718,-5.9944911729,2.7017870391
H,0,1.1092663948,-5.5153353255,3.0397338917

Nuc 2.5 with Histidine B3LYP/6-31G*

Anhisdis2.5
E(RB3LYP) = -3183.64130469

Zero-point correction= 0.251939 (Hartree/Particle)
Thermal correction to Energy= 0.271684
Thermal correction to Enthalpy= 0.272628
Thermal correction to Gibbs Free Energy= 0.200838
Sum of electronic and zero-point Energies= -3183.389366
Sum of electronic and thermal Energies= -3183.369621
Sum of electronic and thermal Enthalpies= -3183.368677
Sum of electronic and thermal Free Energies= -3183.440467

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.484	70.771	151.095

C,0,-0.5556168179,1.0182288768,-1.687844932
C,0,0.228850549,1.251462813,-0.455999538
O,0,1.3432011542,1.8335292072,-0.6548958565
C,0,1.7080057015,1.7856239605,-2.1158376571
C,0,0.5628525265,0.9598207538,-2.7741309418
C,0,1.8397374551,3.2043416669,-2.6276667864
O,0,2.8042942496,3.8844350396,-1.8524644659
O,0,0.9181239099,-0.3391596968,-3.1125436042
N,0,-1.3725467686,-4.3677264281,1.33096324
C,0,-0.924101944,-5.305525871,2.2424449479
C,0,0.4075619561,-5.0320682459,2.4122156882
N,0,0.7729183298,-3.9575776756,1.6307863548
C,0,-0.3170077818,-3.5783814775,0.9911315254
H,0,-2.3128280775,-4.2880576578,0.972935178
H,0,2.7793704474,0.4425690383,1.8592529519
H,0,2.6580341314,1.2443345054,-2.0913427759
H,0,2.1333983164,3.1230761609,-3.6867222316
H,0,0.8579231565,3.7099851706,-2.5972239503
H,0,0.2304428259,1.4535587131,-3.6938416288
H,0,-1.2208015076,1.8847187424,-1.831512489
H,0,-1.1595099953,0.1118712972,-1.6509967836
H,0,1.0739980257,-0.8267749859,-2.2561974247
H,0,2.9673630124,4.7487340424,-2.2592372998
O,0,0.9027660456,-1.1539962115,-0.5540053405
O,0,2.9975454979,-2.5558607083,0.7072836768
H,0,2.2482440506,-3.0738165546,1.1209289393
O,0,3.5996818851,-0.1592323967,-0.628224205
O,0,2.0025760733,-0.1127806587,1.6757190146
H,0,-0.0633864654,1.1206279602,0.5810447911
As,0,2.4365106116,-0.9994722891,0.1758314549
H,0,-0.3559302671,-2.7502400562,0.2928963608
H,0,-1.5759358398,-6.0532782101,2.6674999644
H,0,1.1229797234,-5.5386832646,3.044325103

Nuc 2.6 with Histidine B3LYP/6-31G*

Anhisdis2.6
E(RB3LYP) = -3183.63874095

Zero-point correction= 0.251779 (Hartree/Particle)
Thermal correction to Energy= 0.271534
Thermal correction to Enthalpy= 0.272478
Thermal correction to Gibbs Free Energy= 0.200736
Sum of electronic and zero-point Energies= -3183.386962
Sum of electronic and thermal Energies= -3183.367207
Sum of electronic and thermal Enthalpies= -3183.366263
Sum of electronic and thermal Free Energies= -3183.438005

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.390	70.789	150.995

C,0,-0.5651049309,1.0693031156,-1.6641529038
C,0,0.2248688442,1.3308412649,-0.4432922754
O,0,1.3533110311,1.8712834846,-0.6574574763
C,0,1.7111796753,1.7874076757,-2.1227588419
C,0,0.5454557483,0.9727932242,-2.7588675786
C,0,1.8687443627,3.1937880588,-2.6600151226
O,0,2.84455089,3.8713392711,-1.8973386105
O,0,0.8708808336,-0.3355334431,-3.081878681
N,0,-1.3506109735,-4.4189225048,1.3045422194
C,0,-0.904606289,-5.3469234414,2.2272414455
C,0,0.4191683398,-5.0518089093,2.4209516339

N,0,0.7823663636,-3.9744349369,1.64241904
C,0,-0.3012074948,-3.6145167318,0.9810842119
H,0,-2.2848128949,-4.3556975265,0.9278526546
H,0,2.7255529214,0.4219736539,1.8976436094
H,0,2.6500497111,1.2273155099,-2.0858126631
H,0,2.1612156779,3.0860259153,-3.7170193071
H,0,0.8962734232,3.7179747049,-2.641124324
H,0,0.2142224391,1.4622172793,-3.6815991908
H,0,-1.2275197756,1.9345214726,-1.8264644846
H,0,-1.1740710935,0.167594018,-1.5973525393
H,0,1.0228878216,-0.818978105,-2.2176786679
H,0,3.0357366149,4.7173751382,-2.3294404818
O,0,0.8840870542,-1.1815100771,-0.5595780159
O,0,2.9972337071,-2.5284957362,0.7472850434
H,0,2.2531662036,-3.0603391175,1.1512481261
O,0,3.563567278,-0.1440495083,-0.6206198428
O,0,1.9371074661,-0.0982020196,1.667279039
H,0,-0.0590244935,1.2144707868,0.5984451971
As,0,2.4051460146,-0.9950251535,0.1806280239
H,0,-0.3389053529,-2.7890390968,0.2792874622
H,0,-1.5524991789,-6.1034394983,2.6427530148
H,0,1.1303042261,-5.545023208,3.0683615663

Nuc 2.7 with Histidine B3LYP/6-31G*

Anhisdis2.7
E(RB3LYP) = -3183.63648089

Zero-point correction= 0.251669
(Hartree/Particle)
Thermal correction to Energy= 0.271434
Thermal correction to Enthalpy= 0.272378
Thermal correction to Gibbs Free Energy= 0.200670
Sum of electronic and zero-point Energies= -
3183.384812
Sum of electronic and thermal Energies= -
3183.365047
Sum of electronic and thermal Enthalpies= -
3183.364103
Sum of electronic and thermal Free Energies= -
3183.435811

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.327	70.811	150.921

C,0,-0.5702276817,1.1078811003,-1.6399474639
C,0,0.2216149835,1.4030908944,-0.4299546732
O,0,1.3612308575,1.9063962901,-0.656434015
C,0,1.7144152495,1.7899924761,-2.1235433674
C,0,0.5319788389,0.987091167,-2.7427372972
C,0,1.8951412738,3.1842792695,-2.6839477949
O,0,2.8820807589,3.8585623462,-1.9331995407
O,0,0.8364638352,-0.3240963127,-3.0676747514
N,0,-1.3349771296,-4.4672088351,1.2840523577
C,0,-0.8885277869,-5.3815918531,2.220035646
C,0,0.4274293543,-5.0642698638,2.4311151207
N,0,0.7855945298,-3.9870171198,1.6500447832
C,0,-0.2934531163,-3.6487684988,0.9699843972
H,0,-2.2641189349,-4.421357677,0.8926675047
H,0,2.6749442472,0.4285968071,1.8965918799
H,0,2.6431350802,1.2132411597,-2.0747683423
H,0,2.1850739844,3.0522581328,-3.7388648702
H,0,0.9313521393,3.7247201305,-2.6745565468
H,0,0.1980082614,1.4795913206,-3.6631086244
H,0,-1.2397037361,1.9642215326,-1.8207059944
H,0,-1.1743909984,0.2054454695,-1.5423067726
H,0,0.9946504658,-0.8157403405,-2.2067307708
H,0,3.0894510694,4.6924357444,-2.3812133122
O,0,0.8722327152,-1.2135709976,-0.5705856547
O,0,2.9926840348,-2.5119446729,0.7766604223
H,0,2.2510651856,-3.0518106728,1.1738399462
O,0,3.5382828231,-0.1344021552,-0.6078582492
O,0,1.8860179762,-0.0856487452,1.6547171685
H,0,-0.0589612879,1.3065320517,0.6153259891
As,0,2.3788154549,-0.9969519268,0.1818849471
H,0,-0.3343294439,-2.8287606525,0.2616528028
H,0,-1.5306239494,-6.1452771235,2.631430838
H,0,1.136365116,-5.5416328848,3.092705518

Nuc 2.2 without Histidine B3LYP/6-31G*

Andis22
E(RB+HF-LYP) = -2957.41754786
Zero-point correction= 0.178824
(Hartree/Particle)
Thermal correction to Energy= 0.193640
Thermal correction to Enthalpy= 0.194585
Thermal correction to Gibbs Free Energy= 0.135927
Sum of electronic and zero-point Energies= -
2957.238724
Sum of electronic and thermal Energies= -
2957.223907
Sum of electronic and thermal Enthalpies= -
2957.222963
Sum of electronic and thermal Free Energies= -
2957.281621

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.511	52.979	123.455

C,0,-0.3038121907,3.804218824,1.4144318138
C,0,-0.088479815,2.7536183271,0.3863327806
O,0,-1.1648732097,2.3880661977,-0.2167716218
C,0,-2.3799379056,2.8861720753,0.4946229256
C,0,-1.8540532676,3.8272286456,1.6183147094
C,0,-3.2788076571,3.5539895304,-0.5208492806
O,0,-3.684732626,2.5902007961,-1.4726426089
O,0,-2.2851027066,3.470410309,2.8917502523
O,0,-1.9662187758,0.8350966039,2.7008702855
As,0,-0.4381253556,0.2356502121,2.5213179758
O,0,0.2266998189,-0.1502541854,4.1064198304
O,0,-0.4133868563,-1.3901388574,1.8112040638
O,0,0.6944489323,1.1180691377,1.6321262824
H,0,0.0495807269,-1.2947912674,0.9613790515
H,0,-2.8338980451,1.9877309991,0.9138769754
H,0,-4.1298428815,3.9683710996,0.0435146879
H,0,-2.7461513103,4.3993395828,-0.989559464
H,0,-2.2192344201,4.8461219686,1.4438730565
H,0,0.0759444537,4.7547172066,1.0119245801
H,0,0.2373188714,3.5921710071,2.3371969607
H,0,-2.1422793376,2.4893317438,2.9985970352
H,0,-4.311400231,3.0090615881,-2.0816634698
H,0,0.7787659224,-0.9434630366,4.0022170974
H,0,0.8373788662,2.5398134921,-0.1318619193

Nuc 2.3 without Histidine B3LYP/6-31G*

Andis23
E(RB+HF-LYP) = -2957.41396619

Zero-point correction= 0.178482
(Hartree/Particle)
Thermal correction to Energy= 0.193498
Thermal correction to Enthalpy= 0.194442
Thermal correction to Gibbs Free Energy= 0.134096
Sum of electronic and zero-point Energies= -
2957.235484
Sum of electronic and thermal Energies= -
2957.220469

Sum of electronic and thermal Enthalpies= -2957.219524
Sum of electronic and thermal Free Energies= -2957.279870

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.422	53.116	127.009

C,0,-0.3007240591,3.7441215575,1.4490466521
C,0,-0.0931718223,2.7678252561,0.3520695802
O,0,-1.1632462954,2.432053068,-0.2655906112
C,0,-2.3818789872,2.8977888219,0.4686196307
C,0,-1.8545497464,3.8000364313,1.6231904832
C,0,-3.2895969317,3.5932804604,-0.5186879685
O,0,-3.6952428733,2.6599998274,-1.5000171064
O,0,-2.3212681264,3.4240377943,2.8773063137
O,0,-1.981902577,0.8063977659,2.6059507037
As,0,-0.4555518402,0.1846004558,2.4826664831
O,0,0.1520659901,-0.0617598138,4.119770857
O,0,-0.4542224548,-1.4774294347,1.8691081407
O,0,0.7090597655,0.984111027,1.5623538746
H,0,0.0268989596,-1.4345385619,1.0249923797
H,0,-2.8214757235,1.9788677541,0.8585843877
H,0,-4.1384042424,3.982703526,0.0663340572
H,0,-2.7655030423,4.457885784,-0.9613639709
H,0,-2.1915880074,4.8311323502,1.464285138
H,0,0.1241625887,4.7091646199,1.136767436
H,0,0.2139659471,3.4360358401,2.3604909699
H,0,-2.1682508434,2.441795122,2.9724430061
H,0,-4.3401442609,3.0899446711,-2.0816706524
H,0,1.0115584689,-0.5110394609,4.0561975859
H,0,0.8388111139,2.5337161382,-0.1462243701

Nuc 2.4 without Histidine B3LYP/6-31G*

Andis24

E(RB+HF-LYP) = -2957.41070550

Zero-point correction= 0.178405 (Hartree/Particle)
Thermal correction to Energy= 0.193366
Thermal correction to Enthalpy= 0.194311
Thermal correction to Gibbs Free Energy= 0.135067
Sum of electronic and zero-point Energies= -2957.232300
Sum of electronic and thermal Energies= -2957.217339
Sum of electronic and thermal Enthalpies= -2957.216395
Sum of electronic and thermal Free Energies= -2957.275638

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.339	53.201	124.689

C,0,-0.3122415509,3.7921619726,1.4109057814
C,0,-0.1088420511,2.8205910401,0.3135142358
O,0,-1.1774435283,2.4485421905,-0.2756867395
C,0,-2.3959576047,2.9111939958,0.4668266667
C,0,-1.8641645983,3.8252912424,1.6102216328
C,0,-3.3161128024,3.5926172734,-0.5185892719
O,0,-3.7150784761,2.6519823171,-1.4950860854
O,0,-2.3022788182,3.4446046215,2.8716536423
O,0,-1.9014034873,0.8468678709,2.5898545775
As,0,-0.3757338678,0.2101169698,2.5036157291
O,0,0.1924183622,-0.0968138466,4.1469415454
O,0,-0.3767937943,-1.4610611955,1.9001067271
O,0,0.7959257548,1.0111223823,1.6047223503
H,0,0.1457765916,-1.4342229806,1.0804347522
H,0,-2.8191053485,1.9882188886,0.8651175872
H,0,-4.1661584804,3.97393348,0.0700162918
H,0,-2.804567712,4.4624429253,-0.9658584719
H,0,-2.2197737924,4.8504083195,1.4527370811
H,0,0.0996760405,4.7630642445,1.0993931338
H,0,0.2225487894,3.4809790532,2.3106712399
H,0,-2.1275548851,2.4643369801,2.964190619
H,0,-4.3634111251,3.0740164418,-2.0787571377
H,0,0.7259288708,-0.9084632535,4.1194289257
H,0,0.8241485137,2.5588010668,-0.1697528127

Nuc 2.5 without Histidine B3LYP/6-31G*

E(RB+HF-LYP) = -2957.40809802

Zero-point correction= 0.178099 (Hartree/Particle)
Thermal correction to Energy= 0.193079
Thermal correction to Enthalpy= 0.194024
Thermal correction to Gibbs Free Energy= 0.134875
Sum of electronic and zero-point Energies= -2957.229999
Sum of electronic and thermal Energies= -2957.215019
Sum of electronic and thermal Enthalpies= -2957.214074
Sum of electronic and thermal Free Energies= -2957.273223

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.159	53.296	124.488

C,0,-0.3354116908,3.8081107111,1.3694653092
C,0,-0.1540545076,2.8015911768,0.3039475918
O,0,-1.2313175943,2.3946048758,-0.2368198072
C,0,-2.4388849757,2.917908901,0.4889781672
C,0,-1.8755207865,3.7912024381,1.6484611957
C,0,-3.2967772447,3.6621795104,-0.5094149969
O,0,-3.6991001504,2.7642066093,-1.5224576919
O,0,-2.2267147026,3.3361765052,2.9110068074
O,0,-1.9193903262,0.7592386582,2.4844577878
As,0,-0.3965838085,0.1143173833,2.3732900384
O,0,0.1983212397,-0.558286388,3.9077188626
O,0,-0.5442823678,-1.38886213,1.4591659777
O,0,0.853041893,1.0834767004,1.8151853211
H,0,0.1567091706,-1.9847753199,1.7717896018
H,0,-2.9187615482,2.0129293389,0.8621120433
H,0,-4.1503319699,4.0638750485,0.0603841355
H,0,-2.7360516998,4.5220569843,-0.9159117591
H,0,-2.265355842,4.8120521523,1.5595192331
H,0,0.0220571681,4.7806718435,0.9998831437
H,0,0.2523834346,3.5433659979,2.2509000491
H,0,-2.0668807122,2.3457525166,2.9311688445
H,0,-4.3135238313,3.2247317459,-2.1136744248
H,0,0.9742001785,-0.0183983267,4.1367036
H,0,0.7720316741,2.4826040672,-0.1592360298

Nuc 2.6 without Histidine B3LYP/6-31G*

Andis26
E(RB+HF-LYP) = -2957.40489985

Zero-point correction= 0.177882 (Hartree/Particle)
Thermal correction to Energy= 0.192147
Thermal correction to Enthalpy= 0.193091
Thermal correction to Gibbs Free Energy= 0.135565
Sum of electronic and zero-point Energies= -2957.227018

Sum of electronic and thermal Energies= -2957.212753
Sum of electronic and thermal Enthalpies= -2957.211809
Sum of electronic and thermal Free Energies= -2957.269335

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	120.574	51.418	121.074

C,0,-0.3413352377,3.7526474863,1.3807986968
C,0,-0.1740247429,2.8123000212,0.2567166786
O,0,-1.2512332665,2.4408104879,-0.301633204
C,0,-2.45543979,2.9340759497,0.452292032
C,0,-1.8876331527,3.7954033524,1.6194883347
C,0,-3.3444622298,3.6766125379,-0.5180721019
O,0,-3.7640061241,2.7821829884,-1.5279419876
O,0,-2.2958558843,3.362770634,2.8726421744
O,0,-1.8019212861,0.8331467616,2.3822908449
As,0,-0.2783434988,0.1833446673,2.4793054727
O,0,0.1115629863,-0.0132972092,4.1931522332
O,0,-0.2541676002,-1.527039517,1.9931691767
O,0,0.9627057151,0.9256551803,1.6381706731
H,0,0.3560711715,-1.5634198478,1.2368396097
H,0,-2.9095536903,2.0142758345,0.8208689483
H,0,-4.1864015812,4.0643945096,0.0779386755
H,0,-2.8037738271,4.5454827276,-0.931921425
H,0,-2.2367799103,4.8292063607,1.5135529931
H,0,0.0822246023,4.7268449431,1.0959715476
H,0,0.2153196248,3.3969041823,2.2522476091
H,0,-2.0969803071,2.381498203,2.9155653939
H,0,-4.4025553921,3.2393609515,-2.0957713514
H,0,0.6642798836,-0.8082585402,4.2730104594
H,0,0.7521045376,2.4858293352,-0.2020594838

Nuc 2.7 without Histidine B3LYP/6-31G*

Andis27
E(RB+HF-LYP) = -2957.40287086

Zero-point correction= 0.177792 (Hartree/Particle)
Thermal correction to Energy= 0.192892
Thermal correction to Enthalpy= 0.193836
Thermal correction to Gibbs Free Energy= 0.134027
Sum of electronic and zero-point Energies= -2957.225078
Sum of electronic and thermal Energies= -2957.209979
Sum of electronic and thermal Enthalpies= -2957.209035
Sum of electronic and thermal Free Energies= -2957.268844

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.042	53.382	125.880

C,0,-0.3462170736,3.7780916942,1.3601054855
C,0,-0.1859856023,2.8170845294,0.2551011677
O,0,-1.2631328814,2.4165418756,-0.2776839447
C,0,-2.4668643727,2.9376846487,0.4674528333
C,0,-1.8873830763,3.7904058335,1.634986091
C,0,-3.3307021056,3.6953647615,-0.5142416993
O,0,-3.743071211,2.8116766498,-1.535389556
O,0,-2.2499356717,3.3264877773,2.888940351
O,0,-1.8183583677,0.8099464604,2.374990213
As,0,-0.3097854643,0.1158495151,2.3827124134
O,0,0.13420322,-0.5522073242,3.9705430647
O,0,-0.4606686202,-1.3949268812,1.477976082
O,0,1.0004635971,1.0324727019,1.8975076102
H,0,0.1955974537,-2.0130243286,1.8400274341
H,0,-2.9389698217,2.0252369537,0.8317391307
H,0,-4.1778724307,4.0898553859,0.0700904442
H,0,-2.773357844,4.5607510791,-0.9135668863
H,0,-2.2577890986,4.819182026,1.5541949398
H,0,0.0519250121,4.7549569263,1.0491127567
H,0,0.2336943136,3.4382918269,2.2233196988
H,0,-2.048089118,2.3399579645,2.901451747
H,0,-4.3721766195,3.276258977,-2.1077261958
H,0,0.9346692425,-0.0639763238,4.2287444094
H,0,0.7396075401,2.458768271,-0.1837645906