

SUPPORTING INFORMATION

Arsenate and phosphate as nucleophiles at the transition states of human purine nucleoside phosphorylase

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1. Comparison between arsenate and phosphate ions

O,0,-0.5861441149,1.5233286418,2.3073655835

A. Phosphate dianion

Phosphate dianion B3LYP/6-31G*

phosarsbbb1
E(RB+HF-LYP) = -642.817443435

Zero-point correction=	0.025266
(Hartree/Particle)	
Thermal correction to Energy=	0.030190
Thermal correction to Enthalpy=	0.031135
Thermal correction to Gibbs Free Energy=	-0.002939
Sum of electronic and zero-point Energies=	-
642.792177	
Sum of electronic and thermal Energies=	-
642.787253	
Sum of electronic and thermal Enthalpies=	-
642.786309	
Sum of electronic and thermal Free Energies=	-
642.820383	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	18.945	16.818	71.715

O,0,-0.419283131,0.3048102228,-0.0270122134
P,0,-0.1360998213,0.1694780842,1.7288008189
O,0,1.4020314318,-0.0547914664,1.6742509457
O,0,-0.966185659,-1.0496255915,2.1703299385
H,0,0.5209012944,0.1773851091,-0.2362840732

Phosphate dianion B3LYP/6-311++G** (as shown in figure 1)

phosarsbbb2
E(RB+HF-LYP) = -643.017830487

Zero-point correction=	0.024392
(Hartree/Particle)	
Thermal correction to Energy=	0.029680
Thermal correction to Enthalpy=	0.030624
Thermal correction to Gibbs Free Energy=	-0.004260
Sum of electronic and zero-point Energies=	-
642.993438	
Sum of electronic and thermal Energies=	-
642.988151	
Sum of electronic and thermal Enthalpies=	-
642.987207	
Sum of electronic and thermal Free Energies=	-
643.022090	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	18.624	17.572	73.419

O,0,-0.4077474878,0.3026686235,-0.0165469669
P,0,-0.126961091,0.1674173732,1.7426768548
O,0,1.412109486,-0.0591784929,1.729604312
O,0,-0.9694638174,-1.0473241358,2.1732812673
H,0,0.49732181,0.1852382026,-0.3218144208

O,0,-0.5900388998,1.5217634294,2.3102499536

B. Arsenate dianion

Arsenate dianion B3LYP/6-31G*

phosarssbbb3
E(RB+HF-LYP) = -2535.13703846

Zero-point correction= 0.022518
(Hartree/Particle)
Thermal correction to Energy= 0.028051
Thermal correction to Enthalpy= 0.028996
Thermal correction to Gibbs Free Energy= -0.006920
Sum of electronic and zero-point Energies= -
2535.114520
Sum of electronic and thermal Energies= -
2535.108987
Sum of electronic and thermal Enthalpies= -
2535.108043
Sum of electronic and thermal Free Energies= -
2535.143959

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	17.602	18.674	75.591

O,0,-0.4075582828,0.3144145274,-0.1321786661
As,0,-0.1509879129,0.1679713108,1.7530252564
O,0,1.5306777501,-0.0712670368,1.6475016146
O,0,-1.0571125885,-1.1703598341,2.23376889
H,0,0.5470371705,0.1842475714,-0.2811575514
O,0,-0.6468351364,1.6455774613,2.3964914565

Arsenate dianion B3LYP/6-311++G** (as shown in figure 1)

phosarssbbb4
E(RB+HF-LYP) = -2537.43216078

Zero-point correction= 0.021358
(Hartree/Particle)
Thermal correction to Energy= 0.027316
Thermal correction to Enthalpy= 0.028260
Thermal correction to Gibbs Free Energy= -0.008476
Sum of electronic and zero-point Energies= -
2537.410802
Sum of electronic and thermal Energies= -
2537.404845
Sum of electronic and thermal Enthalpies= -
2537.403900
Sum of electronic and thermal Free Energies= -
2537.440636

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	17.141	19.797	77.318

O,0,-0.4057469286,0.3144761151,-0.1359179653
As,0,-0.1360591394,0.1643990186,1.7772506623
O,0,1.5546176297,-0.0789249702,1.7238924377
O,0,-1.0636583191,-1.1750223393,2.2387834682
H,0,0.5178116626,0.1944058728,-0.3889812374
O,0,-0.6517439052,1.6512503029,2.4024236345

2. Potential Energy Surfaces for Arsenolysis vs. Phosphorolysis

A. Lowest Energy Starting Material

B3LYP/6-31G*

E(RB+HF-LYP) = -983.394914064

Zero-point correction= 0.240841
(Hartree/Particle)
Thermal correction to Energy= 0.256514
Thermal correction to Enthalpy= 0.257458
Thermal correction to Gibbs Free Energy= 0.196971
Sum of electronic and zero-point Energies= -
983.154073
Sum of electronic and thermal Energies= -
983.138400
Sum of electronic and thermal Enthalpies= -
983.137456
Sum of electronic and thermal Free Energies= -
983.197943

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	160.965	61.117	127.306

C,0,3.2302631632,6.8851058247,-1.5007148654
C,0,2.9776130829,5.3804028374,-1.2565992502
O,0,1.9816050137,5.3159089707,-0.2614246106
C,0,2.0204946029,6.5235192222,0.5561980708
C,0,3.0929128995,7.4277739158,-0.0700075737
C,0,0.6085967873,7.0989167628,0.582440977
O,0,0.1441901214,7.4495463577,-0.7124691366
N,0,2.4722104327,4.6519791294,-2.4263199854
C,0,1.4531469156,3.7154229039,-2.4457656101
N,0,1.2783416631,3.1570003187,-3.6206414118
C,0,2.2333619329,3.7355722475,-4.4208692813
C,0,2.9886959319,4.6612580376,-3.6997547162
N,0,4.0255157303,5.4332532376,-4.1496756103
C,0,4.2955658327,5.2366448596,-5.4115732686
N,0,3.6269089688,4.3615429165,-6.2070128177
C,0,2.5255829247,3.5156652554,-5.8199934576
O,0,2.0135747182,2.7781862603,-6.638813755
O,0,4.3079852002,7.2349788722,0.6346698595
O,0,4.5075944137,7.1978541643,-1.9965215952
H,0,-0.0649721212,6.3756595361,1.0663989021
H,0,0.5992721242,8.0164797637,1.1796377601
H,0,2.3349491408,6.2464405455,1.5689238866
H,0,3.9069418105,4.9016669425,-0.9192684599
H,0,5.100932006,5.7971317544,-5.8776681623
H,0,2.7917519406,8.4842986556,-0.0668876099
H,0,2.4214417763,7.2845583913,-2.127189573
H,0,4.6007858283,6.7289532663,-2.8558249423
H,0,5.014714719,7.4092254932,-0.0138554307
H,0,3.8970873443,4.2660688473,-7.1802677642
H,0,0.0782416023,6.6191942755,-1.2111661019
H,0,0.8853314933,3.4999544344,-1.5531444662

B3LYP/6-31+G**

E(RB3LYP) = -983.471364636

Zero-point correction= 0.239725
 (Hartree/Particle)
 Thermal correction to Energy= 0.255668
 Thermal correction to Enthalpy= 0.256612
 Thermal correction to Gibbs Free Energy= 0.194992
 Sum of electronic and zero-point Energies= -
 983.231640
 Sum of electronic and thermal Energies= -
 983.215697
 Sum of electronic and thermal Enthalpies= -
 983.214753
 Sum of electronic and thermal Free Energies= -
 983.276373

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.434	61.682	129.691

C,0,3.236893831,6.8617175092,-1.525734687
 C,0,2.9387351202,5.3663343702,-1.2815501785
 O,0,1.8959970758,5.3528356652,-0.3296470634
 C,0,2.0138708086,6.5198498528,0.5372205958
 C,0,3.0715254371,7.4342596322,-0.1070136212
 C,0,0.6231510618,7.1199734525,0.6944756394
 O,0,0.0823192138,7.5923932728,-0.5336745371
 N,0,2.4589150643,4.6353211138,-2.4603128972
 C,0,1.456805059,3.6792002987,-2.4859326566
 N,0,1.3074679912,3.1131498088,-3.6617640533
 C,0,2.2617981096,3.7027591546,-4.454265167
 C,0,2.9923760821,4.6459395825,-3.7278888358
 N,0,4.0237414353,5.4281732361,-4.1720833693
 C,0,4.3146520488,5.2285630421,-5.430046904
 N,0,3.6678542273,4.3385380982,-6.228865067
 C,0,2.5774182858,3.4821347676,-5.8474157906
 O,0,2.0846062257,2.7291430348,-6.6691489077
 O,0,4.278543925,7.308797359,0.632940327
 O,0,4.5297931943,7.1472944052,-2.0033704941
 H,0,-0.0399716474,6.3768111335,1.1581553205
 H,0,0.6812904054,7.9844534743,1.3631310412
 H,0,2.3859366959,6.1931800455,1.5156775859
 H,0,3.835786722,4.8610744988,-0.8963950094
 H,0,5.1184924776,5.7967667768,-5.8883983251
 H,0,2.7424403184,8.4798552431,-0.138899217
 H,0,2.4559603093,7.2744037461,-2.178440299
 H,0,4.6236309005,6.7002648822,-2.871201234
 H,0,5.0079436743,7.5090352349,0.0243192272
 H,0,3.9521625874,4.2422138935,-7.1976660974
 H,0,-0.1074946875,6.8245974817,-1.0898123742
 H,0,0.8779970473,3.4611289333,-1.6015529511

**B. A_ND_N mechanism – phosphate grid
 – B3LYP/6-31G***

LG 1.9 Nuc 1.9

grid1lg19.1

E(RB+HF-LYP) = -1626.30450556

Zero-point correction= 0.265220
 (Hartree/Particle)
 Thermal correction to Energy= 0.285782
 Thermal correction to Enthalpy= 0.286726
 Thermal correction to Gibbs Free Energy= 0.215530

Sum of electronic and zero-point Energies= -
 1626.039285
 Sum of electronic and thermal Energies= -
 1626.018724
 Sum of electronic and thermal Enthalpies= -
 1626.017779
 Sum of electronic and thermal Free Energies= -
 1626.088976

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.331	79.497	149.845

C,0,0.8670627822,1.4989604038,-0.2946585882
 C,0,0.5015384403,0.3509703833,-1.2720409554
 O,0,1.3696469843,-0.7034621642,-1.1361542767
 C,0,2.643330721,-0.2052457921,-0.650923624
 C,0,2.3627893211,1.1150624161,0.1069562032
 C,0,3.2395064472,-1.3243747223,0.186628198
 O,0,2.4012697022,-1.7190747376,1.2703889204
 N,0,-0.8460277872,-0.5273953846,-0.608834974
 C,0,-0.9717874284,-1.8885125284,-0.2618644165
 N,0,-2.1203464303,-2.3911512637,0.1954286996
 C,0,-2.826381876,-1.2620451757,0.5200254633
 C,0,-2.0454121193,-0.112631877,0.2343517272
 N,0,-2.4308876151,1.1915565669,0.4340967915
 C,0,-3.6218027688,1.3121349079,0.922567497
 N,0,-4.4533057764,0.257508171,1.2298353702
 C,0,-4.1481855371,-1.1268501587,1.06558805
 O,0,-4.9952693497,-1.9647365859,1.387952792
 O,0,3.3592685259,2.0794798544,-0.0875526927
 O,0,0.60225634,2.802881393,-0.6811189881
 H,0,3.4576685082,-2.1919040728,-0.4621932397
 H,0,4.1879602144,-0.9779999413,0.615349179
 H,0,3.2756519231,0.0185974364,-1.5150273951
 H,0,-4.0310650778,2.3024921489,1.119819517
 H,0,2.3523170542,0.9061137458,1.1850181883
 H,0,0.2635940411,1.3517217909,0.6043343158
 H,0,1.0409709765,3.049546916,-1.544642841
 H,0,3.5825812139,2.1236866617,-1.0690848714
 H,0,-5.3756659975,0.4339713686,1.6084608373
 H,0,1.495780291,-1.6631433731,0.9161962609
 H,0,-0.1676057502,-2.5084271919,-0.6380258627
 O,0,1.4558498909,1.0282423278,-2.7689010395
 P,0,2.4020453456,2.1806264113,-3.2548553317
 O,0,2.5721917194,1.9284935801,-4.9168924148
 O,0,1.7668421539,3.5518614,-3.0490124792
 O,0,3.8462756419,1.9922314388,-2.7305504372
 H,0,-0.2309385193,0.3626261232,-2.0520636238
 H,0,3.4805282644,1.5928571434,-4.9669337989

LG 1.9 Nuc 2.1

grid1lg19.2

E(RB+HF-LYP) = -1626.31390345

Zero-point correction= 0.264562
 (Hartree/Particle)
 Thermal correction to Energy= 0.286088
 Thermal correction to Enthalpy= 0.287032
 Thermal correction to Gibbs Free Energy= 0.212065
 Sum of electronic and zero-point Energies= -
 1626.049341
 Sum of electronic and thermal Energies= -
 1626.027816
 Sum of electronic and thermal Enthalpies= -
 1626.026872
 Sum of electronic and thermal Free Energies= -
 1626.101838

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.523	81.571	157.781

C,0,0.8637162099,1.4814818271,-0.2917754619
C,0,0.4645040926,0.306819683,-1.2171479885
O,0,1.3466431879,-0.7226530941,-1.1228975759
C,0,2.6368049278,-0.2151414299,-0.6740124799
C,0,2.3645233129,1.0970819254,0.0970748523
C,0,3.277434896,-1.3316222321,0.131021329
O,0,2.487117725,-1.751553701,1.2428457121
N,0,-0.9211854581,-0.5541157214,-0.2431604685
C,0,-1.0154720577,-1.9135389306,-0.1666592266
N,0,-2.1487173571,-2.4025613053,0.3368076152
C,0,-2.8703438509,-1.12659889032,0.6036133513
C,0,-2.1182278685,-0.1225507265,0.2391341156
N,0,-2.5216764291,1.1840355555,0.3604799103
C,0,-3.70830436,1.3134302227,0.8578574389
N,0,-4.5151482917,0.2656201046,1.242291051
C,0,-4.187537917,-1.1211322771,1.1594901282
O,0,-5.0132179929,-1.9524739178,1.5441895307
O,0,3.3561727334,2.0609113918,-0.0961542949
O,0,0.5912570075,2.7687653362,-0.7160349892
H,0,3.4871089358,-2.1903984535,-0.531342898
H,0,4.2337829048,-0.9707058242,0.528115989
H,0,3.2247662499,0.0222206394,-1.5647102936
H,0,-4.1329768658,2.3067407715,0.9980672098
H,0,2.3591797335,0.8754796979,1.1734748404
H,0,0.2735873085,-1.3590329195,0.6227030053
H,0,1.0557393679,3.012775279,-1.5740489619
H,0,3.5849611519,2.1125733523,-1.0819109114
H,0,-5.4349977838,0.4496050034,1.6235811228
H,0,1.5687875301,-1.711865711,0.9233413829
H,0,-0.2027915749,-2.5373908609,-0.5168402771
O,0,1.5188017418,1.0120491338,-2.8907980717
P,0,2.4556284993,2.1889155289,-3.2837906496
O,0,2.7217319622,2.0513429888,-4.9526867746
O,0,1.802384514,3.5472304532,-3.0206082875
O,0,3.8885642855,2.0058005203,-2.7111999555
H,0,-0.1762882421,0.37741110868,-2.0736461249
H,0,3.6659322413,1.8300372877,-4.9649967335

LG 1.9 Nuc 2.3

grid1lg19.3

E(RB+HF-LYP) = -1626.32006768

Zero-point correction=	0.263920
(Hartree/Particle)	
Thermal correction to Energy=	0.285486
Thermal correction to Enthalpy=	0.286430
Thermal correction to Gibbs Free Energy=	0.211389
Sum of electronic and zero-point Energies=	-
1626.056148	
Sum of electronic and thermal Energies=	-
1626.034582	
Sum of electronic and thermal Enthalpies=	-
1626.033638	
Sum of electronic and thermal Free Energies=	-
1626.108679	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.145	81.622	157.937

C,0,0.8528955582,1.4731586546,-0.2894099391
C,0,0.4370990895,0.2789893618,-1.1799340209
O,0,1.3325057897,-0.7317416621,-1.1107075678
C,0,2.6302544947,-0.2131322512,-0.6831221592
C,0,2.3562164865,1.0929731424,0.0959927074

C,0,3.2996947902,-1.3249496121,0.1028124609
O,0,2.5361545289,-1.7623342376,1.2274958175
N,0,-0.975287713,-0.5732951737,-0.2371870263
C,0,-1.0534195831,-1.9301719354,-0.1233573373
N,0,-2.1763715182,-2.4090159856,0.4089085673
C,0,-2.9029043325,-1.2705725718,0.6527897557
C,0,-2.1668991112,-0.1310322811,0.2469885647
N,0,-2.5761090409,1.1753783625,0.3351529997
C,0,-3.7568743234,1.3104169578,0.8452900638
N,0,-4.5501178029,0.2685615852,1.270676228
C,0,-4.2136415152,-1.1178343352,1.223144745
O,0,-5.0265410561,-1.9439563681,1.6424313327
O,0,3.3392126529,2.0618720516,-0.0983986998
O,0,0.5818446688,2.7443608545,-0.7560062269
H,0,3.5091314912,-2.1772727203,-0.5672998669
H,0,4.257450829,-0.9515371549,0.483982629
H,0,3.1896424582,0.0343411768,-1.589629565
H,0,-4.1866012325,2.3043379097,0.9626161465
H,0,2.3538972989,0.8644848842,1.1713210679
H,0,0.2668783788,1.3755170878,0.6318413867
H,0,1.0700356917,2.9809362417,-1.6120765439
H,0,3.5726425825,2.1120378601,-1.0874359272
H,0,-5.4657181354,0.4572221197,1.6599173712
H,0,1.612490504,-1.7412979292,0.9230360466
H,0,-0.2386255066,-2.5554429264,-0.4657368136
O,0,1.5745953485,0.9514082035,-3.0624724309
P,0,2.4962278913,2.1637016219,-3.3266087206
O,0,2.8717431726,2.164256038,-4.9829210391
O,0,1.8066972082,3.4963959782,-3.005725122
O,0,3.9057153566,1.9874790831,-2.6861642059
H,0,-0.1299662742,0.3916202143,-2.0872256519
H,0,3.8282953447,2.0088053754,-4.9433128662

LG 1.9 Nuc 2.5

grid1lg19.4

E(RB+HF-LYP) = -1626.32352444

Zero-point correction=	0.263280
(Hartree/Particle)	
Thermal correction to Energy=	0.284926
Thermal correction to Enthalpy=	0.285871
Thermal correction to Gibbs Free Energy=	0.210173
Sum of electronic and zero-point Energies=	-
1626.060245	
Sum of electronic and thermal Energies=	-
1626.038598	
Sum of electronic and thermal Enthalpies=	-
1626.037654	
Sum of electronic and thermal Free Energies=	-
1626.113351	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.794	81.614	159.319

C,0,0.8429103849,1.475354951,-0.2792448503
C,0,0.4260393119,0.2653561526,-1.1466611168
O,0,1.330251718,-0.7355641927,-1.0763464066
C,0,2.6316773002,-0.2012948633,-0.6674736628
C,0,2.3516893745,1.1087011279,0.1024588359
C,0,3.3187282419,-1.301165506,0.1190731512
O,0,2.5616841455,-1.7438580676,1.246740436
N,0,-1.0171946272,-0.5841939944,-0.2492549803
C,0,-1.1024564858,-1.9416929836,-0.1578054422
N,0,-2.2238933567,-2.4167999531,0.3787870741
C,0,-2.9369725704,-1.275644971,0.6502162581
C,0,-2.197228518,-0.1351404212,0.2557485635
N,0,-2.5913620156,1.1727826631,0.3724533982
C,0,-3.7643033528,1.3092402799,0.9005546331

N,0,-4.5617121947,0.2673882381,1.3167784402
 C,0,-4.2392241466,-1.1211884089,1.2399862865
 O,0,-5.0535338759,-1.9473647167,1.6548566287
 O,0,3.3208733889,2.0841260676,-0.1120951698
 O,0,0.5700591157,2.72715609,-0.7887777479
 H,0,3.5372963675,-2.1529937255,-0.5482653577
 H,0,4.2719313153,-0.9135974293,0.4969107442
 H,0,3.1750421791,0.0424337378,-1.585276068
 H,0,-4.1824483038,2.3048635463,1.0417821006
 H,0,2.3556204629,0.8877467461,1.17967939
 H,0,0.2605291797,1.3967867498,0.6471827119
 H,0,1.0722582017,2.9432878556,-1.6538807512
 H,0,3.5443508899,2.1200812851,-1.1092730263
 H,0,-5.4704008421,0.4576112021,1.7212277779
 H,0,1.6391793948,-1.7430471155,0.9377178135
 O,0,-0.2948115532,-2.5657654955,-0.5182522236
 O,0,1.6196948416,0.8487663207,-3.264399435
 P,0,2.5126778539,2.0944306876,-3.3916878907
 O,0,2.9972523127,2.2216211098,-5.0168052066
 O,0,1.7782534815,3.3974291867,-3.0283844121
 O,0,3.8920735962,1.9360985969,-2.6762133018
 H,0,-0.0724454312,0.4016357271,-2.0950847945
 H,0,3.960158686,2.1810811422,-4.9073062395

LG 1.9 Nuc 2.7

grid1lg19.5

E(RB+HF-LYP) = -1626.32505364

Zero-point correction=	0.262866
(Hartree/Particle)	
Thermal correction to Energy=	0.284570
Thermal correction to Enthalpy=	0.285514
Thermal correction to Gibbs Free Energy=	0.209966
Sum of electronic and zero-point Energies=	-
1626.062187	
Sum of electronic and thermal Energies=	-
1626.040484	
Sum of electronic and thermal Enthalpies=	-
1626.039539	
Sum of electronic and thermal Free Energies=	-
1626.115088	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.570	81.570	159.005

C,0,0.832343946,1.4784826793,-0.2710433288
 C,0,0.419451287,0.2588390556,-1.1248570179
 O,0,1.3305900239,-0.7342010332,-1.0581034698
 C,0,2.6321247675,-0.1910354184,-0.6524298527
 C,0,2.3453289183,1.1226285757,0.1095558716
 C,0,3.324780577,-1.283507953,0.1388510236
 O,0,2.567219162,-1.7264261262,1.2662030104
 N,0,-1.0431232032,-0.5918232555,-0.2604231236
 C,0,-1.13826867,-1.9498115032,-0.1923190562
 N,0,-2.259304851,-2.4216048121,0.3464364186
 C,0,-2.9586550908,-1.2781973548,0.6444084656
 C,0,-2.2128900746,-0.1376725551,0.2634702856
 N,0,-2.5914796158,1.1715291634,0.4082409161
 C,0,-3.7576262108,1.3097546858,0.9510426749
 N,0,-4.5610809646,0.2684543664,1.3559509913
 C,0,-4.2533057327,-1.1216888719,1.2507562104
 O,0,-5.0709415085,-1.9474284157,1.6587741727
 O,0,3.3029851853,2.1031979792,-0.1218288789
 O,0,0.561720425,2.7155039364,-0.812963118
 H,0,3.550687334,-2.1361639406,-0.5245825856
 H,0,4.2740936376,-0.8877108381,0.5176579794
 H,0,3.1716994851,0.0494846742,-1.5742011023

H,0,-4.1638227248,2.3067469907,1.1150525047
 H,0,2.3542628531,0.909734375,1.1885380868
 H,0,0.2503345042,1.4150092408,0.6570719703
 H,0,1.0647745541,2.9054110694,-1.6936251162
 H,0,3.5178171021,2.1260658018,-1.1254810814
 H,0,-5.4635570575,0.4602527202,1.7734011374
 H,0,1.6468003634,-1.7395282612,0.9512954659
 H,0,-0.3381604836,-2.5736770475,-0.5693257303
 O,0,1.6833591763,0.7472217188,-3.4602399245
 P,0,2.5255444347,2.0273797195,-3.4545694385
 O,0,3.1054032079,2.2773900185,-5.0349063818
 O,0,1.7286120164,3.2894985722,-3.0632929716
 O,0,3.8692499982,1.8960822551,-2.6635433121
 H,0,-0.0407800609,0.4037744609,-2.0954538359
 H,0,4.0560577596,2.3427029478,-4.853851699

LG 1.9 Nuc 2.9

grid1lg19.6

E(RB+HF-LYP) = -1626.32534512

Zero-point correction=	0.262557
(Hartree/Particle)	
Thermal correction to Energy=	0.284336
Thermal correction to Enthalpy=	0.285280
Thermal correction to Gibbs Free Energy=	0.209037
Sum of electronic and zero-point Energies=	-
1626.062788	
Sum of electronic and thermal Energies=	-
1626.041009	
Sum of electronic and thermal Enthalpies=	-
1626.040065	
Sum of electronic and thermal Free Energies=	-
1626.116308	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.424	81.508	160.468

C,0,0.8289681007,1.4901803121,-0.2698022495
 C,0,0.4102294413,0.2697845704,-1.1180174013
 O,0,1.3272061303,-0.7147986831,-1.0834834555
 C,0,2.6268243863,-0.1869636784,-0.6460257254
 C,0,2.3419314683,1.1318125692,0.1092501822
 C,0,3.2928113686,-1.2867232235,0.1568206185
 O,0,2.5220377554,-1.7106611018,1.2825653085
 N,0,-1.0499404365,-0.5903258589,-0.2588846611
 C,0,-1.1376003241,-1.9487950104,-0.1912700504
 N,0,-2.2522014972,-2.4245724842,0.3565065636
 C,0,-2.9537411415,-1.2841156396,0.6610132959
 C,0,-2.216463805,-0.1401342103,0.2754076758
 N,0,-2.5989881893,1.1674112353,0.422851849
 C,0,-3.7621119216,1.3003944465,0.9736729206
 N,0,-4.5579791134,0.2556140735,1.3839350714
 C,0,-4.2450297622,-1.1332881042,1.2765049965
 O,0,-5.055780857,-1.9626844952,1.6897891904
 O,0,3.2972718431,2.1093721447,-0.137198586
 O,0,0.5702643243,2.7189124686,-0.8326986176
 H,0,3.5093858546,-2.1465591219,-0.5002223346
 H,0,4.2458584225,-0.9051981103,0.5406976248
 H,0,3.1879498595,0.0484100666,-1.5575835359
 H,0,-4.1715600594,2.2955675476,1.1402388244
 H,0,2.3540150011,0.9272365602,1.1898167063
 H,0,0.2459914081,1.4403145868,0.6588116106
 H,0,1.0747593763,2.8831214395,-1.5753350324
 H,0,3.5017408438,2.118145836,-1.1464987188
 H,0,-5.458714031,0.4435187801,1.8069185521
 H,0,1.6048470253,-1.7341277897,0.9597982594
 H,0,-0.3384270168,-2.5686407216,-0.5769665822

O,0,1.7281709535,0.7031611828,-3.6646241207
 P,0,2.5412860433,1.9881450721,-3.5184406624
 O,0,3.2073839759,2.3615856291,-5.040543496
 O,0,1.7107878796,3.2188172556,-3.0873385985
 O,0,3.8458200374,1.8353408955,-2.6621504357
 H,0,-0.0528909761,0.425551694,-2.087748653
 H,0,4.1381321019,2.469857487,-4.79009835

LG 1.9 Nuc 3.1

grid1lg19.7

E(RB+HF-LYP) = -1626.32688428

Zero-point correction= 0.262172
 (Hartree/Particle)
 Thermal correction to Energy= 0.283806
 Thermal correction to Enthalpy= 0.284750
 Thermal correction to Gibbs Free Energy= 0.209297
 Sum of electronic and zero-point Energies= -
 1626.064713
 Sum of electronic and thermal Energies= -
 1626.043079
 Sum of electronic and thermal Enthalpies= -
 1626.042134
 Sum of electronic and thermal Free Energies= -
 1626.117587

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.091	81.050	158.804

C,0,1.0509156765,1.5484516414,-0.2587410404
 C,0,0.6963633882,0.3645590494,-1.1814165566
 O,0,1.6477519214,-0.5729125703,-1.1795046704
 C,0,2.7344257381,-0.238355536,-0.2573273119
 C,0,2.5820973854,1.2692564927,0.0742746739
 C,0,2.6835092005,-1.2069157066,0.9165361976
 O,0,1.5483432379,-1.0466518422,1.7590239383
 N,0,-0.771483716,-0.5654328873,-0.4129512957
 C,0,-0.9917163078,-1.8668065094,-0.7732767625
 N,0,-2.1512623692,-2.3836893441,-0.385939914
 C,0,-2.7534035739,-1.3329679848,0.2641233213
 C,0,-1.910872336,-0.1991291454,0.2439042407
 N,0,-2.173418915,-1.0229757705,0.8049530708
 C,0,-3.3310052013,1.0845846216,1.3797551451
 N,0,-4.2268528282,0.0433018866,1.4475459848
 C,0,-4.0359173301,-1.2663056587,0.9123299974
 O,0,-4.9218811409,-2.1081137956,1.0603956801
 O,0,3.5044988162,2.0688635587,-0.575735302
 O,0,0.7274102841,2.7968075537,-0.7346046607
 H,0,2.7417466285,-2.2414211378,0.5326726602
 H,0,3.5630711111,-1.0408316506,1.5518441848
 H,0,3.6491260304,-0.3893386991,-0.836791772
 H,0,-3.6507394342,2.0104918786,1.8553037268
 H,0,2.7169779454,1.4166326124,1.156129104
 H,0,0.5010867781,1.394245798,0.6780581752
 H,0,1.117015529,2.9599809009,-1.6899730188
 H,0,3.4255084045,1.8843185546,-1.6023097272
 H,0,-5.1159018808,0.172019707,1.9150244301
 H,0,0.763647638,-1.0494007167,1.1815385167
 H,0,-0.2445318536,-2.407312644,-1.3404199351
 O,0,1.0246779421,0.9246432632,-4.2126727175
 P,0,2.086597198,1.9406700612,-3.8062654034
 O,0,2.8720382658,2.4534756512,-5.2295325953
 O,0,1.5406206979,3.2211505456,-3.1276269726
 O,0,3.3010614961,1.3553821947,-3.0032116484
 H,0,0.2685365734,0.5296780491,-2.1746185985
 H,0,3.7942034703,2.3187636574,-4.9608269845

LG 2.1 Nuc 1.9

gridlg21.1

E(RB+HF-LYP) = -1626.32174866

Zero-point correction= 0.265318
 (Hartree/Particle)
 Thermal correction to Energy= 0.285909
 Thermal correction to Enthalpy= 0.286853
 Thermal correction to Gibbs Free Energy= 0.215529
 Sum of electronic and zero-point Energies= -
 1626.056430
 Sum of electronic and thermal Energies= -
 1626.035840
 Sum of electronic and thermal Enthalpies= -
 1626.034895
 Sum of electronic and thermal Free Energies= -
 1626.106219

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.411	79.293	150.114

C,0,0.8965778144,1.6318854792,-0.5140406463
 C,0,0.6453454047,0.4675954752,-1.4968173413
 O,0,1.5023524281,-0.5462907549,-1.3222041696
 C,0,2.6216323575,-0.1461971299,-0.4782828196
 C,0,2.3401203164,1.2839973645,0.0515561473
 C,0,2.7486961014,-1.2177173097,0.5946281645
 O,0,1.6438539275,-1.2611300365,1.4820708792
 N,0,-0.7530486114,-0.553548274,-0.3086440562
 C,0,-1.0621730053,-1.7864115218,-0.8226764028
 N,0,-2.2637420632,-2.2953734716,-0.5433233226
 C,0,-2.8177097371,-1.3147075173,0.2407797802
 C,0,-1.8877292403,-0.2525347834,0.3869328847
 N,0,-2.0908430315,0.8913368259,1.1266958732
 C,0,-3.2511275253,0.9475011052,1.6954440235
 N,0,-4.217391293,-0.0284801046,1.5984363802
 C,0,-4.1032894113,-1.2552175169,0.8747614701
 O,0,-5.0547991757,-2.042565492,0.8925490746
 O,0,3.3731288506,2.1875763748,-0.2265338074
 O,0,0.6672501147,2.9282812061,-0.955027255
 H,0,2.9002480807,-2.197242925,0.1039436065
 H,0,3.6420735664,-1.0098135721,1.1995351639
 H,0,3.5048854993,-0.1208909613,-1.1236450017
 H,0,-3.5192405309,1.8111061473,2.3038487521
 H,0,2.2550761412,1.2480204648,1.1437223249
 H,0,0.1991255407,1.4882960751,0.3113699466
 H,0,1.231816948,3.1663195418,-1.7434735018
 H,0,3.6262587003,2.0886515532,-1.1952157107
 H,0,-5.1036954859,0.0876498607,2.0737993832
 H,0,0.838056064,-1.1329904391,0.9382051505
 H,0,-0.3424849232,-2.3067955152,-1.4456916981
 O,0,1.3537148343,1.1349857054,-3.128625981
 P,0,2.5437955879,2.1274155899,-3.4330074365
 O,0,2.8058311833,1.9285867825,-5.083799499
 O,0,2.1370192455,3.5740787299,-3.189258045
 O,0,3.871374433,1.6621583475,-2.795634573
 H,0,-0.2048518589,0.3242374005,-2.1262483512
 H,0,3.5861372232,1.3528949158,-5.0964632263

LG 2.1 Nuc 2.1

gridlg21.2

E(RB+HF-LYP) = -1626.32175573

Zero-point correction= 0.264412
 (Hartree/Particle)
 Thermal correction to Energy= 0.286086
 Thermal correction to Enthalpy= 0.287031
 Thermal correction to Gibbs Free Energy= 0.210007

Sum of electronic and zero-point Energies= -
 1626.057344
 Sum of electronic and thermal Energies= -
 1626.035669
 Sum of electronic and thermal Enthalpies= -
 1626.034725
 Sum of electronic and thermal Free Energies= -
 1626.111749

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.522	81.460	162.110

C,0,0.888919946,1.6247046392,-0.528192421
 C,0,0.6128931373,0.4294865482,-1.4592977501
 O,0,1.4831453112,-0.5554128346,-1.3233277741
 C,0,2.6200212315,-0.1482780608,-0.4941760518
 C,0,2.338665922,1.282612221,0.0328538349
 C,0,2.7658296561,-1.2201391049,0.574272497
 O,0,1.6719771284,-1.2713963988,1.4772480396
 N,0,-0.8244748018,-0.5758093015,-0.304589508
 C,0,-1.1245811102,-1.8246678058,-0.7805335116
 N,0,-2.3115374673,-2.3386002363,-0.4561534724
 C,0,-2.8618180649,-1.3399509616,0.3085207174
 C,0,-1.9481152738,-0.2597617937,0.4010286205
 N,0,-2.1517603683,0.9065740243,1.1023416949
 C,0,-3.3021222934,0.9663710834,1.6909285833
 N,0,-4.2544492325,-0.0266764263,1.6482022611
 C,0,-4.1363609356,-1.2763118403,0.9660186511
 O,0,-5.0742259431,-2.0762390255,1.0282885253
 O,0,3.3657815531,2.1850921315,-0.2483178497
 O,0,0.6545922422,2.9012089945,-1.009586955
 H,0,2.9168540464,-2.1988272571,0.0829300438
 H,0,3.6636418283,-1.0062607896,1.1692202108
 H,0,3.4829086352,-0.1195511878,-1.1658165993
 H,0,-3.5717278841,1.8477345979,2.2721979912
 H,0,2.2546058123,1.2446726101,1.1256290251
 H,0,0.1984382663,1.5027355042,0.3096097386
 H,0,1.2337405195,3.1316644345,-1.8004619551
 H,0,3.6217919001,2.0925364411,-1.2239211531
 H,0,-5.1337690164,0.0946254389,2.1352272096
 H,0,0.8564381969,-1.1699422889,0.9456546062
 H,0,-0.4108992167,-2.3526685751,-1.4040068959
 O,0,1.427024485,1.0930902068,-3.2777634611
 P,0,2.586711984,2.1192315327,-3.4746885933
 O,0,2.9847147354,2.0311689091,-5.114681587
 O,0,2.1413118903,3.5496298355,-3.1703602408
 O,0,3.9050746645,1.674854774,-2.785694543
 H,0,-0.1638981562,0.3378302654,-2.1879995376
 H,0,3.8569011423,1.6093373164,-5.0709362305

LG 2.1 Nuc 2.3

gridlg21.3

E(RB+HF-LYP) = -1626.32231452

Zero-point correction=	0.263683
(Hartree/Particle)	
Thermal correction to Energy=	0.285387
Thermal correction to Enthalpy=	0.286331
Thermal correction to Gibbs Free Energy=	0.209717
Sum of electronic and zero-point Energies=	-
1626.058631	
Sum of electronic and thermal Energies=	-
1626.036927	
Sum of electronic and thermal Enthalpies=	-
1626.035983	
Sum of electronic and thermal Free Energies=	-
1626.112598	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.083	81.486	161.249

C,0,0.88626134,1.6320890066,-0.5332509243
 C,0,0.5955737075,0.4178894499,-1.4309979045
 O,0,1.4845799276,-0.5402768592,-1.3306040862
 C,0,2.6164362808,-0.142022565,-0.4814281839
 C,0,2.3423260613,1.2982310672,0.0239316682
 C,0,2.7369140454,-1.2077071406,0.5952950619
 O,0,1.6378640833,-1.2363885739,1.4940920211
 N,0,-0.8691767412,-0.5915225659,-0.3149372088
 C,0,-1.1726084427,-1.8383371453,-0.7912816627
 N,0,-2.3506220922,-2.353838529,-0.4417290425
 C,0,-2.888010088,-1.3568054511,0.3349580194
 C,0,-1.9789208472,-0.2727922259,0.4106465877
 N,0,-2.1705091649,0.8924379836,1.1152295108
 C,0,-3.3090499603,0.947597124,1.7272923017
 N,0,-4.2576795859,-0.0490416402,1.7040264361
 C,0,-4.149325386,-1.298248308,1.0192489446
 O,0,-5.0816151257,-2.1018524827,1.0997543068
 O,0,3.3638166134,2.1922179239,-0.2850241902
 O,0,0.6527579255,2.8887217248,-1.0568700805
 H,0,2.8772268104,-2.1923738981,0.1134107058
 H,0,3.6330696729,-1.0018698119,1.1949473487
 H,0,3.4814074725,-0.1292643875,-1.150428362
 H,0,-3.5697494343,1.8279825175,2.3137544541
 H,0,2.2645536327,1.2769617249,1.1181212208
 H,0,0.2005617334,1.5305766622,0.3135250209
 H,0,1.2514935681,3.1054940779,-1.8505917679
 H,0,3.6081336814,2.0820020829,-1.2690349372
 H,0,-5.1269585067,0.0688596034,2.2096451588
 H,0,0.8238157446,-1.1559151254,0.9580019059
 H,0,-0.4694233601,-2.3617364043,-1.4301763508
 O,0,1.4663070549,1.0391792848,-3.46712645
 P,0,2.6085273064,2.0793392322,-3.5382562069
 O,0,3.1385209238,2.1075231036,-5.1480766953
 O,0,2.1399742728,3.4948300885,-3.1733669687
 O,0,3.8998768178,1.6311937487,-2.7882225261
 H,0,-0.1071263897,0.3765704435,-2.2398639488
 H,0,4.0530209185,1.8049638836,-5.0349470162

LG 2.1 Nuc 2.5

gridlg21.4

E(RB+HF-LYP) = -1626.32351965

Zero-point correction=	0.263117
(Hartree/Particle)	
Thermal correction to Energy=	0.284629
Thermal correction to Enthalpy=	0.285573
Thermal correction to Gibbs Free Energy=	0.211033
Sum of electronic and zero-point Energies=	-
1626.060402	
Sum of electronic and thermal Energies=	-
1626.038891	
Sum of electronic and thermal Enthalpies=	-
1626.037947	
Sum of electronic and thermal Free Energies=	-
1626.112486	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.607	81.259	156.882

C,0,0.9801658535,1.64118094,-0.4378649832
 C,0,0.6561259347,0.4491474288,-1.3526050817
 O,0,1.5710602864,-0.4817644639,-1.3336725474
 C,0,2.6647583221,-0.1601193552,-0.4005579667
 C,0,2.4682324792,1.3140553273,0.0356797178

C,0,2.6322939839,-1.1954769893,0.713733541
 O,0,1.5210755454,-1.0762220969,1.5869819039
 N,0,-0.8230024585,-0.6017556746,-0.2953537834
 C,0,-1.1208295774,-1.8333939973,-0.8136146501
 N,0,-2.3093489169,-2.3467023283,-0.5043338043
 C,0,-2.860599796,-1.3635639968,0.2816434054
 C,0,-1.9496207813,-0.2875660867,0.4072581811
 N,0,-2.1501314893,0.86215251,1.1325307444
 C,0,-3.3044405871,0.9108166005,1.7155379725
 N,0,-4.2574965456,-0.0790216597,1.6451953718
 C,0,-4.1384359456,-1.3135549923,0.9358741315
 O,0,-5.0744468662,-2.1149644063,0.9767844133
 O,0,3.4710063775,2.1613901584,-0.4152219925
 O,0,0.7230390718,2.8968009454,-0.9469741576
 H,0,2.6806932085,-2.2051325832,0.2666001835
 H,0,3.5313393655,-1.0665480321,1.3309723774
 H,0,3.5702399058,-0.2481121201,-1.0053471622
 H,0,-3.57529312,1.77966174,2.3142284557
 H,0,2.4741918902,1.3619664606,1.1323117175
 H,0,0.3389472027,1.5180941857,0.4420610197
 H,0,1.2738600335,3.0985277728,-1.7941925454
 H,0,3.598752408,2.002419604,-1.4238476617
 H,0,-5.1392411429,0.033335886,2.1301329765
 H,0,0.7176263427,-1.0087629902,1.0309635994
 H,0,-0.4053195762,-2.342476011,-1.4498571132
 O,0,1.2817698351,1.0187500968,-3.7050760709
 P,0,2.4463740412,2.0187719086,-3.6421814551
 O,0,3.0444101057,2.1989747326,-5.2209376599
 O,0,2.0250616507,3.4174381763,-3.150366652
 O,0,3.7116943427,1.4794414065,-2.8986794359
 H,0,0.0183334998,0.4825744501,-2.2199329837
 H,0,3.9693995862,1.9443050734,-5.0782058456

LG 2.1 Nuc 2.7

gridlg21.5

E(RB+HF-LYP) = -1626.32471629

Zero-point correction= 0.262554
 (Hartree/Particle)
 Thermal correction to Energy= 0.284094
 Thermal correction to Enthalpy= 0.285039
 Thermal correction to Gibbs Free Energy= 0.210264
 Sum of electronic and zero-point Energies= -
 1626.062162
 Sum of electronic and thermal Energies= -
 1626.040622
 Sum of electronic and thermal Enthalpies= -
 1626.039678
 Sum of electronic and thermal Free Energies= -
 1626.114452

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.272	81.212	157.376

C,0,1.014898916,1.6374946307,-0.3863758755
 C,0,0.6853263775,0.4558333227,-1.3076799319
 O,0,1.6099788569,-0.4638665359,-1.3178816221
 C,0,2.6899475635,-0.1666038156,-0.3605611891
 C,0,2.516380288,1.3182194741,0.0494931733
 C,0,2.6107771774,-1.1910109468,0.7623548745
 O,0,1.4938832016,-1.0314082658,1.6217289394
 N,0,-0.8229165226,-0.6082211826,-0.3061843869
 C,0,-1.125574468,-1.8326720192,-0.8377967355
 N,0,-2.3169918189,-2.339912865,-0.5325172113
 C,0,-2.8632304766,-1.3596600299,0.2611969714
 C,0,-1.94841599,-0.2891115754,0.3961087907
 N,0,-2.1415473093,0.8555653898,1.1301849663
 C,0,-3.2959778991,0.9058547175,1.7129808067

N,0,-4.2537686987,-0.0784818637,1.6349435184
 C,0,-4.1407254744,-1.3085851241,0.9169177767
 O,0,-5.080019257,-2.1057754479,0.9514977724
 O,0,3.4996630322,2.1481529988,-0.4644397929
 O,0,0.7474334039,2.888944587,-0.8960204982
 H,0,2.6347484632,-2.2051964384,0.323915909
 H,0,3.5050842441,-1.0844868073,1.3904890492
 H,0,3.6044760177,-0.2854177041,-0.9459909722
 H,0,-3.5623068858,1.7716517893,2.3179294031
 H,0,2.5609670324,1.393556883,1.1441666767
 H,0,0.3933737624,1.5081109617,0.5070081508
 H,0,1.2536619028,3.0658045953,-1.785472761
 H,0,3.5681479553,1.9755672514,-1.4825405795
 H,0,-5.1351718637,0.0349863733,2.1202950835
 H,0,0.6945299311,-0.9832625618,1.0584624831
 H,0,-0.4123104947,-2.3389455815,-1.4784881927
 O,0,1.2466078953,0.9540927137,-3.9012688248
 P,0,2.3726743276,1.9738306317,-3.7106104492
 O,0,3.0536044557,2.2715448428,-5.2391509755
 O,0,1.8988594072,3.3379063544,-3.160969006
 O,0,3.6196634569,1.4360551308,-2.9308111801
 H,0,0.1032004889,0.5305027093,-2.2189839618
 H,0,3.9833134714,2.0736110279,-5.0462640386

LG 2.1 Nuc 2.9

gridlg21.6

E(RB+HF-LYP) = -1626.32471290

Zero-point correction= 0.261962
 (Hartree/Particle)
 Thermal correction to Energy= 0.283667
 Thermal correction to Enthalpy= 0.284611
 Thermal correction to Gibbs Free Energy= 0.208887
 Sum of electronic and zero-point Energies= -
 1626.062751
 Sum of electronic and thermal Energies= -
 1626.041046
 Sum of electronic and thermal Enthalpies= -
 1626.040102
 Sum of electronic and thermal Free Energies= -
 1626.115826

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.004	81.255	159.376

C,0,1.036176566,1.6363830956,-0.3615421925
 C,0,0.7071858151,0.4608522287,-1.2866951828
 O,0,1.6313797278,-0.458801525,-1.3053740213
 C,0,2.70121439,-0.1741707153,-0.3322877391
 C,0,2.5437997435,1.3187488472,0.0557861324
 C,0,2.5898986846,-1.1875126231,0.7980909715
 O,0,1.4647938675,-1.0035093055,1.6419712097
 N,0,-0.8305105664,-0.6024924321,-0.3302536527
 C,0,-1.1331754039,-1.8268580211,-0.8611858259
 N,0,-2.320001817,-2.3367898717,-0.5438798218
 C,0,-2.8614783703,-1.3583641226,0.2553858291
 C,0,-1.949879731,-0.2845603033,0.382209482
 N,0,-2.1388461692,0.8591322459,1.1183074719
 C,0,-3.2875703723,0.9050789308,1.7127217925
 N,0,-4.2424902768,-0.0824932972,1.6439480586
 C,0,-4.1324302913,-1.3121096997,0.9246044103
 O,0,-5.0680415793,-2.1127400843,0.9683336886
 O,0,3.5155223749,2.1324388602,-0.4994387992
 O,0,0.7663930997,2.8850258638,-0.8732127873
 H,0,2.6039699339,-2.2056485503,0.3688096983
 H,0,3.4770033306,-1.0898598053,1.4376533546
 H,0,3.6217204002,-0.3148342437,-0.9031463146
 H,0,-3.5506669373,1.7697804676,2.3205451374

H,0,2.6107598763,1.4153055042,1.1480030649
H,0,0.4242185836,1.5047623321,0.5381716113
H,0,1.2396957771,3.0420088838,-1.7906525789
H,0,3.538124787,1.9460206843,-1.5224219177
H,0,-5.1191629548,0.0275657144,2.1385880226
H,0,0.6711847086,-0.9700406271,1.070369723
H,0,-0.4242196361,-2.3303156871,-1.5086428591
O,0,1.2313281431,0.9290448347,-4.100244006
P,0,2.3245133988,1.9445281613,-3.7740134279
O,0,3.1059038043,2.3375131886,-5.2326960258
O,0,1.8077701886,3.2773638178,-3.1805800997
O,0,3.5283281056,1.3842119382,-2.9394270923
H,0,0.1525457132,0.5549202626,-2.2172149584
H,0,4.0272875561,2.1850826724,-4.9709241957

LG 2.1 Nuc 3.1

gridlg21.7

E(RB+HF-LYP) = -1626.32392738

Zero-point correction= 0.261549
(Hartree/Particle)
Thermal correction to Energy= 0.283345
Thermal correction to Enthalpy= 0.284289
Thermal correction to Gibbs Free Energy= 0.207762
Sum of electronic and zero-point Energies= -
1626.062378
Sum of electronic and thermal Energies= -
1626.040582
Sum of electronic and thermal Enthalpies= -
1626.039638
Sum of electronic and thermal Free Energies= -
1626.116165

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.802	81.247	161.064

C,0,1.0365676616,1.6382762436,-0.3638142548
C,0,0.7025856774,0.4597739554,-1.2812892312
O,0,1.6206444215,-0.4622610251,-1.3067981452
C,0,2.6958948311,-0.1812705381,-0.3354646077
C,0,2.545209925,1.3139896888,0.0498441761
C,0,2.5846898449,-1.193074043,0.7958728546
O,0,1.4640207742,-1.0049074475,1.6448546949
N,0,-0.8430172878,-0.5976596055,-0.3310572197
C,0,-1.1372139158,-1.8319903741,-0.8433803624
N,0,-2.3167406795,-2.3483304377,-0.5098906886
C,0,-2.8614155711,-1.3643575305,0.2802640325
C,0,-1.9596726366,-0.2802321953,0.3857418005
N,0,-2.1541517171,0.8718335606,1.1070617755
C,0,-3.29850224,0.9144843468,1.7100854032
N,0,-4.2440328671,-0.0833763699,1.6626147149
C,0,-4.1276134301,-1.321333322,0.9589789694
O,0,-5.054619354,-2.1305213601,1.0205738675
O,0,3.5146639327,2.1215622792,-0.5145463238
O,0,0.7734303651,2.8808204109,-0.8879335963
H,0,2.5943793529,-2.2121392011,0.3689499679
H,0,3.4748511292,-1.0963210002,1.4312390245
H,0,3.6121397456,-0.3260044943,-0.9116117826
H,0,-3.5654410163,1.7848019151,2.3080881608
H,0,2.6157291873,1.4118648573,1.1419364346
H,0,0.4262118582,1.5149845222,0.5386698363
H,0,1.2369451065,3.0224879411,-1.8207566704
H,0,3.5141985473,1.9325821688,-1.5428839569
H,0,-5.1176890914,0.0248531823,2.162981802
H,0,0.6673038679,-0.9740839236,1.0779571419
H,0,-0.428181473,-2.3379678976,-1.4887598339
O,0,1.2674812666,0.9452488736,-4.2904751189
P,0,2.3223026764,1.941785157,-3.8278487137

O,0,3.2175006645,2.4136455924,-5.1967613516
O,0,1.7633864601,3.2470614003,-3.2061659735
O,0,3.4652580788,1.3468091993,-2.9288920608
H,0,0.1393642061,0.555104762,-2.2066794502
H,0,4.1157761689,2.2685283288,-4.8610391551

LG 2.3 Nuc 1.9

gridlg23.1

E(RB+HF-LYP) = -1626.34068665

Zero-point correction= 0.265234
(Hartree/Particle)
Thermal correction to Energy= 0.285753
Thermal correction to Enthalpy= 0.286697
Thermal correction to Gibbs Free Energy= 0.215738
Sum of electronic and zero-point Energies= -
1626.075453
Sum of electronic and thermal Energies= -
1626.054934
Sum of electronic and thermal Enthalpies= -
1626.053990
Sum of electronic and thermal Free Energies= -
1626.124949

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.312	79.089	149.345

C,0,1.0090944175,1.6656058587,-0.5012403575
C,0,0.7526981913,0.5406356515,-1.5156377918
O,0,1.5718385105,-0.4890257757,-1.3288180824
C,0,2.6693576061,-0.1483690536,-0.4223043319
C,0,2.449754448,1.3080632889,0.0555978084
C,0,2.6636105383,-1.1988011538,0.680810603
O,0,1.554085788,-1.1080914176,1.5509634568
N,0,-0.7431189905,-0.616521051,-0.2066254979
C,0,-1.0631791119,-1.8006815135,-0.8163221013
N,0,-2.2991441465,-2.2788848833,-0.6491198317
C,0,-2.8657856331,-1.3300738529,0.1651138582
C,0,-1.9056126559,-0.3204192391,0.4389011262
N,0,-2.1105635902,0.784698034,1.2362406354
C,0,-3.3023333413,0.8545574668,1.7346971887
N,0,-4.2966445462,-0.0731533814,1.5169865502
C,0,-4.1844151112,-1.2568540124,0.7235460645
O,0,-5.166426074,-2.0015730907,0.6333640163
O,0,3.498509711,2.1714912866,-0.2872055754
O,0,0.7779640161,2.9775669801,-0.8931717179
H,0,2.7293125914,-2.1995287044,0.213363675
H,0,3.5672806054,-1.0642662507,1.2926014472
H,0,3.5862835944,-0.2065044399,-1.0156130225
H,0,-3.5772847567,1.6903691828,2.3781859747
H,0,2.389087495,1.3223314225,1.1491729785
H,0,0.3054938642,1.4687332862,0.3122736565
H,0,1.3339906759,3.2244096652,-1.6845672248
H,0,3.7080142399,2.0367908399,-1.2603435284
H,0,-5.2070587318,0.051352477,1.9419091092
H,0,0.7528077035,-0.9820539955,0.9892606426
H,0,-0.3254833009,-2.3106456464,-1.4278850029
O,0,1.2947677934,1.1996148766,-3.2132543961
P,0,2.5520182991,2.1360816285,-3.4684122974
O,0,2.7794158508,2.0008778011,-5.1268051004
O,0,2.231634116,3.5890403798,-3.1559133338
O,0,3.8399061891,1.5507336795,-2.8584980294
H,0,-0.1795887112,0.352264315,-2.0015800505
H,0,3.4719568944,1.3248969613,-5.1900053576

LG 2.3 Nuc 2.1

gridlg23.2

E(RB+HF-LYP) = -1626.33471648

Zero-point correction= 0.264422
 (Hartree/Particle)
 Thermal correction to Energy= 0.285951
 Thermal correction to Enthalpy= 0.286895
 Thermal correction to Gibbs Free Energy= 0.211986
 Sum of electronic and zero-point Energies= -
 1626.070294
 Sum of electronic and thermal Energies= -
 1626.048765
 Sum of electronic and thermal Enthalpies= -
 1626.047821
 Sum of electronic and thermal Free Energies= -
 1626.122730

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.437	81.213	157.659

C,0,0.9891769593,1.6572050017,-0.5265982397
 C,0,0.7261071151,0.4940688075,-1.4887929912
 O,0,1.5628972551,-0.5010203158,-1.3343075299
 C,0,2.6644811733,-0.1468540338,-0.4250232416
 C,0,2.4358446397,1.3144734979,0.0345663022
 C,0,2.6599603209,-1.190639576,0.6830956249
 O,0,1.5542067453,-1.0954775722,1.5579833837
 N,0,-0.7836960194,-0.6515319032,-0.1856842793
 C,0,-1.1183602935,-1.8315988435,-0.7947905428
 N,0,-2.3545819988,-2.2997309928,-0.6097049477
 C,0,-2.9045537109,-1.3443962976,0.209136023
 C,0,-1.9366478334,-0.3404428133,0.4697734941
 N,0,-2.1230203329,0.768153825,1.265490798
 C,0,-3.3087641738,0.8477751742,1.7772330822
 N,0,-4.3111163348,-0.0741120211,1.5743902751
 C,0,-4.2165409063,-1.2608152382,0.7831816653
 O,0,-5.2025353728,-2.0005780724,0.7077088847
 O,0,3.4764934638,2.1761826831,-0.3148685333
 O,0,0.747717347,2.9474482966,-0.9664020501
 H,0,2.7255701889,-2.194244994,0.2224860798
 H,0,3.5649032379,-1.0505245638,1.2908386179
 H,0,3.57206449,-0.2070596091,-1.0309658065
 H,0,-3.5704451917,1.68758723,2.42069793
 H,0,2.36970689,1.335272669,1.128194539
 H,0,0.2891029097,1.483587335,0.2975251701
 H,0,1.3241721258,3.1864000738,-1.7565479738
 H,0,3.6848767648,2.0435680416,-1.296145972
 H,0,-5.2156258377,0.0582258407,2.0095286712
 H,0,0.7454802179,-0.9936603989,1.0034899755
 H,0,-0.3920541578,-2.3471313656,-1.41539283
 O,0,1.3508941582,1.1597318802,-3.3799652789
 P,0,2.5806367844,2.123825338,-3.5190439585
 O,0,2.9603303785,2.0859106622,-5.1610669991
 O,0,2.2239305716,3.5613252102,-3.1487119643
 O,0,3.8594218821,1.5589275693,-2.8515021262
 H,0,-0.1479000415,0.3371173954,-2.0853109619
 H,0,3.7801110559,1.5676996998,-5.15482813

LG 2.3 Nuc 2.3

grid1lg23.3

E(RB+HF-LYP) = -1626.33077790

Zero-point correction= 0.263595
 (Hartree/Particle)
 Thermal correction to Energy= 0.285189
 Thermal correction to Enthalpy= 0.286133
 Thermal correction to Gibbs Free Energy= 0.211213
 Sum of electronic and zero-point Energies= -
 1626.067183

Sum of electronic and thermal Energies= -
 1626.045589
 Sum of electronic and thermal Enthalpies= -
 1626.044645
 Sum of electronic and thermal Free Energies= -
 1626.119565

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.959	81.329	157.683

C,0,0.9908100363,1.6574386248,-0.5215744155
 C,0,0.7138768969,0.4742863754,-1.4500931202
 O,0,1.5711487013,-0.4925169144,-1.3387560079
 C,0,2.6717865518,-0.142856195,-0.4165845474
 C,0,2.4486689122,1.3248059982,0.0260152693
 C,0,2.6490111094,-1.1810645081,0.6958597308
 O,0,1.5441716235,-1.0674515605,1.5701126939
 N,0,-0.8136218301,-0.6775771283,-0.1733959041
 C,0,-1.1556085961,-1.8544585423,-0.7838249511
 N,0,-2.3913713735,-2.3167577022,-0.5879704449
 C,0,-2.9319550921,-1.3580859724,0.2340031545
 C,0,-1.9609370042,-0.3567985851,0.4874427829
 N,0,-2.1366043183,0.7535406831,1.2818727119
 C,0,-3.3189667058,0.8381795182,1.8010687753
 N,0,-4.3251747827,-0.0808215018,1.6068035284
 C,0,-4.2402202764,-1.2692247585,0.8169543359
 O,0,-5.22786848,-2.0064495588,0.7494346979
 O,0,3.4790904578,2.1800499148,-0.3514564191
 O,0,0.7421112762,2.9300450948,-0.9967456372
 H,0,2.7036888734,-2.1879696671,0.2416918772
 H,0,3.5541308058,-1.0479890018,1.3043111454
 H,0,3.5761933101,-0.2156609707,-1.0249335783
 H,0,-3.573403704,1.6803009615,2.4441546671
 H,0,2.3943283634,1.3576519481,1.1204325296
 H,0,0.3018859679,1.499595986,0.3172333081
 H,0,1.3251372328,3.1584909431,-1.7986829135
 H,0,3.6679167907,2.0377538525,-1.3426989328
 H,0,-5.2264549238,0.0557914599,2.0473766296
 H,0,0.7317450772,-0.9882348234,1.0183266535
 H,0,-0.4357261977,-2.3715538229,-1.4105472478
 O,0,1.3716791676,1.1205417252,-3.5571402378
 P,0,2.5795286177,2.096553297,-3.5754352217
 O,0,3.0914280028,2.1715049622,-5.185366732
 O,0,2.1966166492,3.5164269223,-3.1421808106
 O,0,3.8361781545,1.5275214285,-2.8559404038
 H,0,-0.0978598009,0.3609735599,-2.1404607814
 H,0,3.956884977,1.7386855777,-5.1196400203

LG 2.3 Nuc 2.5

grid1lg23.4

E(RB+HF-LYP) = -1626.32854804

Zero-point correction= 0.262850
 (Hartree/Particle)
 Thermal correction to Energy= 0.284445
 Thermal correction to Enthalpy= 0.285389
 Thermal correction to Gibbs Free Energy= 0.210572
 Sum of electronic and zero-point Energies= -
 1626.065698
 Sum of electronic and thermal Energies= -
 1626.044103
 Sum of electronic and thermal Enthalpies= -
 1626.043159
 Sum of electronic and thermal Free Energies= -
 1626.117976

	E (Thermal)	CV	S
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Total	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
	178.492	81.353	157.465

C,0,1.014613669,1.6535880891,-0.4824669683
 C,0,0.7268913416,0.4690479059,-1.4007396105
 O,0,1.605468992,-0.4735406203,-1.3370837688
 C,0,2.6944599031,-0.1439915311,-0.3881488325
 C,0,2.4898738718,1.333740384,0.0307469011
 C,0,2.627068534,-1.1723587918,0.7320859432
 O,0,1.5190805315,-1.0189402921,1.5962649022
 N,0,-0.8273442268,-0.7014936845,-0.1742889911
 C,0,-1.1780822903,-1.8716219477,-0.7920928721
 N,0,-2.4160353494,-2.3242607991,-0.592979978
 C,0,-2.9474468715,-1.3639149161,0.2337467599
 C,0,-1.9707033066,-0.3699501575,0.4884412577
 N,0,-2.134976932,0.7390183503,1.286031966
 C,0,-3.3160314343,0.8313247833,1.8072082434
 N,0,-4.328939563,-0.0797354835,1.612444784
 C,0,-4.2540695098,-1.2673378297,0.8202789746
 O,0,-5.2459478204,-1.9980315704,0.7534917456
 O,0,3.5023414657,2.1769508856,-0.403801359
 O,0,0.7515854467,2.913209992,-0.9762474746
 H,0,2.6573532466,-2.1841972409,0.2873577861
 H,0,3.5292078616,-1.0605611519,1.3488623725
 H,0,3.6054403676,-0.2441385792,-0.9820735194
 H,0,-3.5629804011,1.6740206759,2.4522488927
 H,0,2.4688647743,1.3896064211,1.1258529184
 H,0,0.3464469952,1.4972488631,0.3743405916
 H,0,1.3126338265,3.1228790613,-1.8139357609
 H,0,3.6436618206,2.0193232775,-1.408348485
 H,0,-5.228599995,0.0628690683,2.0544954641
 H,0,0.7074027201,-0.9664771729,1.0407452306
 H,0,-0.4637606931,-2.3896889662,-1.4241296114
 O,0,1.3570926619,1.0471552175,-3.7499169485
 P,0,2.5257046012,2.0460693134,-3.6445625478
 O,0,3.1465340413,2.2424675279,-5.209157995
 O,0,2.0955221804,3.4379955492,-3.1467372794
 O,0,3.7686979574,1.4868957638,-2.8833591472
 H,0,-0.0168041956,0.4102290462,-2.1743550637
 H,0,4.058020249,1.9412681796,-5.0705523602

LG 2.3 Nuc 2.7

grid1lg23.5

E(RB+HF-LYP) = -1626.32726116

Zero-point correction=	0.262077
(Hartree/Particle)	
Thermal correction to Energy=	0.283774
Thermal correction to Enthalpy=	0.284719
Thermal correction to Gibbs Free Energy=	0.209264
Sum of electronic and zero-point Energies=	-
1626.065184	
Sum of electronic and thermal Energies=	-
1626.043487	
Sum of electronic and thermal Enthalpies=	-
1626.042543	
Sum of electronic and thermal Free Energies=	-
1626.117998	

Total	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
	178.071	81.374	158.808

C,0,1.0291788444,1.6603053985,-0.4517899537
 C,0,0.7415990416,0.47899205,-1.369148104
 O,0,1.6338044118,-0.4477839543,-1.3355642396
 C,0,2.7064780976,-0.1383704411,-0.3597571024
 C,0,2.5147141319,1.3464154051,0.0419042332
 C,0,2.5999913153,-1.1622262353,0.7616984297

O,0,1.4823223162,-0.9861132729,1.6090792174
 N,0,-0.8443954474,-0.7073508622,-0.1998708831
 C,0,-1.2044123834,-1.870555513,-0.8249336634
 N,0,-2.440033627,-2.321370049,-0.6113827509
 C,0,-2.9584119304,-1.3660764288,0.2297287462
 C,0,-1.9784404904,-0.3748449817,0.4786292067
 N,0,-2.1289900204,0.7276117564,1.2870803715
 C,0,-3.302494555,0.8170017446,1.8257298238
 N,0,-4.3188465794,-0.0913855104,1.6382181164
 C,0,-4.2562711971,-1.273483944,0.8368248159
 O,0,-5.2485488572,-2.0037876083,0.7796857827
 O,0,3.5133838591,2.1782658001,-0.4356265802
 O,0,0.7647249311,2.9093758013,-0.9659088884
 H,0,2.6190268281,-2.1756185737,0.3203631986
 H,0,3.4938857447,-1.0656773492,1.392673919
 H,0,3.6255100972,-0.2580758561,-0.9370297816
 H,0,-3.5389931199,1.6548240447,2.4808070257
 H,0,2.5161865643,1.4204775635,1.1365751202
 H,0,0.3716887597,1.5113472283,0.4146724854
 H,0,1.3039359033,3.0916816568,-1.8372830606
 H,0,3.6150003166,2.0040674309,-3.4491519912
 H,0,-5.2114875387,0.0479064173,2.0953391542
 H,0,0.6767847156,-0.9524282136,1.0444016228
 H,0,-0.4995653071,-2.3839965752,-1.4710192547
 O,0,1.3620363808,0.9809032854,-3.9485155503
 P,0,2.4891684298,1.9921229043,-3.7109498599
 O,0,3.2230099362,2.2888796725,-5.2119880191
 O,0,2.0069719581,3.3578795052,-3.1743022268
 O,0,3.6991110005,1.4376358046,-2.8874281505
 H,0,0.0613754029,0.4651360289,-2.2074315837
 H,0,4.1432465362,2.0729834906,-4.9946634653

LG 2.3 Nuc 2.9

grid1lg23.6

E(RB+HF-LYP) = -1626.32603090

Zero-point correction=	0.261473
(Hartree/Particle)	
Thermal correction to Energy=	0.283296
Thermal correction to Enthalpy=	0.284240
Thermal correction to Gibbs Free Energy=	0.207943
Sum of electronic and zero-point Energies=	-
1626.064558	
Sum of electronic and thermal Energies=	-
1626.042735	
Sum of electronic and thermal Enthalpies=	-
1626.041791	
Sum of electronic and thermal Free Energies=	-
1626.118088	

Total	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
	177.771	81.378	160.580

C,0,1.0436501239,1.6708402416,-0.4353709845
 C,0,0.7528263213,0.493351274,-1.3529664151
 O,0,1.6463154314,-0.429959222,-1.3364047109
 C,0,2.7096249028,-0.1387220509,-0.3434735698
 C,0,2.5348592955,1.3521185133,0.0452422915
 C,0,2.5728992593,-1.1571735348,0.7796185684
 O,0,1.4499402613,-0.9608569316,1.6156134856
 N,0,-0.8610714552,-0.6937285403,-0.2232876782
 C,0,-1.2175232692,-1.8611495809,-0.8423142481
 N,0,-2.4450131529,-2.3233812191,-0.6090486207
 C,0,-2.9607359731,-1.3714882129,0.2375865016
 C,0,-1.9885596781,-0.3692648471,0.4703016283
 N,0,-2.1382947077,0.7329054781,1.2788558657
 C,0,-3.3043366113,0.810369798,1.8353438589
 N,0,-4.3134313437,-0.1092113699,1.6647862682

C,0,-4.2501721752,-1.2920675882,0.8647295183
 O,0,-5.2344929066,-2.0337377096,0.8242077605
 O,0,3.5278596872,-2.1687878643,-0.4630414185
 O,0,0.7843765043,2.9133288566,-0.9628682961
 H,0,2.5806272017,-2.1722626548,0.3422838635
 H,0,3.4615203793,-1.0726866438,1.4196164237
 H,0,3.632688942,-0.2768581663,-0.9096248118
 H,0,-3.5396746235,1.6466028286,2.4927836408
 H,0,2.551587957,1.4395211937,1.139139227
 H,0,0.3934937242,1.5291766852,0.4377455271
 H,0,1.3034518844,3.0713830706,-1.8609522911
 H,0,3.5946461853,1.9776758081,-1.4822586895
 H,0,-5.2001166789,0.0207640291,2.1360481077
 H,0,0.648901279,-0.9360065203,1.0450205167
 H,0,-0.5170019124,-2.3684240353,-1.4977931966
 O,0,1.3729181708,0.9602985867,-4.1471467483
 P,0,2.4663629556,1.9588719414,-3.7734309145
 O,0,3.3145173292,2.3422936728,-5.1943209649
 O,0,1.9467823925,3.3000967339,-3.2004036584
 O,0,3.6208518784,1.3770528538,-2.8854554806
 H,0,0.1005730045,0.5032677763,-2.2180626925
 H,0,4.221393887,2.1629392415,-4.9010315035

LG 2.3 Nuc 3.1

grid1lg23.7

E(RB+HF-LYP) = -1626.32466505

Zero-point correction=	0.260999
(Hartree/Particle)	
Thermal correction to Energy=	0.282003
Thermal correction to Enthalpy=	0.282947
Thermal correction to Gibbs Free Energy=	0.208846
Sum of electronic and zero-point Energies=	-
1626.063666	
Sum of electronic and thermal Energies=	-
1626.042662	
Sum of electronic and thermal Enthalpies=	-
1626.041718	
Sum of electronic and thermal Free Energies=	-
1626.115819	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.960	79.354	155.960

C,0,1.0385084544,1.6618575925,-0.4383355904
 C,0,0.7526894845,0.4781903969,-1.346990623
 O,0,1.6491525956,-0.4390709297,-1.3373910165
 C,0,2.7108371277,-0.1443322426,-0.3410697406
 C,0,2.5337118097,1.3492106026,0.040430238
 C,0,2.5723384905,-1.159440755,0.784851259
 O,0,1.4465688936,-0.9645921191,1.6173607186
 N,0,-0.8661370654,-0.7056551546,-0.2209757038
 C,0,-1.2277610814,-1.877717558,-0.828169265
 N,0,-2.4549592252,-2.3348482131,-0.5847905906
 C,0,-2.9644949814,-1.3743133009,0.2558915574
 C,0,-1.9896552591,-0.3719988135,0.4751156161
 N,0,-2.1332198616,0.7375177066,1.2743171337
 C,0,-3.2965063179,0.8223857964,1.8355118126
 N,0,-4.3081036349,-0.0966632303,1.6780663907
 C,0,-4.2508913345,-1.286864426,0.8885603062
 O,0,-5.2365873945,-2.0268941044,0.8587561885
 O,0,3.5206310262,2.1630322447,-0.4790249132
 O,0,0.7726437039,2.8950620371,-0.979853302
 H,0,2.5852506397,-2.1763610924,0.3519704832
 H,0,3.4589235832,-1.0690109741,1.4268094068
 H,0,3.6338089821,-0.2841601094,-0.9064393705
 H,0,-3.5269817267,1.6650748325,2.4863207707
 H,0,2.5518854831,1.4414486875,1.1341460952

H,0,0.3926226941,1.5242895077,0.4385777014
 H,0,1.2820929644,3.0478906558,-1.8927188802
 H,0,3.566751618,1.9624350843,-1.5032085876
 H,0,-5.1923485797,0.0395808732,2.1521632586
 H,0,0.6460348139,-0.9474280926,1.0461168256
 H,0,-0.5312791684,-2.3927807346,-1.4819654665
 O,0,1.4157386799,0.9749813044,-4.3342239563
 P,0,2.4590300388,1.9605844034,-3.8266059828
 O,0,3.4153883971,2.4293099013,-5.1522926504
 O,0,1.8883101821,3.269830031,-3.2229605698
 O,0,3.5540692884,1.3510958558,-2.8788511506
 H,0,0.096509899,0.4847621174,-2.2115011542
 H,0,4.2976712508,2.2582598389,-4.7879310883

LG 2.5 Nuc 1.9

grid1lg25.1

E(RB+HF-LYP) = -1626.35492381

Zero-point correction=	0.265045
(Hartree/Particle)	
Thermal correction to Energy=	0.286514
Thermal correction to Enthalpy=	0.287458
Thermal correction to Gibbs Free Energy=	0.212424
Sum of electronic and zero-point Energies=	-
1626.089878	
Sum of electronic and thermal Energies=	-
1626.068410	
Sum of electronic and thermal Enthalpies=	-
1626.067466	
Sum of electronic and thermal Free Energies=	-
1626.142500	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.790	81.007	157.922

C,0,1.1040094688,1.7019679658,-0.4992341765
 C,0,0.8317494443,0.6115313069,-1.5397884845
 O,0,1.5995587982,-0.4498079365,-1.3328005197
 C,0,2.6999443167,-0.1550603173,-0.4101010452
 C,0,2.5288084244,1.30940012,0.0629461707
 C,0,2.6279384593,-1.2041694223,0.6926961161
 O,0,1.5233025312,-1.0516825969,1.5567095536
 N,0,-0.7974862609,-0.6665506719,-0.1390414684
 C,0,-1.1292754654,-1.7940736724,-0.838700719
 N,0,-2.3851592798,-2.2426725771,-0.7456989462
 C,0,-2.9513801691,-1.3315986147,0.1106130689
 C,0,-1.9702779706,-0.3743971092,0.4844220531
 N,0,-2.168625929,0.6837770944,1.3451972901
 C,0,-3.3748830345,0.7598962239,1.8070986945
 N,0,-4.3888496976,-0.1185169075,1.4952983293
 C,0,-4.2858220518,-1.2508810933,0.628348515
 O,0,-5.2867016722,-1.9561701692,0.459663698
 O,0,3.6017463944,2.1397846847,-0.2870054547
 O,0,0.891278812,3.027993388,-0.854696548
 H,0,2.6425291399,-2.2059719362,0.2227282148
 H,0,3.5351770723,-1.1204391075,1.3085611872
 H,0,3.6227559121,-0.2526099392,-0.9888797165
 H,0,-3.6473800495,1.5607139839,2.4947946209
 H,0,2.4693215988,1.3308982211,1.1561811107
 H,0,0.3845254748,1.4778228368,0.297195699
 H,0,1.4495693632,3.2765788259,-1.6448020689
 H,0,3.7916540783,2.0055107313,-1.2626246885
 H,0,-5.3094888091,0.0076525465,1.8970367845
 H,0,0.7177246911,-0.9360697429,0.9930363296
 H,0,-0.3858952882,-2.2865179984,-1.4579972401
 O,0,1.3251875922,1.2506746536,-3.2596755778
 P,0,2.6166383147,2.1611381164,-3.4723773771
 O,0,2.8390415054,2.0692551735,-5.1315673007

O,0,2.3364660526,3.6119575653,-3.1194395125
 O,0,3.8747328324,1.5151455594,-2.8687797755
 H,0,-0.1428165498,0.4188431762,-1.9419592591
 H,0,3.4726264215,1.3413152587,-5.2276913969

LG 2.5 Nuc 2.1

grid1lg25.2

E(RB+HF-LYP) = -1626.34551380

Zero-point correction= 0.264311
 (Hartree/Particle)
 Thermal correction to Energy= 0.285819
 Thermal correction to Enthalpy= 0.286763
 Thermal correction to Gibbs Free Energy= 0.211895
 Sum of electronic and zero-point Energies= -
 1626.081203
 Sum of electronic and thermal Energies= -
 1626.059695
 Sum of electronic and thermal Enthalpies= -
 1626.058750
 Sum of electronic and thermal Free Energies= -
 1626.133619

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.354	81.124	157.573

C,0,1.0722896462,1.6824084763,-0.5210485944
 C,0,0.8019471605,0.5555964679,-1.5141761505
 O,0,1.5896416289,-0.4702273201,-1.337462835
 C,0,2.6957203058,-0.1553408551,-0.4132805772
 C,0,2.5066635408,1.3119271256,0.043727249
 C,0,2.6345284456,-1.200454754,0.6932153436
 O,0,1.5360913045,-1.0530873657,1.5652934942
 N,0,-0.8175745313,-0.7207194879,-0.1006117238
 C,0,-1.1717857892,-1.8398666486,-0.8027017115
 N,0,-2.4355675665,-2.262690702,-0.7071144337
 C,0,-2.9823923038,-1.3398011056,0.149679097
 C,0,-1.9837407373,-0.4023220125,0.5227550575
 N,0,-2.1592595988,0.6607755559,1.3815343696
 C,0,-3.3639175918,0.7623492006,1.8430903058
 N,0,-4.3948135422,-0.0965946984,1.5337096413
 C,0,-4.315132236,-1.2319006495,0.6682501719
 O,0,-5.3288147585,-1.9177472557,0.5005265315
 O,0,3.5660452149,2.1484567843,-0.3122285316
 O,0,0.8410108538,2.9888925982,-0.915233574
 H,0,2.6555848422,-2.2043292574,0.2283780679
 H,0,3.545496615,-1.104870986,1.3011746402
 H,0,3.6081963477,-0.2485670337,-1.0073220548
 H,0,-3.6201477908,1.5703434886,2.528377529
 H,0,2.4427805801,1.3386964658,1.1368845877
 H,0,0.3586276046,1.4694843153,0.2863546696
 H,0,1.4122832412,3.2344011137,-1.7073368538
 H,0,3.7546720121,2.01862666,-1.2957516151
 H,0,-5.3129359933,0.0499395288,1.9343635928
 H,0,0.719033872,-0.963266631,1.0133525568
 H,0,-0.4398184767,-2.3471749619,-1.4238797979
 O,0,1.368022589,1.2172864225,-3.4251242658
 P,0,2.62780252,2.1575233271,-3.5191516794
 O,0,3.0059403689,2.1623157625,-5.1590535254
 O,0,2.3032909318,3.5898841218,-3.1066744546
 O,0,3.8806221866,1.5328716385,-2.8624997637
 H,0,-0.1241862283,0.385277291,-2.0282454719
 H,0,3.7860398021,1.5865730007,-5.1821031312

LG 2.5 Nuc 2.3

grid1lg25.3

E(RB+HF-LYP) = -1626.33864873

Zero-point correction= 0.263467
 (Hartree/Particle)
 Thermal correction to Energy= 0.285041
 Thermal correction to Enthalpy= 0.285986
 Thermal correction to Gibbs Free Energy= 0.211026
 Sum of electronic and zero-point Energies= -
 1626.075181
 Sum of electronic and thermal Energies= -
 1626.053607
 Sum of electronic and thermal Enthalpies= -
 1626.052663
 Sum of electronic and thermal Free Energies= -
 1626.127623

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.866	81.265	157.767

C,0,1.0667759557,1.6742883735,-0.519625546
 C,0,0.788763994,0.5266550206,-1.4791724056
 O,0,1.5974184076,-0.4713066246,-1.3414016513
 C,0,2.7023029348,-0.1545997752,-0.4050659184
 C,0,2.5129502842,1.3182817844,0.0340789768
 C,0,2.626426141,-1.1930034483,0.7063539378
 O,0,1.5279963155,-1.0302482879,1.5752537299
 N,0,-0.8387067115,-0.7601141479,-0.0843385661
 C,0,-1.2079520896,-1.8748358831,-0.7856957238
 N,0,-2.4754451798,-2.2823446928,-0.6829027077
 C,0,-3.0077545102,-1.3515835859,0.1749848316
 C,0,-1.9985945169,-0.424372019,0.5419715685
 N,0,-2.1575321358,0.6430857056,1.3977862815
 C,0,-3.3595031655,0.7601987917,1.8630563517
 N,0,-4.4007986987,-0.0881380546,1.5605793027
 C,0,-4.3373764394,-1.2274420496,0.698976809
 O,0,-5.3583823484,-1.9028202288,0.537321355
 O,0,3.5597647586,2.1519107924,-0.3472140751
 O,0,0.8226039708,2.9648992694,-0.9438183325
 H,0,2.641116597,-2.1998695511,0.2484829132
 H,0,3.5362153158,-1.100311271,1.3159872377
 H,0,3.6112358012,-0.2576006783,-1.0019410862
 H,0,-3.603895701,1.5737584324,2.5458568558
 H,0,2.4586501114,1.3560101438,1.1277887897
 H,0,0.3638504913,1.4707284974,0.3018654994
 H,0,1.3958372302,3.2021366187,-1.7503552375
 H,0,3.7293362856,2.0184386929,-1.3411052747
 H,0,-5.3158182652,0.0706723678,1.9637140271
 H,0,0.7074737586,-0.9668913002,1.0250523498
 H,0,-0.4850268921,-2.3910781787,-1.4102401558
 O,0,1.3928095202,1.1750313149,-3.6016084858
 P,0,2.6198692232,2.1353695338,-3.5732293047
 O,0,3.132565086,2.2525215259,-5.1774360893
 O,0,2.2552149027,3.5452750997,-3.0975581412
 O,0,3.8580101032,1.5186235763,-2.8668495713
 H,0,-0.0839375439,0.3896664104,-2.0887464119
 H,0,3.9857814797,1.793675445,-5.1311399721

LG 2.5 Nuc 2.5

grid1lg25.4

E(RB+HF-LYP) = -1626.33397018

Zero-point correction= 0.262594
 (Hartree/Particle)
 Thermal correction to Energy= 0.284237
 Thermal correction to Enthalpy= 0.285182
 Thermal correction to Gibbs Free Energy= 0.210008
 Sum of electronic and zero-point Energies= -
 1626.071376
 Sum of electronic and thermal Energies= -
 1626.049733

Sum of electronic and thermal Enthalpies= -
1626.048789
Sum of electronic and thermal Free Energies= -
1626.123962

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.362	81.375	158.217

C,0,1.0632625742,1.6669455715,-0.5044944034
C,0,0.7845482264,0.5091845678,-1.4455139561
O,0,1.615839955,-0.4633546408,-1.3480557713
C,0,2.7116861015,-0.1522849589,-0.3915541394
C,0,2.5229467657,1.3253081068,0.0340017177
C,0,2.6158248067,-1.1876734814,0.721010932
O,0,1.5160390304,-0.10117397809,1.5853322977
N,0,-0.853737865,-0.7949368529,-0.079760217
C,0,-1.2380543814,-1.9062810316,-0.7783530023
N,0,-2.5085879823,-2.2993333819,-0.6660723838
C,0,-3.0260872393,-1.3599702837,0.1920261267
C,0,-2.0067135378,-0.4419491549,0.5504943395
N,0,-2.1488768725,0.6303173569,1.4024419835
C,0,-3.3474057376,0.7625407239,1.8728695548
N,0,-4.3987021757,-0.0761793309,1.5795507928
C,0,-4.351695332,-1.2202328696,0.7231397618
O,0,-5.379579885,-1.8862225246,0.5699467941
O,0,3.5545845391,2.1570710233,-0.3769981331
O,0,0.8066268285,2.941836892,-0.9573203739
H,0,2.623421814,-2.1957230396,0.2660890794
H,0,3.523597709,-1.1022618328,1.3343745161
H,0,3.6220272477,-0.2645342313,-0.9840147437
H,0,-3.5795960517,1.5820397317,2.5526198406
H,0,2.4823919257,1.3733548173,1.1282747485
H,0,0.3737226414,1.4700710385,0.3310779962
H,0,1.3743737305,3.1657964907,-1.7872529624
H,0,3.6995297877,2.0153981752,-1.3813602577
H,0,-5.3099952321,0.094391658,1.9863692183
H,0,0.6936176946,-0.9723211962,1.0360875513
H,0,-0.5244971714,-2.4313453325,-1.4063385109
O,0,1.4144475505,1.1209721946,-3.7862274731
P,0,2.5979404715,2.1017834549,-3.6309858159
O,0,3.2357263281,2.3295393141,-5.1820274674
O,0,2.1784805032,3.484700165,-3.1032229117
O,0,3.8169574157,1.4991019735,-2.8685851055
H,0,-0.0265265116,0.4113929232,-2.1451667076
H,0,4.1347067984,1.9892653654,-5.052736755

LG 2.5 Nuc 2.7

grid1lg25.5

E(RB+HF-LYP) = -1626.33086393

Zero-point correction=	0.261738
(Hartree/Particle)	
Thermal correction to Energy=	0.283516
Thermal correction to Enthalpy=	0.284460
Thermal correction to Gibbs Free Energy=	0.208564
Sum of electronic and zero-point Energies=	-
1626.069126	
Sum of electronic and thermal Energies=	-
1626.047348	
Sum of electronic and thermal Enthalpies=	-
1626.046404	
Sum of electronic and thermal Free Energies=	-
1626.122300	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.909	81.461	159.738

C,0,1.0603831781,1.6717022442,-0.4896324566
C,0,0.7861201747,0.5120982057,-1.4244297096
O,0,1.6340260287,-0.4418731339,-1.3579126571
C,0,2.7153995383,-0.1436531502,-0.3766701525
C,0,2.5288375044,1.3373319781,0.0395002554
C,0,2.5951336362,-1.1791569873,0.7332999275
O,0,1.4904526395,-0.992835733,1.5889918581
N,0,-0.8684035258,-0.8082767682,-0.0943318518
C,0,-1.2635936856,-1.9171595413,-0.791042359
N,0,-2.5330234963,-2.3067360235,-0.6619614355
C,0,-3.0374306475,-1.3665016185,0.2033615663
C,0,-2.0129723345,-0.4503738963,0.5490842793
N,0,-2.1411668714,0.6213943714,1.403301689
C,0,-3.3331725401,0.7553850238,1.8897786511
N,0,-4.3893163399,-0.0816182919,1.6103033073
C,0,-4.3555270781,-1.2256667228,0.7532625622
O,0,-5.3854546645,-1.8909931246,0.6144103893
O,0,3.5482853754,2.1651196828,-0.3984884508
O,0,0.8030851718,2.9345112219,-0.9686399277
H,0,2.5972192737,-2.1868424349,0.2779683609
H,0,3.4982731516,-1.1034983293,1.3545319902
H,0,3.6306089316,-0.2643658881,-0.9593840141
H,0,-3.5547105355,1.5749561314,2.5728497263
H,0,2.4995001909,1.3948574664,1.1340050237
H,0,0.3775094868,1.4849310031,0.353539899
H,0,1.3616408807,3.1365042948,-1.8246435557
H,0,3.6690871454,2.0068537063,-1.4107002844
H,0,-5.2945289774,0.0895887551,2.0302636197
H,0,0.6704183985,-0.9691486692,1.0359595538
H,0,-0.5594285052,-2.4429915084,-1.4288006504
O,0,1.4392466831,1.0754848578,-3.9829488083
P,0,2.5810531468,2.0589883636,-3.6901545945
O,0,3.3485447266,2.3829996854,-5.1662414035
O,0,2.1115822498,3.4173012085,-3.1262110926
O,0,3.7572813135,1.4522918452,-2.8571373614
H,0,0.0329197396,0.4521543565,-2.1952194128
H,0,4.2543651064,2.119050394,-4.950360352

LG 2.5 Nuc 2.9

grid1lg25.6

E(RB+HF-LYP) = -1626.32858267

Zero-point correction=	0.261070
(Hartree/Particle)	
Thermal correction to Energy=	0.282976
Thermal correction to Enthalpy=	0.283920
Thermal correction to Gibbs Free Energy=	0.207188
Sum of electronic and zero-point Energies=	-
1626.067513	
Sum of electronic and thermal Energies=	-
1626.045606	
Sum of electronic and thermal Enthalpies=	-
1626.044662	
Sum of electronic and thermal Free Energies=	-
1626.121394	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.570	81.484	161.496

C,0,1.0717033177,1.6786310163,-0.4697198634
C,0,0.7995285843,0.5221092757,-1.4039060156
O,0,1.6549497734,-0.4227218063,-1.3585089523
C,0,2.7233989634,-0.140039328,-0.3571085057
C,0,2.5476636549,1.3461332428,0.0468886341
C,0,2.5730529475,-1.1714595442,0.7531561952
O,0,1.4601306475,-0.9686090849,1.5940699861
N,0,-0.8795584561,-0.8086703254,-0.1156150115
C,0,-1.2817824174,-1.9141606034,-0.8138766093

N,O,-2.5489822633,-2.3047602827,-0.670620213
 C,O,-3.0437856561,-1.3683845248,0.2046114813
 C,O,-2.0170530608,-0.4523151516,0.5416413157
 N,O,-2.1353707555,0.6154958501,1.4018508389
 C,O,-3.3213416769,0.7456276826,1.904002027
 N,O,-4.3795119442,-0.091865036,1.6345433367
 C,O,-4.3549551919,-1.232343464,0.7724897469
 O,O,-5.3849615763,-1.8992674439,0.6444214992
 O,O,3.557402436,2.1640045495,-0.4235700237
 O,O,0.8160576184,2.9337369279,-0.9643107766
 H,O,2.5684802128,-2.180119316,0.3004260915
 H,O,3.4687873538,-1.1060531005,1.3861515028
 H,O,3.6438907625,-0.2761144084,-0.9275326972
 H,O,-3.5352143748,1.5619124866,2.5933403643
 H,O,2.5342386147,1.4172180204,1.1411865284
 H,O,0.3962914103,1.4978463617,0.3805866575
 H,O,1.3519287069,3.1109535924,-1.8516649781
 H,O,3.6414411481,1.9893409119,-1.4428186642
 H,O,-5.2793490323,0.0757368097,2.0673427668
 H,O,0.6458826179,-0.9575655279,1.0326525292
 H,O,-0.5850603695,-2.4364448978,-1.4625195833
 O,O,1.4544268166,1.0410047806,-4.1809289476
 P,O,2.5493734209,2.0180626851,-3.754265909
 O,O,3.4344458092,2.4274397946,-5.1425831174
 O,O,2.030407981,3.3508322202,-3.1613295758
 O,O,3.6712707352,1.3969587875,-2.8525712799
 H,O,0.0835326492,0.4898419377,-2.2150387025
 H,O,4.3308850625,2.2126745324,-4.8412059158

LG 2.5 Nuc 3.1

grid1lg25.7

E(RB+HF-LYP) = -1626.32673925

Zero-point correction= 0.260566
 (Hartree/Particle)
 Thermal correction to Energy= 0.282576
 Thermal correction to Enthalpy= 0.283520
 Thermal correction to Gibbs Free Energy= 0.205618
 Sum of electronic and zero-point Energies= -
 1626.066173
 Sum of electronic and thermal Energies= -
 1626.044164
 Sum of electronic and thermal Enthalpies= -
 1626.043219
 Sum of electronic and thermal Free Energies= -
 1626.121122

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.319	81.444	163.959

C,O,1.0762410262,1.6750502327,-0.4590881206
 C,O,0.8083861709,0.5221457808,-1.3943231852
 O,O,1.6656515589,-0.4193688277,-1.3608519921
 C,O,2.7270025767,-0.1454151023,-0.3482319073
 C,O,2.5581291694,1.3444929623,0.0484535673
 C,O,2.5579742237,-1.1733237147,0.7625510013
 O,O,1.4392551824,-0.9599118364,1.5931843361
 N,O,-0.8923279782,-0.8097571988,-0.1359098432
 C,O,-1.3003681977,-1.9228308396,-0.8186544706
 N,O,-2.5640648811,-2.315576583,-0.6538341496
 C,O,-3.0497423549,-1.3722760559,0.2192354086
 C,O,-2.0219260185,-0.4498473605,0.5334041065
 N,O,-2.1313655463,0.6256037843,1.3849353682
 C,O,-3.3106327966,0.7569537821,1.9023360333
 N,O,-4.3696927895,-0.0862475672,1.6554789621
 C,O,-4.3535265662,-1.2347125624,0.8039149804
 O,O,-5.3828174791,-1.9060370231,0.696280195
 O,O,3.5595744892,2.156747283,-0.442625657

O,O,0.8199208766,2.9246974782,-0.9616128578
 H,O,2.5499482403,-2.1831571484,0.3128322141
 H,O,3.4484506471,-1.112831081,1.4033203189
 H,O,3.6505663167,-0.291397964,-0.9110393936
 H,O,-3.5173442738,1.5790636867,2.5868530544
 H,O,2.5549612344,1.4230162754,1.1426028046
 H,O,0.4066063877,1.4944792179,0.3956844906
 H,O,1.3279495901,3.0760052199,-1.8791504926
 H,O,3.6169891423,1.9760768894,-1.4687493735
 H,O,-5.263969588,0.0828265209,2.0991167598
 H,O,0.629154432,-0.9537673453,1.0264189932
 H,O,-0.6111078016,-2.4491663103,-1.4719564472
 O,O,1.5266295565,0.9985655586,-4.3720988962
 P,O,2.5392723814,1.9887842983,-3.8138382325
 O,O,3.5181118027,2.5043645356,-5.1020103797
 O,O,1.9317242727,3.2773827514,-3.1988613744
 O,O,3.6158466376,1.3741878253,-2.8497726758
 H,O,0.1068817495,0.5032330362,-2.2208277778
 H,O,4.3959030766,2.3666150217,-4.7134992079

LG 2.7 Nuc 1.9

grid1lg27.1

E(RB+HF-LYP) = -1626.36424458

Zero-point correction= 0.264921
 (Hartree/Particle)
 Thermal correction to Energy= 0.286396
 Thermal correction to Enthalpy= 0.287340
 Thermal correction to Gibbs Free Energy= 0.212372
 Sum of electronic and zero-point Energies= -
 1626.099324
 Sum of electronic and thermal Energies= -
 1626.077849
 Sum of electronic and thermal Enthalpies= -
 1626.076905
 Sum of electronic and thermal Free Energies= -
 1626.151872

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.716	80.930	157.783

C,O,1.1932493418,1.7656900202,-0.5527332251
 C,O,0.8966431602,0.6739119345,-1.5813234081
 O,O,1.6142428468,-0.412421751,-1.3308783063
 C,O,2.7170675279,-0.1383766368,-0.4023609236
 C,O,2.6033214782,1.3454926175,0.0226096558
 C,O,2.5834269368,-1.1486553947,0.731613301
 O,O,1.4865407494,-0.9139292603,1.5835762227
 N,O,-0.8687106759,-0.6817576086,-0.0530293918
 C,O,-1.189619207,-1.7715462869,-0.8119103917
 N,O,-2.4479910899,-2.2214283651,-0.7591293039
 C,O,-3.0255798569,-1.3503807299,0.1301518348
 C,O,-2.0492460453,-0.4129780442,0.5635523909
 N,O,-2.2607393602,0.6063742926,1.4674173645
 C,O,-3.4741005653,0.6619301525,1.9136044865
 N,O,-4.4832698273,-0.2011754059,1.5476902106
 C,O,-4.3673077593,-1.292830518,0.6317287261
 O,O,-5.3657667819,-1.9888870068,0.4162977489
 O,O,3.7038006975,2.1248829206,-0.3572234311
 O,O,1.0060861372,3.0928950588,-0.9154822402
 H,O,2.551768906,-2.1634917323,0.2912580285
 H,O,3.4917426206,-1.0909675145,1.3492694678
 H,O,3.6416029968,-0.2962350622,-0.9649891196
 H,O,-3.7577294322,1.431533682,2.6319389337
 H,O,2.5461738314,1.4062257837,1.114362284
 H,O,0.4639421353,1.5507817323,0.2404564309
 H,O,1.5682305452,3.3184336382,-1.7103308305
 H,O,3.8800137923,1.9598728594,-1.3307075363

H,0,-5.4096514849,-0.0934334989,1.9415163955
H,0,0.6733346169,-0.835400623,1.0200556759
H,0,-0.4369488029,-2.2372440306,-1.4405962166
O,0,1.373948323,1.2509962512,-3.3275055314
P,0,2.6947433691,2.1257811206,-3.5363865976
O,0,2.913206798,2.0205974329,-5.1937593344
O,0,2.4536191541,3.5845294148,-3.1893430491
O,0,3.9284170932,1.4431834601,-2.9261326684
H,0,-0.1020986675,0.4859134628,-1.9338831909
H,0,3.5158809684,1.266781255,-5.2897283014

LG 2.7 Nuc 2.1

grid1lg27.2

E(RB+HF-LYP) = -1626.35291706

Zero-point correction= 0.264082
(Hartree/Particle)
Thermal correction to Energy= 0.285625
Thermal correction to Enthalpy= 0.286569
Thermal correction to Gibbs Free Energy= 0.211431
Sum of electronic and zero-point Energies= -
1626.088835
Sum of electronic and thermal Energies= -
1626.067292
Sum of electronic and thermal Enthalpies= -
1626.066348
Sum of electronic and thermal Free Energies= -
1626.141486

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.232	81.089	158.141

C,0,1.1581783116,1.7447786428,-0.5703810639
C,0,0.8623750926,0.6211828821,-1.5538701206
O,0,1.5954059162,-0.4347317823,-1.3313647557
C,0,2.7098771376,-0.1415989717,-0.4073001371
C,0,2.5776027834,1.3440013927,0.006982093
C,0,2.5937802295,-1.1516807532,0.7279992836
O,0,1.5056026747,-0.9243595628,1.5921822084
N,0,-0.8784273283,-0.745447695,-0.0072851898
C,0,-1.2217075104,-1.8310380186,-0.7626757486
N,0,-2.4899580162,-2.2504989902,-0.7110324728
C,0,-3.0498031592,-1.3606561194,0.1711742651
C,0,-2.0544395735,-0.4440404631,0.6029893527
N,0,-2.2445835092,0.5869283995,1.4977908675
C,0,-3.4587907868,0.6760269706,1.936552233
N,0,-4.4864255387,-0.1653511357,1.5722629267
C,0,-4.3926189138,-1.2666874894,0.6653714617
O,0,-5.4056464554,-1.9403097756,0.4497448454
O,0,3.6654214973,2.131505784,-0.374052346
O,0,0.9528479529,3.0545162325,-0.9647592189
H,0,2.5670260077,-2.1675289919,0.2902950536
H,0,3.5087478941,-1.0836818733,1.3340003442
H,0,3.6218101428,-0.2914183228,-0.9906295818
H,0,-3.7272614313,1.4586029425,2.6464178187
H,0,2.5146670155,1.4054038453,1.0985387151
H,0,0.433926205,1.5364136719,0.2326434319
H,0,1.5232078139,3.2777355312,-1.7655654063
H,0,3.8398355544,1.9783900158,-1.3560185278
H,0,-5.4123717379,-0.0304580971,1.9587398898
H,0,0.679793791,-0.870651016,1.0435090137
H,0,-0.4792364843,-2.3178843308,-1.3877569409
O,0,1.4165184402,1.2145279385,-3.4905850394
P,0,2.7001662027,2.128329085,-3.5801063556
O,0,3.0716638225,2.1240946304,-5.2198003634
O,0,2.4064901683,3.5678876944,-3.1710853194
O,0,3.9329598724,1.4720870892,-2.9209207526
H,0,-0.0936709159,0.452981076,-2.0174233051

H,0,3.8192813047,1.5072971845,-5.2549149983

LG 2.7 Nuc 2.3

grid1lg27.3

E(RB+HF-LYP) = -1626.34436004

Zero-point correction= 0.263214
(Hartree/Particle)
Thermal correction to Energy= 0.284840
Thermal correction to Enthalpy= 0.285784
Thermal correction to Gibbs Free Energy= 0.210378
Sum of electronic and zero-point Energies= -
1626.081146
Sum of electronic and thermal Energies= -
1626.059520
Sum of electronic and thermal Enthalpies= -
1626.058576
Sum of electronic and thermal Free Energies= -
1626.133982

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.740	81.265	158.704

C,0,1.1222175192,1.7217694983,-0.5819955531
C,0,0.8395521087,0.5763448751,-1.5356748071
O,0,1.5988412287,-0.4488756184,-1.3437832615
C,0,2.7083100879,-0.1394594079,-0.4058079473
C,0,2.550606375,1.3462166106,0.000131327
C,0,2.5976160748,-1.1527001094,0.7265722481
O,0,1.510688933,-0.9354504467,1.5941547882
N,0,-0.8872034618,-0.8047697125,0.0137880153
C,0,-1.2566588251,-1.8882668404,-0.7322367648
N,0,-2.5330536162,-2.2790940598,-0.6713173103
C,0,-3.0696701107,-1.3692025229,0.2052217248
C,0,-2.0539882895,-0.470790007,0.625171678
N,0,-2.2171170287,0.5732541925,1.5094275103
C,0,-3.4277888722,0.6945251544,1.9505833797
N,0,-4.4746145898,-0.1278432972,1.5987042942
C,0,-4.4086434978,-1.240388855,0.70297277
O,0,-5.4363578421,-1.8937058918,0.4973618207
O,0,3.6210253744,2.1475004426,-0.3851038124
O,0,0.8974694195,3.0148421411,-1.0055772971
H,0,2.5793727014,-2.167987758,0.2875671126
H,0,3.5135343439,-1.0775789762,1.3298521687
H,0,3.6176750545,-0.2786653497,-0.9947215489
H,0,-3.6762981045,1.4908955287,2.6521070881
H,0,2.4824672918,1.4087054825,1.0915484064
H,0,0.4003726639,1.5144263886,0.2258052898
H,0,1.4773831131,3.2360212744,-1.8131836225
H,0,3.7919753091,1.9993157086,-1.375351842
H,0,-5.3963146258,0.0327955909,1.9855379762
H,0,0.678610316,-0.9044223688,1.0529552981
H,0,-0.5282230277,-2.3967920614,-1.356891991
O,0,1.457361027,1.1702905714,-3.6700455176
P,0,2.6983460804,2.117287531,-3.6241090222
O,0,3.2252401434,2.2227516408,-5.2225885672
O,0,2.3441102405,3.5327977035,-3.1591383979
O,0,3.9155207814,1.4832053928,-2.9008465914
H,0,-0.0606218388,0.4256750811,-2.1051914935
H,0,4.0605020134,1.7320400942,-5.1762313882

LG 2.7 Nuc 2.5

grid1lg27.4

E(RB+HF-LYP) = -1626.33825313

Zero-point correction= 0.262344
(Hartree/Particle)
Thermal correction to Energy= 0.284054

Thermal correction to Enthalpy= 0.284998
 Thermal correction to Gibbs Free Energy= 0.209245
 Sum of electronic and zero-point Energies= -
 1626.075909
 Sum of electronic and thermal Energies= -
 1626.054200
 Sum of electronic and thermal Enthalpies= -
 1626.053255
 Sum of electronic and thermal Free Energies= -
 1626.129008

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.246	81.395	159.434

C,0,1.1039018665,1.706775519,-0.5741808692
 C,0,0.826881884,0.5509533685,-1.5093752235
 O,0,1.6107300406,-0.4496238371,-1.3545067361
 C,0,2.7123736404,-0.1382742849,-0.3983962415
 C,0,2.5448695319,1.3492052165,-0.0009144376
 C,0,2.5937509813,-1.152163773,0.7323975608
 O,0,1.5073048245,-0.9327484335,1.599377448
 N,0,-0.8926485982,-0.8539668195,0.0266618079
 C,0,-1.2819260672,-1.937375222,-0.7094939969
 N,0,-2.564111684,-2.3055219838,-0.6409824394
 C,0,-3.0829607601,-1.3778563021,0.2279885093
 C,0,-2.052232398,-0.4926343471,0.6366853079
 N,0,-2.1946018667,0.5636257022,1.5093787515
 C,0,-3.4022893554,0.7111331529,1.9510512701
 N,0,-4.4633874852,-0.0972805292,1.610714795
 C,0,-4.4185633234,-1.2210018768,0.7275569433
 O,0,-5.4570238055,-1.8593254035,0.5315203236
 O,0,3.5989276672,2.1556244597,-0.4056970438
 O,0,0.8636686446,2.985143556,-1.0220745765
 H,0,2.5749830684,-2.1672210789,0.293380426
 H,0,3.5093046614,-1.0785206854,1.3361366009
 H,0,3.6214596421,-0.2771858294,-0.9871631374
 H,0,-3.6355228525,1.5200700649,2.6431977207
 H,0,2.4836717674,1.4160211495,1.0909270067
 H,0,0.3919183397,1.4999695464,0.2442358207
 H,0,1.4407271333,3.1972187546,-1.8495619136
 H,0,3.7523885113,2.003765192,-1.4056288604
 H,0,-5.3815311769,0.0842258627,1.9968250153
 H,0,0.6718545843,-0.9237176398,1.0623947792
 H,0,-0.5642611835,-2.4639361766,-1.3317798866
 O,0,1.4842537884,1.1231012812,-3.8525578093
 P,0,2.6777291239,2.0923911373,-3.6738402984
 O,0,3.3373477447,2.3116068082,-5.2149853959
 O,0,2.2641382529,3.4799368994,-3.1555875466
 O,0,3.8733155406,1.4721072719,-2.8923319431
 H,0,-0.0159920507,0.4291134899,-2.169072907
 H,0,4.223795838,1.9410334096,-5.0826326644

LG 2.7 Nuc 2.7

grid1lg27.5

E(RB+HF-LYP) = -1626.33405525

Zero-point correction= 0.261510
 (Hartree/Particle)
 Thermal correction to Energy= 0.283340
 Thermal correction to Enthalpy= 0.284284
 Thermal correction to Gibbs Free Energy= 0.207894
 Sum of electronic and zero-point Energies= -
 1626.072545
 Sum of electronic and thermal Energies= -
 1626.050715
 Sum of electronic and thermal Enthalpies= -
 1626.049771

Sum of electronic and thermal Free Energies= -
 1626.126162

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.799	81.494	160.778

C,0,-0.9273135293,0.3023566286,1.1380022001
 C,0,-0.7344597934,-0.2053262922,-0.2692482298
 O,0,-0.9627445747,0.652242769,-1.1835492582
 C,0,-1.4775161717,1.9356016351,-0.6124071375
 C,0,-1.6923907129,1.6818742983,0.900386151
 C,0,-0.465412256,3.0123402227,-0.9814664576
 O,0,0.7365868993,2.9608203751,-0.2524061279
 N,0,1.8809276873,0.3622484204,-0.6264724249
 C,0,2.2434484264,-0.092092726,-1.8634105479
 N,0,3.4405238592,-0.6713497518,-1.9835755038
 C,0,3.9260192069,-0.5970374924,-0.7012897742
 C,0,2.9661209088,0.0395611631,0.1261254493
 N,0,3.1031044383,0.2964785791,1.4722503793
 C,0,4.2276245839,-0.1133575963,1.26522636412
 N,0,5.2169263917,-0.7386815666,1.2406881089
 C,0,5.1777482634,-1.0390104326,-0.1568571934
 O,0,6.1545436885,-1.5928628925,-0.669377731
 O,0,-3.0217438028,1.7247804172,1.190725949
 O,0,-1.4156802449,-0.5767314798,2.0733099824
 H,0,-0.2911108866,2.9724171808,-2.0728344877
 H,0,-0.9328589162,3.9834504583,-0.7656611634
 H,0,-2.4347933728,2.0717701462,-1.1190725943
 H,0,4.4438099763,0.029234158,3.0238463381
 H,0,-1.1560944734,2.4520032504,1.4661469995
 H,0,0.1043818147,0.5715025756,1.4260130134
 H,0,-2.3488219463,-0.9432793951,1.7848410832
 H,0,-3.5451548626,1.0917894654,0.6628569826
 H,0,6.0704274873,-1.0324231357,1.6992624635
 H,0,1.1528149731,2.070348867,-0.3948511465
 H,0,1.5672600746,0.0131670886,-2.7067270162
 O,0,-2.6889721448,-1.9002249467,-1.0420368515
 P,0,-3.8089879595,-1.275958586,-0.1941783423
 O,0,-5.2584702832,-2.0018931931,-0.6826321614
 O,0,-3.6715870811,-1.5381114617,1.320743414
 O,0,-4.0896789753,0.2282400328,-0.511044464
 H,0,-0.423191149,-1.1918811749,-0.5790380973
 H,0,-5.755551895,-1.2193208604,-0.9673369516

LG 2.7 Nuc 2.9

grid1lg27.6

E(RB+HF-LYP) = -1626.33108791

Zero-point correction= 0.260743
 (Hartree/Particle)
 Thermal correction to Energy= 0.282695
 Thermal correction to Enthalpy= 0.283639
 Thermal correction to Gibbs Free Energy= 0.206560
 Sum of electronic and zero-point Energies= -
 1626.070344
 Sum of electronic and thermal Energies= -
 1626.048393
 Sum of electronic and thermal Enthalpies= -
 1626.047449
 Sum of electronic and thermal Free Energies= -
 1626.124528

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.394	81.533	162.227

C,0,-0.9314224827,0.338034724,1.1502156963
 C,0,-0.7401961952,-0.1729398757,-0.2518292229

O,0,-0.9884482757,0.6666998973,-1.1729186981
 C,0,-1.47779114,1.9638330697,-0.6073684939
 C,0,-1.7163922549,1.7078069469,0.9022563729
 C,0,-0.4399868118,3.0203823105,-0.9649186782
 O,0,0.75128233,2.948245249,-0.2206179574
 N,0,1.8797238751,0.3543156671,-0.636561612
 C,0,2.2464490819,-0.1013547869,-1.8719685886
 N,0,3.445106452,-0.6775149768,-1.9870306047
 C,0,3.9263244349,-0.6005378863,-0.7031319507
 C,0,2.9626542987,0.0339478898,0.1207550359
 N,0,3.0946788142,0.2940592163,1.4665475168
 C,0,4.2191464562,-0.111347876,1.9634519771
 N,0,5.2124151547,-0.7344459001,1.2426491336
 C,0,5.1783931654,-1.0369529984,-0.1545886223
 O,0,6.1586338586,-1.5872661592,-0.6638289212
 O,0,-3.0518091963,1.7171112018,1.2563062751
 O,0,-1.4169568232,-0.5466611948,2.077869089
 H,0,-0.2530093354,2.9764705029,-2.0538479636
 H,0,-0.8928989669,3.999892948,-0.7561978719
 H,0,-2.4249638377,2.1179208956,-1.1273116277
 H,0,4.4318148851,0.0338430661,3.0223442152
 H,0,-1.2048155491,2.4869199789,1.4790545977
 H,0,0.0949589838,0.6246823235,1.4404217288
 H,0,-2.3329942897,-0.9582580658,1.7560939546
 H,0,-3.5360966607,1.052493707,0.6254503754
 H,0,6.0657089327,-1.0243253959,1.70407808
 H,0,1.1682880948,2.0607932217,-0.379592833
 H,0,1.572680544,0.0007321661,-2.7175627279
 O,0,-2.7627274805,-2.0458929896,-1.152613686
 P,0,-3.7788571635,-1.349015825,-0.2472086936
 O,0,-5.3082552039,-1.9720978873,-0.6291043023
 O,0,-3.5761950454,-1.6006014316,1.2673226142
 O,0,-3.985241972,0.1750473109,-0.5461443413
 H,0,-0.4946104025,-1.1815247486,-0.5601337607
 H,0,-5.7848599215,-1.1498095471,-0.8218500861

LG 2.7 Nuc 3.1

grid1lg27.7

E(RB+HF-LYP) = -1626.32889260

Zero-point correction=	0.260108
(Hartree/Particle)	
Thermal correction to Energy=	0.282182
Thermal correction to Enthalpy=	0.283126
Thermal correction to Gibbs Free Energy=	0.204956
Sum of electronic and zero-point Energies=	-
1626.068784	
Sum of electronic and thermal Energies=	-
1626.046711	
Sum of electronic and thermal Enthalpies=	-
1626.045767	
Sum of electronic and thermal Free Energies=	-
1626.123937	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.072	81.513	164.524

C,0,-0.9328645498,0.3770384204,1.1454968034
 C,0,-0.7498048817,-0.1371522649,-0.2528050676
 O,0,-0.9976180613,0.6957500698,-1.1785742831
 C,0,-1.4732207502,1.999145049,-0.6151859008
 C,0,-1.7346735935,1.737375586,0.8905136944
 C,0,-0.4164912989,3.0423132934,-0.9568930407
 O,0,0.7655557702,2.9471163627,-0.2010763922
 N,0,1.8754204474,0.3523732683,-0.6509847508
 C,0,2.255529065,-0.0950775615,-1.8855143211
 N,0,3.4558794595,-0.6689423257,-1.9913559574
 C,0,3.9231620331,-0.6004082494,-0.7016983467

C,0,2.9504724354,0.0275024797,0.1160185917
 N,0,3.0674876302,0.2791515945,1.4646377458
 C,0,4.1864926858,-0.1293488019,1.97128252
 N,0,5.1878019044,-0.7471957394,1.2572370114
 C,0,5.1695690234,-1.0397730178,-0.14242309
 O,0,6.155747449,-1.5854503462,-0.6448324708
 O,0,-3.0743894844,1.7141000319,1.218393688
 O,0,-1.407572509,-0.5053634305,2.0765396307
 H,0,-0.21932781,3.0017358184,-2.0440276216
 H,0,-0.8565572103,4.0274349391,-0.7471012557
 H,0,-2.4108447763,2.1689738174,-1.1476335496
 H,0,4.3872413415,0.0086658792,3.0334151252
 H,0,-1.2470434853,2.5236985463,1.4787031244
 H,0,0.0918734797,0.6798360008,1.426145024
 H,0,-2.2978097493,-0.9710290632,1.7259473688
 H,0,-3.5182913701,1.0076314692,0.594205475
 H,0,6.0358207952,-1.0404039385,1.7262385677
 H,0,1.1774595828,2.0596053948,-0.3732349957
 H,0,1.5906733054,0.0113953171,-2.737585402
 O,0,-2.8545990987,-2.1753311866,-1.2655517902
 P,0,-3.7498562362,-1.4304832678,-0.2852701531
 O,0,-5.3408403737,-1.9620839393,-0.5372753491
 O,0,-3.4491201792,-1.6917186336,1.215281482
 O,0,-3.8983494675,0.1082759109,-0.5564677123
 H,0,-0.5399436602,-1.1564774273,0.5601549247
 H,0,-5.797237509,-1.1101953073,-0.6159261308

LG 2.9 Nuc 1.9

grid1lg29.1

E(RB+HF-LYP) = -1626.36992118

Zero-point correction=	0.264821
(Hartree/Particle)	
Thermal correction to Energy=	0.286332
Thermal correction to Enthalpy=	0.287276
Thermal correction to Gibbs Free Energy=	0.212149
Sum of electronic and zero-point Energies=	-
1626.105100	
Sum of electronic and thermal Energies=	-
1626.083589	
Sum of electronic and thermal Enthalpies=	-
1626.082645	
Sum of electronic and thermal Free Energies=	-
1626.157772	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	179.676	80.873	158.118

C,0,1.290922749,1.8321070488,-0.5991603297
 C,0,0.9455173037,0.7504088992,-1.6224654781
 O,0,1.6018471225,-0.3683879739,-1.3479880547
 C,0,2.7212772144,-0.1353499006,-0.4264084379
 C,0,2.6837243388,1.359208295,-0.0273973544
 C,0,2.5367821098,-1.1165362602,0.7270058214
 O,0,1.4655328269,-0.8025049392,1.5838467806
 N,0,-0.9456728686,-0.6863696656,0.0415839136
 C,0,-1.2632326878,-1.7196264564,-0.7918358005
 N,0,-2.5239184873,-2.1674236238,-0.7771261351
 C,0,-3.1047646156,-1.3548735215,0.1633982902
 C,0,-2.1285373676,-0.4514883142,0.6656380219
 N,0,-2.3444387982,0.5087053649,1.6315359099
 C,0,-3.5614050746,0.5389599705,2.0706137701
 N,0,-4.570019881,-0.2954546973,1.6420011336
 C,0,-4.4503787449,-1.3249125888,0.6570660966
 O,0,-5.4495399015,-2.0015177191,0.3890822002
 O,0,3.8145225232,2.0811112396,-0.4295667991
 O,0,1.1505441972,3.1645155158,-0.9605936907
 H,0,2.4423681527,-2.1350177433,0.3048859569

H,0,3.453509112,-1.101113497,1.3348629523
 H,0,3.6346940601,-0.3518053418,-0.9880373042
 H,0,-3.8492198986,1.2615749319,2.8347899621
 H,0,2.6387003338,1.4424575686,1.0632856781
 H,0,0.5565579947,1.6383118527,0.1972856251
 H,0,1.7146310878,3.3640540662,-1.7624256739
 H,0,3.9719945886,1.8996909255,-1.4029052883
 H,0,-5.499512899,-0.20976737,2.0339230346
 H,0,0.6353554233,-0.7497288548,1.0394045004
 H,0,-0.507157692,-2.1447964525,-1.4444574083
 O,0,1.4280672154,1.2750577105,-3.3836825828
 P,0,2.7769320049,2.1081576975,-3.6004691379
 O,0,2.9722128143,1.9982861825,-5.2589343079
 O,0,2.5859122688,3.5735738749,-3.2513976397
 O,0,3.9887160546,1.382264859,-2.998433134
 H,0,-0.071447515,0.5965510111,-1.9480919322
 H,0,3.5211694317,1.2063455257,-5.3691669981

LG 2.9 Nuc 2.1

grid1lg29.2

E(RB+HF-LYP) = -1626.35753217

Zero-point correction= 0.263986
 (Hartree/Particle)
 Thermal correction to Energy= 0.285562
 Thermal correction to Enthalpy= 0.286506
 Thermal correction to Gibbs Free Energy= 0.210982
 Sum of electronic and zero-point Energies= -
 1626.093546
 Sum of electronic and thermal Energies= -
 1626.071970
 Sum of electronic and thermal Enthalpies= -
 1626.071026
 Sum of electronic and thermal Free Energies= -
 1626.146550

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.193	81.030	158.954

C,0,1.254049194,1.8150508594,-0.6178149672
 C,0,0.9047984485,0.704124617,-1.5958319162
 O,0,1.5722772958,-0.3883701438,-1.3477086553
 C,0,2.7066812955,-0.1408996246,-0.4331088442
 C,0,2.6562442834,1.3568632378,-0.04480135
 C,0,2.5414846476,-1.1219679798,0.7226480228
 O,0,1.4822116637,-0.8125349589,1.5948470015
 N,0,-0.9487743554,-0.7519779486,0.0935551132
 C,0,-1.2869709624,-1.7796958958,-0.7389402617
 N,0,-2.5583280067,-2.1944915079,-0.7303777108
 C,0,-3.1237049303,-1.3644634672,0.2042982334
 C,0,-2.1292443931,-0.48345388,0.7085289556
 N,0,-2.3264521444,0.4873541823,1.6674502391
 C,0,-3.545670755,0.5520731178,2.0965994687
 N,0,-4.5719657419,-0.2589791177,1.6658708359
 C,0,-4.4716529292,-1.2980172116,0.6888699987
 O,0,-5.4855267777,-1.949165385,0.415584018
 O,0,3.777812129,2.0825052999,-0.4488490127
 O,0,1.096143512,3.1315837026,-1.0075178361
 H,0,2.4486345928,-2.1417583622,0.3040447416
 H,0,3.4675504381,-1.0977783075,1.3151565766
 H,0,3.6056682807,-0.3513533436,-1.018093268
 H,0,-3.8203094425,1.287206743,2.8534587226
 H,0,2.6057648611,1.4405784737,1.0457397373
 H,0,0.5253332421,-1.6260335786,0.1890368382
 H,0,1.6665647263,3.3284500503,-1.8167958893
 H,0,3.9322741365,1.9141845061,-1.4314514008
 H,0,-5.5021666336,-0.1454765108,2.0489913895
 H,0,0.6379550596,-0.7849130086,1.0689645022

H,0,-0.5392607131,-2.2268500634,-1.3867135436
 O,0,1.466168847,1.2351320904,-3.5484945812
 P,0,2.7787482962,2.1090461949,-3.6453688918
 O,0,3.132671587,2.0950789406,-5.2880174445
 O,0,2.5336550977,3.5565739288,-3.2325131844
 O,0,3.9925473319,1.4103961577,-2.9966313175
 H,0,-0.0717863698,0.5708900617,-2.0322965786
 H,0,3.8588196587,1.4536885945,-5.3326515812

LG 2.9 Nuc 2.3

grid1lg29.3

E(RB+HF-LYP) = -1626.34802945

Zero-point correction= 0.262972
 (Hartree/Particle)
 Thermal correction to Energy= 0.284671
 Thermal correction to Enthalpy= 0.285615
 Thermal correction to Gibbs Free Energy= 0.209405
 Sum of electronic and zero-point Energies= -
 1626.085058
 Sum of electronic and thermal Energies= -
 1626.063359
 Sum of electronic and thermal Enthalpies= -
 1626.062414
 Sum of electronic and thermal Free Energies= -
 1626.138624

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.634	81.248	160.397

C,0,1.2078682637,1.7946414043,-0.6396374558
 C,0,0.8768681993,0.664418901,-1.5928496647
 O,0,1.5653067758,-0.4030179298,-1.3691107684
 C,0,2.6945098016,-0.1394168211,-0.4361548653
 C,0,2.6155979505,1.3577297403,-0.0519886113
 C,0,2.536178176,-1.1281925674,0.712786804
 O,0,1.4794997216,-0.8322863511,1.5916067044
 N,0,-0.9550583011,-0.8061684299,0.1075662019
 C,0,-1.3183900508,-1.8410674655,-0.7054597893
 N,0,-2.5960369565,-2.2336202576,-0.6776633996
 C,0,-3.1385153677,-1.3775804165,0.2473423527
 C,0,-2.1251428273,-0.5064676302,0.728513391
 N,0,-2.2958075909,0.4843139065,1.6714653372
 C,0,-3.5098574934,0.5784292089,2.109948531
 N,0,-4.5538571746,-0.221604304,1.7023493879
 C,0,-4.4812296466,-1.2778879294,0.7414964783
 O,0,-5.5077131173,-1.9170957586,0.4896956741
 O,0,3.7242406095,2.0982994324,-0.4495390823
 O,0,1.0338720435,3.0967954063,-1.0554476093
 H,0,2.4516250261,-2.1465094666,0.2892382471
 H,0,3.4650929411,-1.0987453272,1.3003197297
 H,0,3.5922761588,-0.3358196777,-1.0267283945
 H,0,-3.7644162713,1.3315101956,2.8559287373
 H,0,2.5514315845,1.4396106754,1.0381712452
 H,0,0.4747618798,1.6041702277,0.1651404074
 H,0,1.6206212272,3.2927269326,-1.8665530432
 H,0,3.8843728741,1.9345401229,-1.4393947365
 H,0,-5.478516127,-0.0843996711,2.0911320015
 H,0,0.6298643101,-0.8211406864,1.0731568999
 H,0,-0.5853262174,-2.3124567944,-1.353141108
 O,0,1.5117424362,1.2050180066,-3.7363710975
 P,0,2.7893051142,2.1051736485,-3.6835190661
 O,0,3.3159411585,2.1972459264,-5.281135981
 O,0,2.4880422937,3.5312078208,-3.2137327725
 O,0,3.9793300684,1.4199761725,-2.9639656275
 H,0,-0.0432789852,0.5454576981,-2.1408639177
 H,0,4.1270419826,1.6668796776,-5.2429349804

LG 2.9 Nuc 2.5

grid1lg29.4

E(RB+HF-LYP) = -1626.34116574

Zero-point correction= 0.262111
 (Hartree/Particle)
 Thermal correction to Energy= 0.283914
 Thermal correction to Enthalpy= 0.284858
 Thermal correction to Gibbs Free Energy= 0.208267
 Sum of electronic and zero-point Energies= -
 1626.079055
 Sum of electronic and thermal Energies= -
 1626.057252
 Sum of electronic and thermal Enthalpies= -
 1626.056308
 Sum of electronic and thermal Free Energies= -
 1626.132899

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.159	81.426	161.200

C,0,1.1529200034,1.7661301422,-0.6592875977
 C,0,0.8586975362,0.6220674728,-1.5992534996
 O,0,1.5777591815,-0.4167674776,-1.3962427963
 C,0,2.6868831561,-0.1338600109,-0.4340787878
 C,0,2.5652488401,1.3607143998,-0.0495842634
 C,0,2.5362251978,-1.1351155761,0.7043752799
 O,0,1.4736616857,-0.8661040332,1.5838218788
 N,0,-0.95783531,-0.8640283555,0.1041913153
 C,0,-1.3550819886,-1.9024324716,-0.6883684382
 N,0,-2.6403029585,-2.265409182,-0.6369287611
 C,0,-3.1506601902,-1.383268571,0.2822001612
 C,0,-2.1124877007,-0.5277419004,0.7355286677
 N,0,-2.2468173262,0.4820265577,1.6635760318
 C,0,-3.4521651317,0.6110545896,2.1171225132
 N,0,-4.5189358582,-0.1724396653,1.7379786797
 C,0,-4.4836462018,-1.2459857362,0.7941379267
 O,0,-5.5269144405,-1.8664596944,0.5675210937
 O,0,3.6560486237,2.126243137,-0.4360725606
 O,0,0.9594379153,3.0535566913,-1.1000353204
 H,0,2.4721692706,-2.1509779553,0.2715927728
 H,0,3.4633693467,-1.0941579058,1.293734966
 H,0,3.5916058382,-0.3060702975,-1.0209331166
 H,0,-3.6790647944,1.3824757856,2.8530481097
 H,0,2.4817329223,1.4376430687,1.0396889408
 H,0,0.413119404,1.5668083071,0.1391281397
 H,0,1.5576352246,3.2476095216,-1.9182377763
 H,0,3.8222038167,1.9658425738,-1.4315224032
 H,0,-5.4346433269,-0.0078731571,2.1372190426
 H,0,0.6231913879,-0.8704362239,1.0666377289
 H,0,-0.6422315747,-2.4009522249,-1.3386369808
 O,0,1.57224221,1.1588462759,-3.9343593807
 P,0,2.7926365469,2.0906656898,-3.7221474534
 O,0,3.4885396969,2.2958961258,-5.247285707
 O,0,2.4104841874,3.4884850515,-3.2084067045
 O,0,3.947062776,1.4262629163,-2.9179514622
 H,0,0.0081944136,0.5159500568,-2.2538031019
 H,0,4.3519620908,1.8764696956,-5.1087009768

LG 2.9 Nuc 2.7

grid1lg29.5

E(RB+HF-LYP) = -1626.33640271

Zero-point correction= 0.261200
 (Hartree/Particle)
 Thermal correction to Energy= 0.283075
 Thermal correction to Enthalpy= 0.284020
 Thermal correction to Gibbs Free Energy= 0.206987

Sum of electronic and zero-point Energies= -
 1626.075203
 Sum of electronic and thermal Energies= -
 1626.053327
 Sum of electronic and thermal Enthalpies= -
 1626.052383
 Sum of electronic and thermal Free Energies= -
 1626.129415

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.632	81.504	162.128

C,0,1.1892515608,1.7816077717,-0.6190998757
 C,0,0.8686579263,0.6447263751,-1.5510485118
 O,0,1.5940861628,-0.3897281362,-1.3959923337
 C,0,2.7011961629,-0.1378838205,-0.4172777715
 C,0,2.6174617294,1.3635313411,-0.0462581389
 C,0,2.5097708625,-1.128367639,0.7249167081
 O,0,1.4521890646,-0.8194716403,1.5963737555
 N,0,-0.9617782907,-0.874795936,0.1074291693
 C,0,-1.3534145283,-1.9238254407,-0.6741900075
 N,0,-2.6370084971,-2.290680434,-0.6203263122
 C,0,-3.1524444192,-1.3993793629,0.2871932084
 C,0,-2.1191814359,-0.534199261,0.7319909198
 N,0,-2.2581668226,0.4849678586,1.6486789241
 C,0,-3.4645844647,0.6137612146,2.0996962965
 N,0,-4.5273771834,-0.1785365753,1.728300177
 C,0,-4.4865172952,-1.2627831113,0.7968937891
 O,0,-5.5262012672,-1.8911674918,0.5770761651
 O,0,3.7001318478,2.1047662744,-0.4863295925
 O,0,0.9963270076,3.0631793365,-1.0669520448
 H,0,2.4158443907,-2.1440140533,0.2978901233
 H,0,3.4352652661,-1.113537472,1.3181326236
 H,0,3.6019113537,-0.3422085059,-0.9992775075
 H,0,-3.6954106186,1.392171233,2.8268945216
 H,0,2.569763684,1.4548685068,1.044366739
 H,0,0.4709335717,1.5856939887,0.200949296
 H,0,1.5672096317,3.2364745217,-1.9258846443
 H,0,3.8067367337,1.9298297493,-1.4954175531
 H,0,-5.4440384827,-0.0138870074,2.1253338481
 H,0,0.6002107081,-0.8431771984,1.0812498731
 H,0,-0.6379636404,-2.4268691182,-1.3180738907
 O,0,1.5213514731,1.1552644615,-4.1207440999
 P,0,2.7236138949,2.0544023198,-3.785738803
 O,0,3.5371391063,2.3433504741,-5.2409657278
 O,0,2.3368984338,3.4356071813,-3.214196176
 O,0,3.8298339578,1.3512005461,-2.9370492195
 H,0,0.0636762458,0.5832698483,-2.2694273048
 H,0,4.4168706399,2.0005068215,-5.0194504623

LG 2.9 Nuc 2.9

grid1lg29.6

E(RB+HF-LYP) = -1626.33309138

Zero-point correction= 0.260414
 (Hartree/Particle)
 Thermal correction to Energy= 0.282406
 Thermal correction to Enthalpy= 0.283351
 Thermal correction to Gibbs Free Energy= 0.205792
 Sum of electronic and zero-point Energies= -
 1626.072678
 Sum of electronic and thermal Energies= -
 1626.050685
 Sum of electronic and thermal Enthalpies= -
 1626.049741
 Sum of electronic and thermal Free Energies= -
 1626.127300

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.213	81.564	163.237

C,0,1.2031244554,1.7690236367,-0.5905978236
 C,0,0.8901933466,0.640078932,-1.5272835307
 O,0,1.6198226763,-0.389885763,-1.3915027297
 C,0,2.7156210252,-0.1499390698,-0.3941580304
 C,0,2.6424552704,1.355627869,-0.0353156515
 C,0,2.5019720461,-1.1343031933,0.7495192728
 O,0,1.4435524671,-0.8081108869,1.6128153113
 N,0,-0.9525106188,-0.8890874669,0.1085919296
 C,0,-1.3495345809,-1.940625271,-0.6673931421
 N,0,-2.6353964703,-2.298116394,-0.6135541956
 C,0,-3.1468433627,-1.3969676706,0.2866596969
 C,0,-2.1092269039,-0.5358633915,0.7278743955
 N,0,-2.2426605972,0.4903343344,1.637266945
 C,0,-3.4493261892,0.6310956635,2.0841879704
 N,0,-4.5166482621,-0.1562489398,1.715708915
 C,0,-4.4811669949,-1.2477496372,0.7924951826
 O,0,-5.5242506474,-1.8709314086,0.575106705
 O,0,3.7104991013,2.0892174579,-0.5134531748
 O,0,1.0013695764,3.0470748336,-1.035546234
 H,0,2.3977006559,-2.1499847704,0.3253475999
 H,0,3.4241873968,-1.1299510435,1.3480345601
 H,0,3.6185353511,-0.3683250151,-0.9675233921
 H,0,-3.6763002649,1.4163870846,2.8050939746
 H,0,2.6159030903,1.4593526285,1.0551096289
 H,0,0.4963181162,1.5619676094,0.2369936432
 H,0,1.5325625045,3.2075314849,-1.9351804397
 H,0,3.7653420152,1.9122620389,-1.5330016647
 H,0,-5.4331629327,0.0180230648,2.1089745705
 H,0,0.5929444627,-0.8427730191,1.0952061552
 H,0,-0.6365565795,-2.4525675063,-1.3069788021
 O,0,1.5050784392,1.1369958956,-4.3174417254
 P,0,2.6506358603,2.0347600757,-3.846889341
 O,0,3.5822590914,2.4190799291,-5.2082071872
 O,0,2.2057104816,3.3865988659,-3.2355904433
 O,0,3.7076732398,1.3200649671,-2.9390745254
 H,0,0.1366956015,0.6097627714,-2.3059566668
 H,0,4.455672603,2.1208589241,-4.9106715964

LG 2.9 Nuc 3.1

grid1lg29.7

E(RB+HF-LYP) = -1626.39164653

Zero-point correction=	0.266607
(Hartree/Particle)	
Thermal correction to Energy=	0.288612
Thermal correction to Enthalpy=	0.289556
Thermal correction to Gibbs Free Energy=	0.212253
Sum of electronic and zero-point Energies=	-
1626.125040	
Sum of electronic and thermal Energies=	-
1626.103035	
Sum of electronic and thermal Enthalpies=	-
1626.102091	
Sum of electronic and thermal Free Energies=	-
1626.179393	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.107	82.311	162.697

C,0,1.5846343606,1.6399451188,-0.4256551216
 C,0,1.3466176529,0.6439606642,-1.5831414314
 O,0,1.8707828906,-0.5777932912,-1.1351714597
 C,0,2.9007816771,-0.3539085051,-0.1450517145
 C,0,2.987646479,1.1738392118,0.0519676443

C,0,2.5404787203,-1.1620347855,1.1020297496
 O,0,1.4242105769,-0.6747609079,1.8036370289
 N,0,-0.7559679663,-0.6007304217,-0.021132419
 C,0,-1.0056903436,-1.710222307,-0.7766848688
 N,0,-2.2592865435,-2.1778917101,-0.8049342608
 C,0,-2.9128142352,-1.2948642458,0.0167737451
 C,0,-1.9820167241,-0.3333369591,0.4985472993
 N,0,-2.27239125,0.6992742296,1.3652677269
 C,0,-3.515895607,0.7469772695,1.719724373
 N,0,-4.4848650041,-0.1375466183,1.2990525505
 C,0,-4.2868088011,-1.2483293007,0.4207180231
 O,0,-5.2583953165,-1.9669529688,0.1558475662
 O,0,4.0469675516,1.7516961829,-0.7092131718
 O,0,1.462030037,3.0058859283,-0.7147725454
 H,0,2.4036614475,-2.2151343521,0.7894196073
 H,0,3.3968882715,-1.1397987455,1.7948982301
 H,0,3.8589763148,-0.7224724561,-0.5439918201
 H,0,-3.8619931656,1.526711452,2.399264658
 H,0,3.1726787367,1.4384246552,1.0975034281
 H,0,0.8620554707,1.4071652447,0.3589283003
 H,0,1.8293593098,3.2116979579,-1.3096037083
 H,0,3.7352311101,1.7042886826,-1.6348334792
 H,0,-5.4394224027,-0.0349464548,1.6200914374
 H,0,0.6605716804,-0.6384385561,1.1636770986
 H,0,-0.2016682034,-2.1758075419,-1.3096037083
 O,0,0.2105521578,1.8006875257,-4.2253623418
 P,0,1.6185477815,2.1283829862,-3.8566015571
 O,0,2.6611682642,1.7066530205,-5.0903330354
 O,0,2.0851030529,3.5009098361,-3.3958986195
 O,0,2.1720982533,1.0422165697,-2.711704257
 H,0,0.3180251509,0.5138379582,-1.9051664868
 H,0,3.3503930849,2.387083254,-5.0418078841

LG 3.1 Nuc 1.9

grid1lg31.1

E(RB+HF-LYP) = -1626.37328129

Zero-point correction=	0.264552
(Hartree/Particle)	
Thermal correction to Energy=	0.286121
Thermal correction to Enthalpy=	0.287065
Thermal correction to Gibbs Free Energy=	0.211524
Sum of electronic and zero-point Energies=	-
1626.108729	
Sum of electronic and thermal Energies=	-
1626.087161	
Sum of electronic and thermal Enthalpies=	-
1626.086217	
Sum of electronic and thermal Free Energies=	-
1626.161757	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.543	80.902	158.988

C,0,1.3630087546,1.882937499,-0.6360257192
 C,0,0.9965469651,0.8133837998,-1.6639072911
 O,0,1.5912877406,-0.3316078127,-1.3599970928
 C,0,2.7116095456,-0.1363901826,-0.4285049002
 C,0,2.7279958662,1.361599196,-0.0406546563
 C,0,2.4814243838,-1.1020047992,0.7307551567
 O,0,1.429442321,-0.7359021332,1.588514719
 N,0,-1.0152551628,-0.7168988397,0.130774155
 C,0,-1.3382797612,-1.6500003099,-0.8102855974
 N,0,-2.6113502555,-2.0583395113,-0.8694209036
 C,0,-3.1934226559,-1.3262396073,0.1336614593
 C,0,-2.2061019224,-0.5067319604,0.7466549532
 N,0,-2.42122593,0.3599174205,1.7976052346
 C,0,-3.6484868552,0.3838271414,2.2076014384

N,0,-4.6682259162,-0.373116447,1.6741134007
 C,0,-4.5505080384,-1.3040320673,0.5952389571
 O,0,-5.5606420256,-1.9198580247,0.2372682166
 O,0,3.8920240447,2.0362914318,-0.4295130962
 O,0,1.2692922253,3.2189580498,-0.9960367624
 H,0,2.3415241404,-2.1171524075,0.3136790005
 H,0,3.4003850133,-1.1239650979,1.3353340995
 H,0,3.6206095239,-0.3916385575,-0.9812515082
 H,0,-3.9368200858,1.0362719063,3.0324010103
 H,0,2.6689829065,1.4540207561,1.0483449304
 H,0,0.6112647986,1.7085345926,0.1500212854
 H,0,1.8478911982,3.399727609,-1.7928452379
 H,0,4.0573613642,1.8483133595,-1.4001020052
 H,0,-5.6054998522,-0.2972818168,2.0491623058
 H,0,0.5836678303,-0.7103753841,1.0623508937
 H,0,-0.5777438232,-2.0309825493,-1.4844455367
 O,0,1.5256801027,1.2995438965,-3.4227886695
 P,0,2.8991363381,2.1001548426,-3.6161923384
 O,0,3.1149159074,1.9891116174,-5.2711660145
 O,0,2.738151807,3.5687590141,-3.2651336886
 O,0,4.0829000113,1.3419299864,-3.0000063248
 H,0,-0.0233966972,0.6976651618,-2.0022790158
 H,0,3.6641006628,1.1962378478,-5.373258697

LG 3.1 Nuc 2.1

grid1lg31.2

E(RB+HF-LYP) = -1626.36031234

Zero-point correction=	0.263705
(Hartree/Particle)	
Thermal correction to Energy=	0.285347
Thermal correction to Enthalpy=	0.286291
Thermal correction to Gibbs Free Energy=	0.210340
Sum of electronic and zero-point Energies=	-
1626.096608	
Sum of electronic and thermal Energies=	-
1626.074966	
Sum of electronic and thermal Enthalpies=	-
1626.074021	
Sum of electronic and thermal Free Energies=	-
1626.149972	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	179.058	81.061	159.852

C,0,1.3247566365,1.8798338862,-0.6712731506
 C,0,0.9557558848,0.7829590911,-1.6572417596
 O,0,1.5515857347,-0.3410905924,-1.3707471329
 C,0,2.6828832647,-0.1368715335,-0.4382523487
 C,0,2.6896831383,1.3640123,-0.059010279
 C,0,2.4617454641,-1.1045083794,0.7197692889
 O,0,1.4157525299,-0.7425463119,1.5852777375
 N,0,-1.0358718287,-0.758710528,0.1501505523
 C,0,-1.3808414068,-1.6938287351,-0.7813633247
 N,0,-2.6585469435,-2.0882474229,-0.821636263
 C,0,-3.2197956469,-1.3433361808,0.1839113976
 C,0,-2.2167613471,-0.5310704931,0.7793860906
 N,0,-2.408741087,0.3452630099,1.8265080051
 C,0,-3.6305722229,0.3855627802,2.2513896907
 N,0,-4.6649034562,-3.2004359354,-1.0637966215
 C,0,-4.5710443175,-1.3030214813,0.6619802616
 O,0,-5.5913731143,-1.9106167346,0.320772726
 O,0,3.8521285039,2.0379411344,-0.4357038304
 O,0,1.2271322243,3.2004359354,-1.0637966215
 H,0,2.3244496121,-2.1202580297,0.3038549552
 H,0,3.3862341265,-1.1210258679,1.3154121609
 H,0,3.5804561365,-0.3874346054,-1.0096966212
 H,0,-3.9013331731,1.0469977201,3.0748458713

H,0,2.6136116292,1.4567910047,1.0290590084
 H,0,0.5686408807,1.7161542445,0.116960781
 H,0,1.8243055735,3.3726903355,-1.8607541167
 H,0,4.0255848575,1.8621801178,-1.4136737736
 H,0,-5.5965085858,-0.2747392805,2.1220934352
 H,0,0.5622379823,-0.7334009921,1.0702998938
 H,0,-0.6342399098,-2.0883656895,-1.4635741534
 O,0,1.5942174756,1.2676763233,-3.5982240203
 P,0,2.9375462971,2.0990824562,-3.658709921
 O,0,3.3319608527,2.0722095463,-5.2907329175
 O,0,2.7277872957,3.554091346,-3.2521049647
 O,0,4.1093253592,1.3612093093,-2.9784972409
 H,0,-0.0170957105,0.6902661504,-2.1159435879
 H,0,4.0420917604,1.4120885591,-5.3169942344

LG 3.1 Nuc 2.3

grid1lg31.3

E(RB+HF-LYP) = -1626.35037102

Zero-point correction=	0.262848
(Hartree/Particle)	
Thermal correction to Energy=	0.284579
Thermal correction to Enthalpy=	0.285524
Thermal correction to Gibbs Free Energy=	0.209089
Sum of electronic and zero-point Energies=	-
1626.087523	
Sum of electronic and thermal Energies=	-
1626.065792	
Sum of electronic and thermal Enthalpies=	-
1626.064847	
Sum of electronic and thermal Free Energies=	-
1626.141282	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.576	81.234	160.870

C,0,1.2955840755,1.8792560834,-0.6948099335
 C,0,0.9232079033,0.7663871484,-1.6518859562
 O,0,1.5285987229,-0.3416105035,-1.3912776264
 C,0,2.6619050605,-0.1352974688,-0.4463707067
 C,0,2.6615285069,1.3669421809,-0.0722226984
 C,0,2.439711123,-1.1059854929,0.7082798237
 O,0,1.4017778787,-0.7424816847,1.5818549623
 N,0,-1.0503439413,-0.7896243717,0.1630293011
 C,0,-1.4098221927,-1.7343228063,-0.7535983761
 N,0,-2.6895393024,-2.122127855,-0.7751828249
 C,0,-3.2360724297,-1.3622667916,0.2274046118
 C,0,-2.2235311454,-0.5476679835,0.8018004376
 N,0,-2.3992337456,0.3429304861,1.8394457845
 C,0,-3.6161992515,0.3946915253,2.2770801483
 N,0,-4.6593778461,-0.3562936711,1.7828708374
 C,0,-4.5818052118,-1.3101290615,0.7204363276
 O,0,-5.6080008884,-1.9173474625,0.3980574312
 O,0,3.8195060176,2.0407511872,-0.4459663181
 O,0,1.1986318437,3.1874008246,-1.113171541
 H,0,2.2971816197,-2.1200294616,0.2907054814
 H,0,3.368748398,-1.1264515597,1.296293112
 H,0,3.5527065879,-0.3836670459,-1.0279808859
 H,0,-3.8746685148,1.0682809626,3.0944900243
 H,0,2.5754073627,1.4592074986,1.0153032991
 H,0,0.5357351193,1.7239941925,0.0949566223
 H,0,1.8128265804,3.3486970947,-1.9124297421
 H,0,3.9931166162,1.8656835452,-1.4309309391
 H,0,-5.5861593351,-0.257958991,2.17807849
 H,0,0.5415424851,-0.7472218379,1.0774244914
 H,0,-0.6734043951,-2.1418819629,-1.4394552197
 O,0,1.6424686552,1.2563413144,-3.7808778555
 P,0,2.9629223277,2.0916668205,-3.6995785695

O,0,3.5246394198,2.1552848136,-5.2860519752
 O,0,2.7218264253,3.5310247227,-3.23617125
 O,0,4.0988085776,1.346708919,-2.9545031002
 H,0,0.0041417403,0.6960245179,-2.2129918289
 H,0,4.3078796225,1.5857597943,-5.2326170375

LG 3.1 Nuc 2.5

grid1lg31.4

E(RB+HF-LYP) = -1626.34306712

Zero-point correction= 0.261844
 (Hartree/Particle)
 Thermal correction to Energy= 0.283683
 Thermal correction to Enthalpy= 0.284627
 Thermal correction to Gibbs Free Energy= 0.207645
 Sum of electronic and zero-point Energies= -
 1626.081223
 Sum of electronic and thermal Energies= -
 1626.059384
 Sum of electronic and thermal Enthalpies= -
 1626.058440
 Sum of electronic and thermal Free Energies= -
 1626.135422

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.014	81.416	162.022

C,0,1.2770385635,1.8673843682,-0.6951487508
 C,0,0.910043367,0.7489709148,-1.6391431925
 O,0,1.5340296756,-0.3444410656,-1.409823578
 C,0,2.6591682247,-0.1384681583,-0.4421162513
 C,0,2.652095962,1.3649827063,-0.0751687133
 C,0,2.4265301569,-1.1101894156,0.7089029549
 O,0,1.393471452,-0.7415593092,1.5848962193
 N,0,-1.0522050404,-0.8208525377,0.1761342607
 C,0,-1.4230975781,-1.7738854831,-0.7275956088
 N,0,-2.7059387123,-2.1500972635,-0.7396925772
 C,0,-3.2422469291,-1.3723319389,0.254799067
 C,0,-2.2212264505,-0.5596679335,0.8154511649
 N,0,-2.3848026921,0.3459987989,1.8417091461
 C,0,-3.5999047663,0.4149519558,2.2822755917
 N,0,-4.6513092804,-0.3328493791,1.8013032388
 C,0,-4.5860548481,-1.3013573459,0.7513831625
 O,0,-5.6182202185,-1.9037104646,0.4403048811
 O,0,3.7989091997,2.041723756,-0.4638381254
 O,0,1.1692206848,3.1663677429,-1.1269883293
 H,0,2.2780239327,-2.1225058941,0.2896293266
 H,0,3.3569926466,-1.1376115897,1.2943638384
 H,0,3.5495393349,-0.3879809467,-1.0232487815
 H,0,-3.8494342794,1.1018265534,3.0912557373
 H,0,2.5698052307,1.4609424785,1.0125117994
 H,0,0.5205593547,1.706185734,0.0986172496
 H,0,1.7844272179,3.3225016567,-1.9436734208
 H,0,3.9561371266,1.864964373,-1.4584176985
 H,0,-5.575953453,-0.2202790451,2.1979770144
 H,0,0.5293711051,-0.7586610897,1.0863604148
 H,0,-0.6933500502,-2.1967654576,-1.4114670818
 O,0,1.662928802,1.2334283728,-3.9733372672
 P,0,2.9444922061,2.0772683472,-3.7462231074
 O,0,3.6588513182,2.2487330858,-5.2653568021
 O,0,2.6559245665,3.4940625989,-3.2229593208
 O,0,4.0435053286,1.3255552751,-2.9428665623
 H,0,0.0536844808,0.7010648887,-2.2944247373
 H,0,4.4812388305,1.7509683309,-5.1367190015

LG 3.1 Nuc 2.7

grid1lg31.5

E(RB+HF-LYP) = -1626.33796834

Zero-point correction= 0.260863
 (Hartree/Particle)
 Thermal correction to Energy= 0.282765
 Thermal correction to Enthalpy= 0.283709
 Thermal correction to Gibbs Free Energy= 0.206434
 Sum of electronic and zero-point Energies= -
 1626.077105
 Sum of electronic and thermal Energies= -
 1626.055203
 Sum of electronic and thermal Enthalpies= -
 1626.054259
 Sum of electronic and thermal Free Energies= -
 1626.131534

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.438	81.531	162.639

C,0,1.2854390054,1.8581882596,-0.6653467615
 C,0,0.9219651842,0.7443672809,-1.6073548251
 O,0,1.5633073039,-0.3380698447,-1.4150414613
 C,0,2.6751348616,-0.1440855176,-0.4216587009
 C,0,2.675392994,1.3622331482,-0.0650574467
 C,0,2.4167495216,-1.1111440956,0.7277048154
 O,0,1.386385012,-0.7243341973,1.5979957969
 N,0,-1.0435644709,-0.8492633572,0.1834641379
 C,0,-1.421691299,-1.8043708768,-0.7153792308
 N,0,-2.708404373,-2.1657651072,-0.7292753563
 C,0,-3.2396161786,-1.374500839,0.2573759934
 C,0,-2.2121375036,-0.56939103,0.8159723269
 N,0,-2.3683678899,0.3452243189,1.8351984605
 C,0,-3.5842378658,0.4314742047,2.2707149419
 N,0,-4.642221543,-0.3077091913,1.7912698236
 C,0,-4.5843596617,-1.2848976141,0.748895394
 O,0,-5.6217082637,-1.8783551778,0.4389631363
 O,0,3.8058922281,2.0356755223,-0.4930757288
 O,0,1.1659496923,3.1511047309,-1.1011216986
 H,0,2.2542430396,-2.1211350871,0.3086040271
 H,0,3.3445200851,-1.153509354,1.3166702433
 H,0,3.5665606452,-0.4063854679,-0.9949312884
 H,0,-3.8286203849,1.1270563824,3.0737230231
 H,0,2.6151265689,1.4666571491,1.0234785532
 H,0,0.5407295677,1.6852643485,0.1384227343
 H,0,1.7517790895,3.295666197,-1.9594459101
 H,0,3.9145557375,1.8552401995,-1.5010421588
 H,0,-5.5669608006,-0.1814568859,2.183602196
 H,0,0.520832684,-0.7584861367,1.1017998512
 H,0,-0.6949397525,-2.2400513186,-1.3944804295
 O,0,1.6302899919,1.2095898745,-4.1709155791
 P,0,2.868172693,2.0486889161,-3.8065518045
 O,0,3.7209509566,2.3103454308,-5.242190039
 O,0,2.5355929708,3.4439259449,-3.2339139492
 O,0,3.9217655575,1.2861995017,-2.9432266048
 H,0,0.1292620172,0.7268480952,-2.3428845844
 H,0,4.5684770495,1.8938292134,-5.0212957372

LG 3.1 Nuc 2.9

grid1lg31.6

E(RB+HF-LYP) = -1626.33455597

Zero-point correction= 0.260041
 (Hartree/Particle)
 Thermal correction to Energy= 0.282081
 Thermal correction to Enthalpy= 0.283025
 Thermal correction to Gibbs Free Energy= 0.204713
 Sum of electronic and zero-point Energies= -
 1626.074515

Sum of electronic and thermal Energies= -
1626.052475
Sum of electronic and thermal Enthalpies= -
1626.051531
Sum of electronic and thermal Free Energies= -
1626.129843

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.008	81.556	164.821

C,0,1.3482617929,1.8391420315,-0.6105780983
C,0,0.9794046973,0.7455098362,-1.5640914329
O,0,1.6093406382,-0.3438120055,-1.3945494222
C,0,2.7062684224,-0.1797626584,-0.3795191658
C,0,2.7530729555,1.3333731559,-0.0495563494
C,0,2.3953939923,-1.1201716046,0.7797758395
O,0,1.3642097702,-0.6829435065,1.6241193081
N,0,-1.0304515661,-0.8529766763,0.1723729656
C,0,-1.3990107174,-1.8375333243,-0.6984341428
N,0,-2.6834217199,-2.2059309162,-0.7071275484
C,0,-3.2239101445,-1.3870608194,0.2517699362
C,0,-2.2038915264,-0.5596903766,0.7902458096
N,0,-2.3691823877,0.3846120743,1.7803375073
C,0,-3.587782348,0.4786203693,2.2065843732
N,0,-4.6395878301,-0.2799295284,1.744546763
C,0,-4.571715043,-1.2890191576,0.7335945139
O,0,-5.6042741785,-1.8973778608,0.4374785089
O,0,3.8677236328,1.9766371622,-0.5487282156
O,0,1.2179938927,3.1356997194,-1.0206549376
H,0,2.2042049406,-2.1300718414,0.3734448766
H,0,3.3116116689,-1.1859001488,1.3846045925
H,0,3.5966297496,-0.4858658893,-0.9327236775
H,0,-3.8395081754,1.1974435857,2.9864598694
H,0,2.7395480998,1.4608394659,1.0384421097
H,0,0.6254247124,1.641420213,0.2083742134
H,0,1.7325357407,3.2784493281,-1.9356370134
H,0,3.8759542614,1.8103808846,-1.5728940704
H,0,-5.567088285,-0.1456426981,2.1275967341
H,0,0.5027478033,-0.7343940318,1.1206851852
H,0,-0.6670030382,-2.2889231399,-1.3614576104
O,0,1.5222217545,1.2427369557,-4.3691055799
P,0,2.7233399127,2.0528036417,-3.880206912
O,0,3.6874292237,2.3904059626,-5.2295879707
O,0,2.3711902153,3.4234023938,-3.248955426
O,0,3.7206477405,1.2523031772,-2.9762127741
H,0,0.2503800313,0.7740680141,-2.367824144
H,0,4.5435357811,2.0538258387,-4.922922455

LG 3.1 Nuc 3.1

grid1lg31.7

E(RB+HF-LYP) = -1626.39811486

Zero-point correction=	0.266612
(Hartree/Particle)	
Thermal correction to Energy=	0.288654
Thermal correction to Enthalpy=	0.289598
Thermal correction to Gibbs Free Energy=	0.212338
Sum of electronic and zero-point Energies=	-
1626.131503	
Sum of electronic and thermal Energies=	-
1626.109461	
Sum of electronic and thermal Enthalpies=	-
1626.108517	
Sum of electronic and thermal Free Energies=	-
1626.185777	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
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Total	181.133	82.265	162.608
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C,0,1.748620647,1.7660045906,-0.3916672514
C,0,1.4535779829,0.8087100489,-1.5685485691
O,0,1.8783476545,-0.4546701003,-1.1272288003
C,0,2.908087013,-0.3194912885,-0.118927179
C,0,3.1108353644,1.1954691225,0.0881894621
C,0,2.46404522,-1.103103273,1.1177081946
O,0,1.3727978658,-0.5394998138,1.799238715
N,0,-0.837940959,-0.5487743287,0.0176945958
C,0,-1.0312399136,-1.600829841,-0.829221515
N,0,-2.2661185771,-2.1099180107,-0.9197931526
C,0,-2.966288341,-1.3200414367,-0.044019436
C,0,-2.0812778366,-0.3662100997,0.5316012331
N,0,-2.427791712,0.5853563032,1.4677468863
C,0,-3.6787417423,0.5589530834,-1.7980955331
N,0,-4.6051544913,-0.3253469083,1.289953976
C,0,-4.3483190855,-1.3554126118,0.3319981269
O,0,-5.2869463609,-2.0850616321,-0.0104241125
O,0,4.214711902,1.6977135401,-0.6612794421
O,0,1.7197553713,3.1411063625,-0.6587924051
H,0,2.2580103711,-2.1425199836,0.7983677942
H,0,3.3066594671,-1.1432573012,1.8264663845
H,0,3.8400104422,-0.76035044,-0.505842637
H,0,-4.0674227109,1.270273496,2.5278744308
H,0,3.3073936502,1.4390020026,1.1368456203
H,0,1.006767948,1.5654065431,0.3856514898
H,0,2.1015043861,3.3342076722,-1.549962496
H,0,3.9128514617,1.6907269223,-1.5908996539
H,0,-5.5685875376,-0.2838140268,1.5979982046
H,0,0.6036352889,-0.5084691583,1.1642177426
H,0,-0.2001860422,-1.9904142634,-1.4069938516
O,0,0.3941285784,2.0544375394,-4.202123916
P,0,1.8235145673,2.3004283804,-3.8225284347
O,0,2.8121818165,1.7903126275,-5.0633567764
O,0,2.3656214636,3.624937762,-3.3428078729
O,0,2.3003325829,1.1554324754,-2.6894049372
H,0,0.414102188,0.7580993047,-1.883427581
H,0,2.3107665473,1.085274361,-5.5027322104

C. ANDN mechanism – arsenate grid – B3LYP/6-31G*

LG 1.9 Nuc 1.9

grid1aslg19.1

E(RB+HF-LYP) = -3518.62814138

Zero-point correction=	0.262098
(Hartree/Particle)	
Thermal correction to Energy=	0.284293
Thermal correction to Enthalpy=	0.285237
Thermal correction to Gibbs Free Energy=	0.208041
Sum of electronic and zero-point Energies=	-
3518.366043	
Sum of electronic and thermal Energies=	-
3518.343848	
Sum of electronic and thermal Enthalpies=	-
3518.342904	
Sum of electronic and thermal Free Energies=	-
3518.420100	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.397	83.645	162.474

C,0,0.8192244506,1.5005557517,-0.3329002415
C,0,0.466598737,0.325635823,-1.2849794797

O,0,1.3507992496,-0.7141147969,-1.1237252772
 C,0,2.6191976225,-0.1866379114,-0.6553659697
 C,0,2.3149817978,1.1343879898,0.0902354053
 C,0,3.2403914853,-1.2840822781,0.1955380568
 O,0,2.4180712552,-1.6793829971,1.2910189742
 N,0,-0.8644051627,-0.5476170529,-0.2477441527
 C,0,-0.9711497542,-1.9095717051,-0.2081984251
 N,0,-2.1115740392,-2.4144190563,0.2670347881
 C,0,-2.8321066632,-1.2860814921,0.5612415457
 C,0,-2.0681964896,-0.134975689,0.2386445372
 N,0,-2.4711752263,1.1691361469,0.4006114266
 C,0,-3.6615416946,1.2878926253,0.8910494092
 N,0,-4.4767115105,0.231529507,1.2337386569
 C,0,-4.1531334485,-1.1529424024,1.1093318153
 O,0,-4.9871660535,-1.9922795666,1.4604262051
 O,0,3.3004675221,2.1150584187,-0.0840379368
 O,0,0.5396989792,2.7975043397,-0.738109715
 H,0,3.4702200313,-2.1562652916,-0.4427274026
 H,0,4.184991354,-0.9136682699,0.6121498094
 H,0,3.2456101718,0.0288223903,-1.5263523874
 H,0,-4.0837851432,2.2779824126,1.0603097137
 H,0,2.2856699077,0.924941013,1.1679584645
 H,0,0.2108450437,1.3656129814,0.5640753832
 H,0,1.0243448941,3.0809255787,-1.5641696536
 H,0,3.619206887,2.1106613163,-1.041102996
 H,0,-5.3990757187,0.4065238218,1.6130298436
 H,0,1.5089979018,-1.6449372383,0.9436041479
 H,0,-0.1591079993,-2.5290259555,-0.5679778408
 O,0,1.3752399806,0.9629320174,-2.8271286843
 As,0,2.4781050079,2.1936600564,-3.2694467558
 O,0,2.7670849712,1.9559057112,-5.0481535659
 O,0,1.8187659585,3.7071951043,-3.0165330825
 O,0,4.0318840635,1.9063828301,-2.6568216568
 H,0,-0.2702441767,0.30316107,-2.0610889653
 H,0,3.6812202779,1.6262624176,-5.013767834

LG 1.9 Nuc 2.1

grid1aslg19.4
 E(RB+HF-LYP) = -3518.63687328

Zero-point correction= 0.261539
 (Hartree/Particle)
 Thermal correction to Energy= 0.283730
 Thermal correction to Enthalpy= 0.284675
 Thermal correction to Gibbs Free Energy= 0.208433
 Sum of electronic and zero-point Energies= -
 3518.375335
 Sum of electronic and thermal Energies= -
 3518.353143
 Sum of electronic and thermal Enthalpies= -
 3518.352199
 Sum of electronic and thermal Free Energies= -
 3518.428441

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.044	83.626	160.465

C,0,0.8102387371,1.4911559684,-0.347454259
 C,0,0.4369558632,0.284118676,-1.2445687519
 O,0,1.3331342771,-0.7297462238,-1.1096078718
 C,0,2.6118743774,-0.1920338084,-0.6627188698
 C,0,2.3084105114,1.1321418405,0.0783254175
 C,0,3.2599522912,-1.278078249,0.1777572574
 O,0,2.4620867837,-1.6854059157,1.2884354709
 N,0,-0.9403316142,-0.5705764965,-0.2533205207
 C,0,-1.0306254487,-1.9310679592,-0.183514843
 N,0,-2.1563337308,-2.4261234293,0.3306522225
 C,0,-2.8772924737,-1.2941704254,0.6139766949

C,0,-2.1327196081,-0.1456244933,0.246901941
 N,0,-2.5375156411,1.1591696167,0.384377167
 C,0,-3.716919524,1.282265056,0.9002120286
 N,0,-4.5160370005,0.2298991537,1.2879067707
 C,0,-4.1865989504,-1.1554319056,1.1898570687
 O,0,-5.0047623697,-1.9914645159,1.5804248441
 O,0,3.2895290043,2.110801815,-0.0979512219
 O,0,0.519622055,2.7648592707,-0.8042389287
 H,0,3.4928720417,-2.1480676571,-0.4617355689
 H,0,4.2048255785,-0.8912903513,0.5778418996
 H,0,3.2091473223,0.0260450415,-1.5531399573
 H,0,-4.1411999645,2.2736097808,1.0548325408
 H,0,2.2760314373,0.9226218775,1.1567824119
 H,0,0.2073672844,1.3840814068,0.5595823586
 H,0,1.0344068739,3.0437668133,-1.6220987785
 H,0,3.6149378742,2.1100610774,-1.0603136024
 H,0,-5.4300840247,0.4088855421,1.6851770433
 H,0,1.5476571945,-1.6717478674,0.9555251376
 H,0,-0.2198438235,-2.5503143228,-0.5458191853
 O,0,1.4635693157,0.9146154234,-2.9646081124
 As,0,2.5341462913,2.1835600823,-3.3171924101
 O,0,2.9498545874,2.0663825883,-5.0885224845
 O,0,1.8334518285,3.6754575087,-3.0203914064
 O,0,4.0688283485,1.9245897826,-2.6337060253
 H,0,-0.2029191492,0.3186350984,-2.1043986942
 H,0,3.8865279147,1.819087821,-5.0036124234

LG 1.9 Nuc 2.3

grid1aslg19.5
 E(RB+HF-LYP) = -3518.64284228

Zero-point correction= 0.260893
 (Hartree/Particle)
 Thermal correction to Energy= 0.283113
 Thermal correction to Enthalpy= 0.284057
 Thermal correction to Gibbs Free Energy= 0.207583
 Sum of electronic and zero-point Energies= -
 3518.381949
 Sum of electronic and thermal Energies= -
 3518.359729
 Sum of electronic and thermal Enthalpies= -
 3518.358785
 Sum of electronic and thermal Free Energies= -
 3518.435259

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.656	83.605	160.953

C,0,0.8188107544,1.4814267579,-0.3216778331
 C,0,0.420903985,0.2618531345,-1.1880593208
 O,0,1.3268261982,-0.7373105576,-1.0836600427
 C,0,2.6179526072,-0.1956073344,-0.6647366657
 C,0,2.3252942731,1.1268267431,0.0828027225
 C,0,3.2919764791,-1.2800751233,0.1554946087
 O,0,2.5228028099,-1.6974389351,1.2833715757
 N,0,-0.9870824423,-0.5858656395,-0.2346738151
 C,0,-1.0657992035,-1.9442657813,-0.1358474618
 N,0,-2.1877759348,-2.4288180043,0.3931585463
 C,0,-2.913457808,-1.2930906974,0.6515041776
 C,0,-2.1779165102,-0.1491772859,0.257005073
 N,0,-2.5864543538,1.1562856704,0.3626114783
 C,0,-3.7659980278,1.2856388036,0.8770967464
 N,0,-4.558867207,0.2390711785,1.2911288091
 C,0,-4.22325255,-1.1468173904,1.2255940057
 O,0,-5.0358130715,-1.9776190624,1.6362333139
 O,0,3.2966831343,2.1075099896,-0.1121404017
 O,0,0.5264236163,2.7406516092,-0.8104826304
 H,0,3.5164171339,-2.1461967281,-0.4916498705

H,0,4.2422583052,-0.8869568901,0.5353578303
 H,0,3.185687534,0.0253163664,-1.5739646474
 H,0,-4.1947375788,2.2782892483,1.0080413462
 H,0,2.3100714684,0.9152721999,1.1616697013
 H,0,0.2293298127,1.391133335,0.5974620571
 H,0,1.0453363269,3.0086449122,-1.6399932177
 H,0,3.6021384009,2.1159542896,-1.0865817322
 H,0,-5.4737221212,0.4232150274,1.6842492454
 H,0,1.6023159999,-1.6995598816,0.9683619088
 H,0,-0.2515191178,-2.5653748192,-0.4866092252
 O,0,1.5087937257,0.8316629295,-3.1327460213
 As,0,2.537579595,2.1485108479,-3.368403731
 O,0,3.0533551756,2.1732696794,-5.1204604267
 O,0,1.7865326755,3.606629787,-3.0094271359
 O,0,4.0553739302,1.9194048894,-2.6300463111
 H,0,-0.1425672104,0.3451098913,-2.1006511624
 H,0,4.0043436657,2.0171644602,-4.9896653338

LG 1.9 Nuc 2.5

grid1aslg19.6

E(RB+HF-LYP) = -3518.64651502

Zero-point correction= 0.260278
 (Hartree/Particle)
 Thermal correction to Energy= 0.282569
 Thermal correction to Enthalpy= 0.283513
 Thermal correction to Gibbs Free Energy= 0.206577
 Sum of electronic and zero-point Energies= -
 3518.386237
 Sum of electronic and thermal Energies= -
 3518.363946
 Sum of electronic and thermal Enthalpies= -
 3518.363002
 Sum of electronic and thermal Free Energies= -
 3518.439938

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.315	83.570	161.924

C,0,0.8325691711,1.4751074302,-0.2761316002
 C,0,0.4254798595,0.2535505401,-1.1329594717
 O,0,1.3374046511,-0.7407487241,-1.0375976689
 C,0,2.6372656853,-0.1909077574,-0.6455169141
 C,0,2.3494539312,1.1316019245,0.1031520868
 C,0,3.3323278311,-1.270787391,0.1621917152
 O,0,2.5772103543,-1.6970249636,1.2970631081
 N,0,-1.0187787063,-0.5947610563,-0.2360298365
 C,0,-1.1024419679,-1.9522567578,-0.1427968797
 N,0,-2.2281346546,-2.4279228335,0.384049608
 C,0,-2.9464467893,-1.2874110484,0.6446409935
 C,0,-2.2049650736,-0.1464313088,0.2549766572
 N,0,-2.602119114,1.1610496574,0.3649660467
 C,0,-3.7809084971,1.2966733478,0.8801292908
 N,0,-4.5809481872,0.2543245959,1.2899871855
 C,0,-4.2554075572,-1.133858374,1.2196521618
 O,0,-5.072332488,-1.9604430025,1.6285194395
 O,0,3.3052599619,2.1180994596,-0.1206257048
 O,0,0.5323298285,2.7229628086,-0.7823369899
 H,0,3.5569075901,-2.1331615309,-0.4893630445
 H,0,4.2825614447,-0.8698146751,0.5332176131
 H,0,3.1821193992,0.030396797,-1.5691519216
 H,0,-4.2021098991,2.2919030439,1.014829597
 H,0,2.3551727594,0.9231227274,1.1828954514
 H,0,0.257931471,1.3877069909,0.6540944706
 H,0,1.0284304215,2.9699382664,-1.6438755554
 H,0,3.5750887465,2.1229581606,-1.1095613146
 H,0,-5.4943148389,0.4438096225,1.6841063032
 H,0,1.6554546685,-1.7101748453,0.9857349113

H,0,-0.289580344,-2.5750603518,-0.4933611653
 O,0,1.527045684,0.7116074402,-3.3299423829
 As,0,2.5012848898,2.0790453885,-3.4279568566
 O,0,3.1018371631,2.2534362301,-5.1457944918
 O,0,1.692553574,3.496560283,-3.0163780606
 O,0,3.9999497029,1.8845145243,-2.6363775349
 H,0,-0.0592470235,0.3762383672,-2.0908617791
 H,0,4.0543408218,2.1708246345,-4.9679213065

LG 1.9 Nuc 2.7

grid1aslg19.7

E(RB+HF-LYP) = -3518.64853511

Zero-point correction= 0.259903
 (Hartree/Particle)
 Thermal correction to Energy= 0.282239
 Thermal correction to Enthalpy= 0.283183
 Thermal correction to Gibbs Free Energy= 0.205494
 Sum of electronic and zero-point Energies= -
 3518.388632
 Sum of electronic and thermal Energies= -
 3518.366297
 Sum of electronic and thermal Enthalpies= -
 3518.365352
 Sum of electronic and thermal Free Energies= -
 3518.443041

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.107	83.458	163.510

C,0,0.8518625198,1.476059135,-0.2316107481
 C,0,0.4479791811,0.2631818527,-1.098250799
 O,0,1.3627573402,-0.7292902011,-1.0145845007
 C,0,2.6631445163,-0.1860975065,-0.6069181982
 C,0,2.3786945217,1.1469995783,0.1262245442
 C,0,3.3377446736,-1.2663795537,0.2171908531
 O,0,2.5617815365,-1.6756516639,1.3438849369
 N,0,-1.0269268969,-0.5931905092,-0.2608300177
 C,0,-1.1226050087,-1.9515369805,-0.2004179397
 N,0,-2.2520638047,-2.4250967086,0.3186589465
 C,0,-2.9566210743,-1.2828047578,0.6090955805
 C,0,-2.2051353145,-0.1406549452,0.2449224358
 N,0,-2.5856158875,1.1679040598,0.3884584175
 C,0,-3.7612131629,1.304073721,0.9109553013
 N,0,-4.5715151013,0.2610987227,1.2979528529
 C,0,-4.2614337468,-1.1285200924,1.193799135
 O,0,-5.0854670605,-1.9558310953,1.5856278838
 O,0,3.3184236599,2.1351847989,-0.1434539776
 O,0,0.546854065,2.719781814,-0.7400513282
 H,0,3.5632216083,-2.1357465719,-0.4244483177
 H,0,4.2864470523,-0.8720082084,0.5991716302
 H,0,3.2205554265,0.0256646282,-1.526953421
 H,0,-4.1704380758,2.3004312415,1.0712734998
 H,0,2.4087464849,0.9606198272,1.2095004512
 H,0,0.287869735,1.3792683626,0.7047322965
 H,0,1.0084081532,2.9356185763,-1.63865816
 H,0,3.5415581374,2.1244363083,-1.147244231
 H,0,-5.4814192218,0.4512065218,1.6997482795
 H,0,1.6459558303,-1.6926225197,1.0153619001
 H,0,-0.3160829206,-2.5731717863,-0.567055834
 O,0,1.5034146454,0.6046151502,-3.5598498732
 As,0,2.4370386868,1.9969876176,-3.5017988056
 O,0,3.1125133759,2.3216010376,-5.1705505538
 O,0,1.5857791214,3.3747155684,-3.0303435863
 O,0,3.9113668866,1.8080791539,-2.658354397
 H,0,0.0194375101,0.4115064021,-2.0849439103
 H,0,4.0572270778,2.3042366425,-4.9405741859

LG 1.9 Nuc 2.9

grid1aslg19.8
E(RB+HF-LYP) = -3518.65067929

Zero-point correction= 0.259868
(Hartree/Particle)
Thermal correction to Energy= 0.282049
Thermal correction to Enthalpy= 0.282993
Thermal correction to Gibbs Free Energy= 0.206560
Sum of electronic and zero-point Energies= -
3518.390812
Sum of electronic and thermal Energies= -
3518.368630
Sum of electronic and thermal Enthalpies= -
3518.367686
Sum of electronic and thermal Free Energies= -
3518.444119

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.988	83.059	160.867

C,0,0.9686130119,1.6214242366,-0.2933951425
C,0,0.61845107,0.4345059533,-1.2159661614
O,0,1.5877495336,-0.4804971198,-1.2391378905
C,0,2.6815749729,-0.1513098133,-0.3241888102
C,0,2.4897126379,1.3311292175,0.0872628458
C,0,2.6804077942,-1.167854396,0.8078777331
O,0,1.5607858978,-1.0685855918,1.6821123949
N,0,-0.8140630409,-0.5283906128,-0.4217838642
C,0,-1.0193370929,-1.8254610085,-0.8055030171
N,0,-2.159503556,-2.3732197628,-0.4020372826
C,0,-2.7637721455,-1.3498369137,0.2878844243
C,0,-1.9424831801,-0.1999043967,0.2723684082
N,0,-2.2143497447,1.004456638,0.8675740864
C,0,-3.3563862963,1.029710416,1.4757667011
N,0,-4.229379229,-0.0305529809,1.5440165261
C,0,-4.0286442654,-1.3235154188,0.9720020011
O,0,-4.8941891741,-2.1854731004,1.1251758498
O,0,3.4369282359,2.1815930313,-0.464358844
O,0,0.6711069979,2.8707133764,-0.7941938893
H,0,2.7525256935,-2.1839662111,0.3804628137
H,0,3.5702161053,-1.0069756435,1.4299265846
H,0,3.5823709325,-0.2422906318,-0.9363284028
H,0,-3.6806373825,1.9379292985,1.9815181005
H,0,2.5719445412,1.4165718829,1.1800572664
H,0,0.3871691969,1.4905801352,0.6266952055
H,0,1.1207129036,3.0325425742,-1.7181342302
H,0,3.514315337,1.9602255018,-1.4732649865
H,0,-5.1065431265,0.0688301114,2.040215905
H,0,0.7648060761,-1.0638442279,1.1206457637
H,0,-0.2764901794,-2.3380032033,-1.4035023621
O,0,1.0520324496,0.6919815671,-4.0717842705
As,0,2.2346814796,1.8337602232,-3.7557958049
O,0,3.0831077392,2.2233566102,-5.3310213601
O,0,1.6511244383,3.2979301309,-3.1420727495
O,0,3.5952966228,1.2928582969,-2.8695666323
H,0,0.177906123,0.5889059917,-2.2047595336
H,0,3.9944830922,2.07534346,-5.025101216

LG 1.9 Nuc 3.1

grid1aslg19.9
E(RB+HF-LYP) = -3518.65066814

Zero-point correction= 0.259542
(Hartree/Particle)
Thermal correction to Energy= 0.281847
Thermal correction to Enthalpy= 0.282791
Thermal correction to Gibbs Free Energy= 0.205639

Sum of electronic and zero-point Energies= -
3518.391126
Sum of electronic and thermal Energies= -
3518.368821
Sum of electronic and thermal Enthalpies= -
3518.367877
Sum of electronic and thermal Free Energies= -
3518.445029

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.862	83.111	162.380

C,0,0.9560443378,1.6234544883,-0.29321679
C,0,0.6039102891,0.4327949081,-1.208352801
O,0,1.5723255769,-0.4796377136,-1.2452366964
C,0,2.6735794483,-0.1501476901,-0.335579144
C,0,2.4798346719,1.3307754547,0.0819882839
C,0,2.6835183602,-1.1709792659,0.7918417814
O,0,1.568784792,-1.0812909376,1.6737716368
N,0,-0.8305102321,-0.5296746296,-0.4170985713
C,0,-1.0337994089,-1.8307015825,-0.7883193274
N,0,-2.1686511197,-2.3782064228,-0.3702771077
C,0,-2.7707597621,-1.3507099054,0.3152608813
C,0,-1.9540830362,-0.1981932394,0.2834272902
N,0,-2.225898562,1.010729632,0.8689927798
C,0,-3.3634266074,1.0374973516,1.4855396723
N,0,-4.2318520251,-0.0252139377,1.5703752873
C,0,-4.0309808477,-1.3224457164,1.0083233864
O,0,-4.8923655058,-2.1858186474,1.1744294058
O,0,3.4214154074,2.1843880012,-0.4716836433
O,0,0.6621133157,2.8649969219,-0.8097283957
H,0,2.7595877898,-2.1854376309,0.3614766712
H,0,3.5756811275,-1.0061992804,1.4093378544
H,0,3.5667233232,-0.2349203601,-0.9591744855
H,0,-3.6871089556,1.9493151614,1.9850467663
H,0,2.5647214711,1.4112138621,1.1751669343
H,0,0.3765196202,1.5009542785,0.6293295084
H,0,1.1025871021,3.0023848339,-1.7485384709
H,0,3.4956754237,1.9582466163,-1.4826461028
H,0,-5.1057280642,0.0758213349,2.0720465102
H,0,0.7688143106,-1.0809773499,1.1185057155
H,0,-0.2941900166,-2.3461461738,-1.3879116235
O,0,1.1409655038,0.6518046409,-4.2536096833
As,0,2.2599542163,1.8076277431,-3.8032852877
O,0,3.1969985718,2.3039955248,-5.298180575
O,0,1.5985861792,3.2296028125,-3.1647176085
O,0,3.5850309412,1.2740773742,-2.8571761724
H,0,0.1480051257,0.5874930167,-2.1880195733
H,0,4.0902217079,2.1841941466,-4.9324421455

LG 2.1 Nuc 1.9

grid1aslg21.1
E(RB+HF-LYP) = -3518.64517069

Zero-point correction= 0.262263
(Hartree/Particle)
Thermal correction to Energy= 0.283544
Thermal correction to Enthalpy= 0.284488
Thermal correction to Gibbs Free Energy= 0.211614
Sum of electronic and zero-point Energies= -
3518.382908
Sum of electronic and thermal Energies= -
3518.361627
Sum of electronic and thermal Enthalpies= -
3518.360682
Sum of electronic and thermal Free Energies= -
3518.433557

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.927	81.410	153.378

C,0,0.8374770287,1.6325370572,-0.5475489657
 C,0,0.5935445004,0.4540124105,-1.5180147701
 O,0,1.4587437133,-0.5519498889,-1.332306077
 C,0,2.5907854712,-0.1244712485,-0.5186256573
 C,0,2.2776965737,1.291527374,0.0338900607
 C,0,2.7756440705,-1.2002292771,0.5400460769
 O,0,1.6845244751,-1.2954262438,1.4414069104
 N,0,-0.7891344446,-0.5626406114,-0.3078032102
 C,0,-1.0920986592,-1.8045138512,-0.8035112379
 N,0,-2.2827119528,-2.3248599906,-0.4987905782
 C,0,-2.8355201732,-1.3422993778,0.2835803232
 C,0,-1.9160264033,-0.2676432821,0.4025849432
 N,0,-2.1214197415,0.8826793731,-1.1318209554
 C,0,-3.2731726754,0.9320738559,1.7182912181
 N,0,-4.2288954022,-0.0564965342,1.648360007
 C,0,-4.1114884045,-1.2904218799,0.9374348073
 O,0,-5.0538370841,-2.0878393171,0.9782624481
 O,0,3.30078362,2.2207376696,-0.2034291421
 O,0,0.6011443043,2.9265908194,-0.9974972162
 H,0,2.9563685806,-2.1682121392,0.0370187898
 H,0,3.6688562385,-0.9645104123,1.1345476147
 H,0,3.4511640197,-0.0637166802,-1.1929258197
 H,0,-3.5420304212,1.7998438325,2.3204181601
 H,0,2.171532478,1.2302262025,1.1231414043
 H,0,0.1339339231,-1.4947643752,0.2731050308
 H,0,1.2034112463,3.2032843268,-1.7437871126
 H,0,3.6565138848,2.0855068558,-1.1347767924
 H,0,-5.1091199014,0.0549617586,2.1359910547
 H,0,0.8694111299,-1.1739832204,0.9112788892
 H,0,-0.3763866605,-2.3238157116,-1.4321261369
 O,0,1.2863012415,1.0908560388,-3.168625417
 As,0,2.62210606,2.1452076475,-3.4189964214
 O,0,3.012642877,1.9255841899,-5.1754645989
 O,0,2.1807805681,3.7293503008,-3.1346016841
 O,0,4.0558110247,1.6094679394,-2.6972516907
 H,0,-0.2600510216,0.2939522157,-2.1397525382
 H,0,3.8649603861,1.4645330431,-5.0956774673

LG 2.1 Nuc 1.9 (b)

grid1aslg21.3
 E(RB+HF-LYP) = -3518.64517485

Zero-point correction=	0.262243
(Hartree/Particle)	
Thermal correction to Energy=	0.283533
Thermal correction to Enthalpy=	0.284477
Thermal correction to Gibbs Free Energy=	0.211565
Sum of electronic and zero-point Energies=	-
3518.382932	
Sum of electronic and thermal Energies=	-
3518.361642	
Sum of electronic and thermal Enthalpies=	-
3518.360698	
Sum of electronic and thermal Free Energies=	-
3518.433610	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.920	81.417	153.456

C,0,0.8252862964,1.6332756532,-0.5694789988
 C,0,0.595379712,0.4365335201,-1.5204711471
 O,0,1.4644696565,-0.5615093602,-1.3090161899
 C,0,2.5940026444,-0.1074828084,-0.5069308334
 C,0,2.2653641428,1.3124414849,0.0255651357

C,0,2.794527699,-1.1650991228,0.5668449899
 O,0,1.7022471771,-1.2641283744,1.466928726
 N,0,-0.7919428729,-0.5656910492,-0.3035576863
 C,0,-1.0837239085,-1.818507979,-0.7770155347
 N,0,-2.2693188326,-2.3446345421,-0.4618236466
 C,0,-2.8304725828,-1.3534534014,0.3034570492
 C,0,-1.9208482704,-0.2681921948,0.4022367077
 N,0,-2.1367495856,0.8932286551,1.1105673758
 C,0,-3.2884622395,0.9423969912,1.6970476866
 N,0,-4.2349055947,-0.056301035,1.6459463122
 C,0,-4.1065222323,-1.3015555098,0.9570779099
 O,0,-5.0411038623,-2.1071808781,1.0136495243
 O,0,3.2834193774,2.2463011066,-0.2144214236
 O,0,0.5789021019,2.917475401,-1.0411514329
 H,0,2.9909687752,-2.1374756858,0.0785021484
 H,0,3.682293752,-0.9069063402,1.1599398699
 H,0,3.4518787524,-0.045607717,-1.1845435437
 H,0,-3.565195745,1.8184100042,2.2834767097
 H,0,2.1512593681,1.2636007602,1.1146362184
 H,0,0.1196217807,1.5029324866,0.2505426088
 H,0,1.1789241969,3.187704084,-1.7922208431
 H,0,3.6445748401,2.1080057665,-1.1439111607
 H,0,-5.1157141093,0.0556862783,2.1323883484
 H,0,0.8875933315,-1.1611263438,0.932791451
 H,0,-0.3640272192,-2.3424319013,-1.3972445763
 O,0,1.3072203446,1.0445809016,-3.1738190453
 As,0,2.6226812673,2.1205818904,-3.4376303364
 O,0,3.0258266086,1.874871768,-5.1875259466
 O,0,2.1498449138,3.7015375939,-3.1878643496
 O,0,4.0614095642,1.625790156,-2.6972114456
 H,0,-0.2497683041,0.2607851431,-2.149555947
 H,0,3.8833035264,1.4258122185,-5.0965385242

LG 2.1 Nuc 2.1

grid1aslg21.4
 E(RB+HF-LYP) = -3518.64463080

Zero-point correction=	0.261446
(Hartree/Particle)	
Thermal correction to Energy=	0.283779
Thermal correction to Enthalpy=	0.284723
Thermal correction to Gibbs Free Energy=	0.207083
Sum of electronic and zero-point Energies=	-
3518.383184	
Sum of electronic and thermal Energies=	-
3518.360852	
Sum of electronic and thermal Enthalpies=	-
3518.359908	
Sum of electronic and thermal Free Energies=	-
3518.437547	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.074	83.543	163.406

C,0,0.8202712943,1.6274327987,-0.576522132
 C,0,0.5609257058,0.4014307355,-1.4740228264
 O,0,1.4413389581,-0.57073221,-1.3044285177
 C,0,2.5952203933,-0.1094473048,-0.5290965649
 C,0,2.2664826852,1.306630344,0.0119167893
 C,0,2.8331523622,-1.1709768597,0.5313030022
 O,0,1.7627717528,-1.2911862663,1.4578877748
 N,0,-0.8614524338,-0.5894246657,-0.2886771045
 C,0,-1.1406614816,-1.858212492,-0.721068329
 N,0,-2.3140271185,-2.385242402,-0.3676093089
 C,0,-2.8766438463,-1.3734738391,0.369861207
 C,0,-1.983922829,-0.2725287539,0.4171067307
 N,0,-2.2048852717,0.912345952,1.0814379625
 C,0,-3.3503110084,0.9684253269,1.6799870351

N,0,-4.2823139941,-0.0446952672,1.6804538214
 C,0,-4.1454210069,-1.313796769,1.0387368071
 O,0,-5.0663231722,-2.1296572492,1.1371558839
 O,0,3.2797234751,2.2400850981,-0.2240419199
 O,0,0.5728422707,2.8909883002,-1.088796961
 H,0,3.031198629,-2.1382569733,0.0347640015
 H,0,3.7287656143,-0.9029897494,1.1065954027
 H,0,3.4234696136,-0.0373211485,-1.2420868718
 H,0,-3.6322606434,1.8630985398,2.2344718626
 H,0,2.152246002,1.2462437633,1.1009780434
 H,0,0.1211292496,1.5222518025,0.2559539025
 H,0,1.1863226738,3.1528557088,-1.8429620003
 H,0,3.6373319673,2.1158114947,-1.1637455641
 H,0,-5.1588978487,0.074846904,2.1728189146
 H,0,0.9341179664,-1.2170694002,0.9443210533
 H,0,-0.422600428,-2.3925556816,-1.334125267
 O,0,1.3802655225,0.996813209,-3.3136424853
 As,0,2.6571214853,2.11121753,-3.4779004985
 O,0,3.2018306509,1.9856450728,-5.2085661845
 O,0,2.145318227,3.6748254003,-3.1670772981
 O,0,4.0809406824,1.6417313454,-2.6789797748
 H,0,-0.2138729005,0.2778880723,-2.2015024191
 H,0,4.1030512713,1.6516672536,-5.0612320064

LG 2.1 Nuc 2.3

grid1aslg21.5
 E(RB+HF-LYP) = -3518.64489080

Zero-point correction=	0.260644
(Hartree/Particle)	
Thermal correction to Energy=	0.282138
Thermal correction to Enthalpy=	0.283082
Thermal correction to Gibbs Free Energy=	0.208892
Sum of electronic and zero-point Energies=	-
3518.384247	
Sum of electronic and thermal Energies=	-
3518.362753	
Sum of electronic and thermal Enthalpies=	-
3518.361809	
Sum of electronic and thermal Free Energies=	-
3518.435999	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.044	81.620	156.147

C,0,0.8228972217,1.6359457148,-0.5755400178
 C,0,0.5458232879,0.3946189238,-1.442407518
 O,0,1.4441164048,-0.5527414432,-1.3149036463
 C,0,2.5963232551,-0.1028065581,-0.5198627255
 C,0,2.2751691358,1.31997288,0.0075969254
 C,0,2.8123075534,-1.164818307,0.5435783754
 O,0,1.7392314139,-1.2670061044,1.470394631
 N,0,-0.9038747021,-0.602530496,-0.2960800459
 C,0,-1.1818759313,-1.8722129742,-0.7237717595
 N,0,-2.3454959827,-2.4012428741,-0.3456657991
 C,0,-2.8996794369,-1.3885056969,0.3976571183
 C,0,-2.0147843667,-0.2820491319,0.4256994392
 N,0,-2.2290087324,0.9049113578,1.086421755
 C,0,-3.3646662675,0.9576537696,1.7040040253
 N,0,-4.2902849458,-0.0605612196,1.7256829068
 C,0,-4.1577823533,-1.3321469853,1.0879871476
 O,0,-5.0714253983,-2.1525674006,1.2048686627
 O,0,3.2849385906,2.2460044494,-0.2492626916
 O,0,0.5757645185,2.8802850748,-1.1255525163
 H,0,2.9976392963,-2.1364898834,0.0513323832
 H,0,3.7095632878,-0.9080240548,1.1208353925
 H,0,3.4261201174,-0.0425963209,-1.2322692197
 H,0,-3.6419813667,1.853808002,2.2580768104

H,0,2.1665520809,1.2703256344,1.0982589831
 H,0,0.1287216921,1.5489404941,0.2653793515
 H,0,1.2011161622,3.1303509505,-1.8878765676
 H,0,3.6279668115,2.1133792664,-1.2000975481
 H,0,-5.1590657994,0.0570582202,2.2322235229
 H,0,0.9107787307,-1.2084972404,0.9559057859
 H,0,-0.4718567368,-2.403226229,-1.3487245129
 O,0,1.4249980162,0.9296745575,-3.4992896831
 As,0,2.6693004989,2.0720223752,-3.539082248
 O,0,3.3483131814,2.0761285499,-5.2309001352
 O,0,2.1238084247,3.616640428,-3.1686489368
 O,0,4.0643865213,1.6087407427,-2.6770308323
 H,0,-0.1602402812,0.3219022132,-2.2466600045
 H,0,4.2584305682,1.8043269352,-5.022610648

LG 2.1 Nuc 2.5

grid1aslg21.6
 E(RB+HF-LYP) = -3518.64600993

Zero-point correction=	0.260020
(Hartree/Particle)	
Thermal correction to Energy=	0.282304
Thermal correction to Enthalpy=	0.283249
Thermal correction to Gibbs Free Energy=	0.206209
Sum of electronic and zero-point Energies=	-
3518.385990	
Sum of electronic and thermal Energies=	-
3518.363705	
Sum of electronic and thermal Enthalpies=	-
3518.362761	
Sum of electronic and thermal Free Energies=	-
3518.439801	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.149	83.385	162.144

C,0,0.9313488883,1.6646655223,-0.4685497328
 C,0,0.6245164906,0.4524302469,-1.364419778
 O,0,1.5576306262,-0.4595774841,-1.3364022151
 C,0,2.6502212999,-0.1084915951,-0.4111182249
 C,0,2.4169568299,1.3595257833,0.0292383837
 C,0,2.6520989443,-1.1436761338,0.7029087528
 O,0,1.5444910021,-1.0550918785,1.5850813211
 N,0,-0.8317436045,-0.6071177519,-0.2842994096
 C,0,-1.1108706028,-1.850045565,-0.7861027813
 N,0,-2.2888224277,-2.3797003554,-0.4642511568
 C,0,-2.8525508757,-1.3970370062,0.3134441013
 C,0,-1.9597294424,-0.3040976574,0.4207430681
 N,0,-2.1764800827,0.8516423393,1.1318208751
 C,0,-3.3286052232,0.8881202386,1.7200888539
 N,0,-4.2645137955,-0.1189781801,1.6677829177
 C,0,-4.1278016327,-1.3603854336,0.9736039396
 O,0,-5.0506110902,-2.1761114832,1.0278610051
 O,0,3.414883624,2.230153472,-0.3928018391
 O,0,0.6616447827,2.9114775878,-0.9973249843
 H,0,2.7236890217,-2.1514753283,0.2550008511
 H,0,3.551903527,-0.9913117369,1.3135780851
 H,0,3.5489692394,-0.1689949458,-1.0295032386
 H,0,-3.6115937951,1.7600609205,2.3085754812
 H,0,2.3987159922,1.4001953192,1.125816413
 H,0,0.2800915923,1.5498809747,0.4046931505
 H,0,1.2359233467,3.1356202441,-1.8229917124
 H,0,3.6252409352,2.0320776615,-1.3785705817
 H,0,-5.1459883883,-0.0152209122,2.1551275254
 H,0,0.7357790253,-1.0042876723,1.0354810654
 H,0,-0.3900346272,-2.3542343843,-1.4201892165
 O,0,1.1889242378,0.9096428933,-3.7565724295
 As,0,2.4777077691,1.9842710362,-3.6593044361

O,0,3.216904161,2.1367637489,-5.3221464758
 O,0,2.0196868174,3.5239388472,-3.148883711
 O,0,3.8398542834,1.3974574308,-2.8137940474
 H,0,-0.0179493572,0.4594053139,-2.228195999
 H,0,4.1223569787,1.8631734895,-5.09575766

LG 2.1 Nuc 2.7

grid1aslg21.7

E(RB+HF-LYP) = -3518.64781297

Zero-point correction= 0.259640
 (Hartree/Particle)
 Thermal correction to Energy= 0.281828
 Thermal correction to Enthalpy= 0.282773
 Thermal correction to Gibbs Free Energy= 0.206367
 Sum of electronic and zero-point Energies= -
 3518.388173
 Sum of electronic and thermal Energies= -
 3518.365985
 Sum of electronic and thermal Enthalpies= -
 3518.365040
 Sum of electronic and thermal Free Energies= -
 3518.441446

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.850	83.191	160.809

C,0,0.9769392033,1.6753893721,-0.4009726588
 C,0,0.6729807456,0.4817579691,-1.315450929
 O,0,1.6159299831,-0.4185426213,-1.3143216394
 C,0,2.6807985707,-0.1023482935,-0.3450734757
 C,0,2.4772919921,1.3800054997,0.0585479601
 C,0,2.6081202062,-1.1250506991,0.7788124301
 O,0,1.4842194583,-0.9818835608,1.6321854432
 N,0,-0.8311940261,-0.6007767187,-0.3277413618
 C,0,-1.1251098864,-1.82289629,-0.8691793517
 N,0,-2.3060408908,-2.348476504,-0.553324346
 C,0,-2.853559539,-1.3844619714,0.2588723053
 C,0,-1.9506391568,-0.3036043847,0.3931064948
 N,0,-2.1472755938,0.8298591505,1.1438779336
 C,0,-3.2930081272,0.8578813534,1.745013764
 N,0,-4.2391599675,-0.1377423914,1.669149324
 C,0,-4.121213027,-1.3578105753,0.9347377666
 O,0,-5.0497392729,-2.167353579,0.9742974089
 O,0,3.456161259,2.2262218533,-0.4422680951
 O,0,0.6979372136,2.91927609,-0.927846795
 H,0,2.6503847119,-2.1391107752,0.341788248
 H,0,3.4969655868,-1.0043036497,1.412139659
 H,0,3.5993846776,-0.2070413341,-0.926499012
 H,0,-3.5610173926,1.7124854973,2.3649872656
 H,0,2.5031991873,1.4597751683,1.1533213473
 H,0,0.3445552867,1.548966953,0.4848378777
 H,0,1.2108619526,3.1010194774,-1.8139393228
 H,0,3.589014539,2.0061753361,-1.442787089
 H,0,-5.1136253971,-0.042723409,2.170706215
 H,0,0.6872717691,-0.9572568943,1.0644206264
 H,0,-0.4145990417,-2.3124065657,-1.5256721133
 O,0,1.1363178975,0.7869513881,-3.9578300369
 As,0,2.3776520904,1.8926878129,-3.7374064406
 O,0,3.1967455651,2.1508385722,-5.3497473363
 O,0,1.8623124734,3.4040508068,-3.1850449166
 O,0,3.7238207179,1.329630166,-2.8464089294
 H,0,0.1093820729,0.5426340422,-2.2427098954
 H,0,4.1101786289,1.9728513286,-5.0669121651

LG 2.1 Nuc 2.9

grid1aslg21.8

E(RB+HF-LYP) = -3518.64831220

Zero-point correction= 0.259334
 (Hartree/Particle)
 Thermal correction to Energy= 0.281596
 Thermal correction to Enthalpy= 0.282540
 Thermal correction to Gibbs Free Energy= 0.205833
 Sum of electronic and zero-point Energies= -
 3518.388978
 Sum of electronic and thermal Energies= -
 3518.366716
 Sum of electronic and thermal Enthalpies= -
 3518.365772
 Sum of electronic and thermal Free Energies= -
 3518.442479

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.704	83.176	161.444

C,0,0.9834620549,1.6752756988,-0.3864404758
 C,0,0.6803298766,0.484217759,-1.3017278407
 O,0,1.6220295311,-0.416511104,-1.3089227489
 C,0,2.6847764662,-0.1068959977,-0.3347365316
 C,0,2.4900004553,1.3799342125,0.0598121652
 C,0,2.598866749,-1.1251798591,0.7921404335
 O,0,1.4658781598,-0.9772228873,1.6336664664
 N,0,-0.8460639111,-0.5938963822,-0.3437153959
 C,0,-1.1376048747,-1.8201534264,-0.8761707712
 N,0,-2.3119987883,-2.3494910948,-0.5440016122
 C,0,-2.8558780152,-1.3838685522,0.2687896253
 C,0,-1.9588806286,-0.2968202439,0.3876268229
 N,0,-2.1539941518,0.8397179054,1.1333813949
 C,0,-3.293368434,0.86418707,1.7467518431
 N,0,-4.2339828568,-0.1375011243,1.6869550762
 C,0,-4.1164862503,-1.3611051235,0.9585319536
 O,0,-5.0389037754,-2.1762702497,1.0124540413
 O,0,3.4624460809,2.2175270422,-0.4623193931
 O,0,0.7010689966,2.9137901367,-0.9180066534
 H,0,2.6442240552,-2.1413708312,0.3607925724
 H,0,3.4804978385,-1.0025364888,1.4348012042
 H,0,3.6038537901,-0.2200530295,-0.9134926611
 H,0,-3.5596819571,1.7209003003,2.3644213724
 H,0,2.5272472993,1.4687472247,1.1538104046
 H,0,0.360333389,1.5472359674,0.505922712
 H,0,1.1940692323,3.0766070153,-1.8255287497
 H,0,3.5675414801,1.9897977384,-1.4685495621
 H,0,-5.1034761637,-0.0447657476,2.1975465723
 H,0,0.6741901923,-0.9599654801,1.0593068081
 H,0,-0.4309955539,-2.3092294953,-1.5371341435
 O,0,1.1664668956,0.7493498057,-4.1483695407
 As,0,2.3599824573,1.8667515121,-3.7904765389
 O,0,3.2761370708,2.2331843212,-5.3298876637
 O,0,1.7872766384,3.3452923978,-3.2000557467
 O,0,3.6698809346,1.2985327945,-2.8462749069
 H,0,0.1306421004,0.553486629,-2.2385992311
 H,0,4.1723580871,2.0629692069,-4.992635141

LG 2.3 Nuc 1.9

grid1aslg23.1

E(RB+HF-LYP) = -3518.66401238

Zero-point correction= 0.262245
 (Hartree/Particle)
 Thermal correction to Energy= 0.284348
 Thermal correction to Enthalpy= 0.285292
 Thermal correction to Gibbs Free Energy= 0.207812
 Sum of electronic and zero-point Energies= -
 3518.401768

Sum of electronic and thermal Energies= -
3518.379665
Sum of electronic and thermal Enthalpies= -
3518.378720
Sum of electronic and thermal Free Energies= -
3518.456200

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.431	83.117	163.070

C,0,0.947755997,1.6719597325,-0.5496112726
C,0,0.6892488297,0.5220142813,-1.538756088
O,0,1.5238430727,-0.4945542238,-1.3464693075
C,0,2.6376124772,-0.1221923477,-0.4730521071
C,0,2.3900794359,1.3276078319,0.0145948939
C,0,2.6914437294,-1.171132813,0.6288454202
O,0,1.6000034722,-1.1160686212,1.5252484529
N,0,-0.7582365349,-0.6302204279,-0.1723240492
C,0,-1.0781216978,-1.8226429797,-0.7660558069
N,0,-2.3075971403,-2.3088394934,-0.5750812048
C,0,-2.8696408455,-1.3560195356,0.2374513538
C,0,-1.9129510877,-0.3368091857,0.4877020908
N,0,-2.1145978143,0.7744854722,1.2773757153
C,0,-3.2993772123,0.8400076407,1.7930432339
N,0,-4.2896256119,-0.0971204952,1.5988605814
C,0,-4.180504648,-1.2871933888,0.814298347
O,0,-5.1573490817,-2.0409822757,0.7475276917
O,0,3.4312363253,2.2121944097,-0.3038201512
O,0,0.7029459842,2.9766398825,-0.9629450678
H,0,2.7771284713,-2.1692068301,0.1591556412
H,0,3.604695037,-1.0081955561,1.2188827694
H,0,3.5350149365,-0.1511353682,-1.0978446389
H,0,-3.5711015075,1.6796524538,2.4328580282
H,0,2.3150820479,1.3289691721,1.1073500736
H,0,0.2456402609,1.4897968272,0.2681453138
H,0,1.2940844896,3.2541662478,-1.7189200278
H,0,3.7305933671,2.0358054008,-1.2467487606
H,0,-5.1942166927,0.0241603987,2.0369418753
H,0,0.7838915237,-0.9956419339,0.984731328
H,0,-0.3458599416,-2.3329352201,-1.3837758875
O,0,1.1975267568,1.1364508458,-3.2633191819
As,0,2.5920074138,2.1297744898,-3.4916109803
O,0,2.9210871161,1.9520946918,-5.2616872345
O,0,2.2408783786,3.7225748293,-3.1434222892
O,0,3.9977497038,1.4842150333,-2.8152629243
H,0,-0.249875196,0.3110808593,-2.0038523927
H,0,3.7417506556,1.4319078157,-5.2287872776

LG 2.3 Nuc 2.1

grid1aslg23.2
E(RB+HF-LYP) = -3518.65745474

Zero-point correction= 0.261357
(Hartree/Particle)
Thermal correction to Energy= 0.283582
Thermal correction to Enthalpy= 0.284527
Thermal correction to Gibbs Free Energy= 0.208102
Sum of electronic and zero-point Energies= -
3518.396098
Sum of electronic and thermal Energies= -
3518.373872
Sum of electronic and thermal Enthalpies= -
3518.372928
Sum of electronic and thermal Free Energies= -
3518.449353

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
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Total	177.951	83.314	160.849
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C,0,0.9297329673,1.6655896124,-0.5774033347
C,0,0.6702678946,0.4800077184,-1.5154418271
O,0,1.516546846,-0.5052606855,-1.3481946134
C,0,2.6349913935,-0.1180954528,-0.4736962495
C,0,2.3746557397,1.3345829085,-0.0002395263
C,0,2.6918280404,-1.1632713947,0.6298542786
O,0,1.5970760398,-1.1139493147,1.5238122333
N,0,-0.8073857408,-0.6597091032,-0.1709776794
C,0,-1.1439170998,-1.8496307898,-0.7591561487
N,0,-2.3704418591,-2.3287043463,-0.5395218979
C,0,-2.910903075,-1.3701035502,0.2816834979
C,0,-1.9474622522,-0.3534135218,0.5082850624
N,0,-2.127201107,0.7628069821,1.2950198565
C,0,-3.3012995128,0.8359317249,-0.3161539452
N,0,-4.2981241482,-0.0987466772,1.6656170596
C,0,-4.2099656675,-1.2932003946,0.8851970781
O,0,-5.1898844071,-2.0434655053,0.8410252991
O,0,3.4094080732,2.2192938013,-0.3161539452
O,0,0.6776058377,2.9484082948,-1.0361215228
H,0,2.787250184,-2.1624015315,0.1651799412
H,0,3.6007422915,-0.9898587948,1.2224927179
H,0,3.5225407051,-0.1445401916,-1.1119371693
H,0,-3.5567325955,1.6804762845,2.4737282308
H,0,2.2874115336,1.3391947088,1.0920282315
H,0,0.2261737122,1.503379794,0.2460016375
H,0,1.2841753779,3.219097296,-1.7944845016
H,0,3.7079958114,2.0508723089,-1.2677420602
H,0,-5.1933361772,0.0290616408,2.1208692968
H,0,0.7778009201,-1.0175459992,0.9855041349
H,0,-0.4267628754,-2.3649806864,-1.3905599569
O,0,1.2726227319,1.0801764487,-3.4355888163
As,0,2.627017179,2.1173834284,-3.5420675752
O,0,3.1241955798,2.0516646299,-5.2864087362
O,0,2.2253491839,3.6910575571,-3.1391003922
O,0,4.0175019458,1.5030470747,-2.7926868549
H,0,-0.2108236069,0.3016753575,-2.0960138259
H,0,3.9935946062,1.6278379878,-5.1870899427

LG 2.3 Nuc 2.3

grid1aslg23.3
E(RB+HF-LYP) = -3518.65320765

Zero-point correction= 0.260471
(Hartree/Particle)
Thermal correction to Energy= 0.282789
Thermal correction to Enthalpy= 0.283733
Thermal correction to Gibbs Free Energy= 0.206927
Sum of electronic and zero-point Energies= -
3518.392737
Sum of electronic and thermal Energies= -
3518.370418
Sum of electronic and thermal Enthalpies= -
3518.369474
Sum of electronic and thermal Free Energies= -
3518.446281

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.453	83.423	161.652

C,0,0.9276839912,1.6607009896,-0.5742173597
C,0,0.6604591641,0.4561362346,-1.4801849171
O,0,1.5282634884,-0.499877136,-1.3557973714
C,0,2.6430404082,-0.114386734,-0.4642821937
C,0,2.3824135927,1.3427756077,-0.005685505
C,0,2.6827269272,-1.1569903468,0.6417947267
O,0,1.5883418377,-1.093394249,1.5355413638

N,O,-0.8335807643,-0.6899162318,-0.1594244031
 C,O,-1.1828858846,-1.8746460198,-0.7500647849
 N,O,-2.4106568246,-2.3428442351,-0.5198640241
 C,O,-2.9372752013,-1.3794427442,0.3055840678
 C,O,-1.9666410171,-0.3698727196,0.5256679684
 N,O,-2.1306225588,0.7480281483,1.3120519526
 C,O,-3.3007555064,0.831051373,1.8585158697
 N,O,-4.3053539618,-0.0961783963,1.6980837748
 C,O,-4.231979084,-1.2920351426,0.9182986218
 O,O,-5.2168083416,-2.0351495768,0.8810527151
 O,O,3.4069965792,2.2241077439,-0.3435191124
 O,O,0.6659801354,2.9245157846,-1.0680695986
 H,O,2.7696469794,-2.1586765202,0.1814979939
 H,O,3.5918718201,-0.9901278662,1.235453196
 H,O,3.5294100475,-0.1494646088,-1.1032093515
 H,O,-3.5451227902,-1.6784435061,2.4985697734
 H,O,2.3029092499,1.3572492929,1.0875095714
 H,O,0.2324758019,1.5119303209,0.2605314044
 H,O,1.2757184651,3.1850027878,-1.8420575609
 H,O,3.6872572385,2.0533229557,-1.3079427804
 H,O,-5.196730469,0.0396237314,2.1586052487
 H,O,0.7660433016,-1.0169333346,0.9996855529
 H,O,-0.4748346076,-2.3939606659,-1.3883856447
 O,O,1.3050803274,1.0189473067,-3.6150636381
 As,O,2.6217161538,2.0868496159,-3.6008702881
 O,O,3.2587294766,2.142438614,-5.3042577406
 O,O,2.1761609937,3.6378519888,-3.1370551018
 O,O,3.9936566889,1.4900994764,-2.7924299568
 H,O,-0.1588774752,0.3185313291,-2.1576595313
 H,O,4.1577862879,1.8109573404,-5.1387367774

LG 2.3 Nuc 2.5

grid1aslg23.4
 E(RB+HF-LYP) = -3518.65100951

Zero-point correction= 0.259896
 (Hartree/Particle)
 Thermal correction to Energy= 0.282216
 Thermal correction to Enthalpy= 0.283160
 Thermal correction to Gibbs Free Energy= 0.206361
 Sum of electronic and zero-point Energies= -
 3518.391114
 Sum of electronic and thermal Energies= -
 3518.368794
 Sum of electronic and thermal Enthalpies= -
 3518.367850
 Sum of electronic and thermal Free Energies= -
 3518.444649

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.093	83.427	161.637

C,O,0.9667569586,1.6800955274,-0.524571214
 C,O,0.6779823455,0.4814006109,-1.4266285534
 O,O,1.5656054886,-0.4522637608,-1.3636715297
 C,O,2.6678608895,-0.105004549,-0.4352980551
 C,O,2.439215775,1.3637279106,0.0035694159
 C,O,2.6448318824,-1.142716516,0.6767084316
 O,O,1.5484136615,-1.02396518,1.5624279853
 N,O,-0.8448433185,-0.694532074,-0.1663962722
 C,O,-1.1908574401,-1.8741545042,-0.7685951065
 N,O,-2.4159129735,-2.3461490791,-0.5366264738
 C,O,-2.942578646,-1.390299525,0.2980974183
 C,O,-1.9769131798,-0.3781703973,0.5222768928
 N,O,-2.1409557612,0.7337356599,1.3159930135
 C,O,-3.3103867187,0.8095437663,1.8653790065
 N,O,-4.3118019011,-0.1201545104,1.7018156093
 C,O,-4.2356725735,-1.3122368756,0.9164695907

O,O,-5.2170511404,-2.0588871191,0.8769763998
 O,O,3.4531498904,2.2263104952,-0.39494477
 O,O,0.6990880625,2.935263172,-1.0305488467
 H,O,2.6911518592,-2.149941429,0.2234335903
 H,O,3.5543572619,-1.0138825876,1.2788680792
 H,O,3.5632528451,-0.1750970212,-1.057013924
 H,O,-3.5561904938,1.6526560623,2.5103133706
 H,O,2.3971087124,1.4003407541,1.0986534986
 H,O,0.293374129,1.5333524502,0.3298138762
 H,O,1.2876143594,3.1697203753,-1.843191487
 H,O,3.6743497522,2.0341040362,-1.3767865376
 H,O,-5.2025735305,0.0099341981,2.1652148335
 H,O,0.7275238327,-0.9712575149,1.0219636343
 H,O,-0.4834263182,-2.3843942902,-1.4145816693
 O,O,1.2478031646,0.9663689025,-3.8120238137
 As,O,2.5541702034,2.0203346177,-3.6691020671
 O,O,3.3071043359,2.1880803644,-5.320805781
 O,O,2.1118034777,3.5569798383,-3.1396455414
 O,O,3.8896658408,1.3913805821,-2.8150011217
 H,O,-0.0792200568,0.4052069724,-2.185180449
 H,O,4.2084437938,1.8992382578,-5.0976952731

LG 2.3 Nuc 2.7

grid1aslg23.5
 E(RB+HF-LYP) = -3518.65015452

Zero-point correction= 0.259273
 (Hartree/Particle)
 Thermal correction to Energy= 0.281601
 Thermal correction to Enthalpy= 0.282546
 Thermal correction to Gibbs Free Energy= 0.205701
 Sum of electronic and zero-point Energies= -
 3518.390882
 Sum of electronic and thermal Energies= -
 3518.368553
 Sum of electronic and thermal Enthalpies= -
 3518.367609
 Sum of electronic and thermal Free Energies= -
 3518.444454

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.708	83.395	161.733

C,O,0.9841435256,1.6859449117,-0.4835014919
 C,O,0.7048804043,0.4939272374,-1.3919547186
 O,O,1.6108475762,-0.4190770675,-1.3608013769
 C,O,2.6874535337,-0.0942932712,-0.3930094216
 C,O,2.4692520405,1.3823477857,0.0243204098
 C,O,2.6145326965,-1.1284633541,0.720417809
 O,O,1.501796126,-0.9862532039,1.5814032346
 N,O,-0.8549310782,-0.7042797098,-0.1997797424
 C,O,-1.2190980546,-1.8673828192,-0.8226004009
 N,O,-2.4453258082,-2.3304595145,-0.5823602855
 C,O,-2.9521217327,-1.3845681206,0.2761505642
 C,O,-1.9756252897,-0.3855227574,0.5068167995
 N,O,-2.1174285933,0.7119181142,1.323766681
 C,O,-3.278322582,0.7873462219,1.8911508942
 N,O,-4.290017452,-0.1300740979,1.7238785797
 C,O,-4.2355899277,-1.3075739977,0.9151712451
 O,O,-5.2221509186,-2.0468255511,0.8479606045
 O,O,3.4667709869,2.2346740927,-0.4243524725
 O,O,0.709336277,2.9302816042,-1.0073462878
 H,O,2.6523125574,-2.1374362958,0.2705160473
 H,O,3.5123908882,-1.0162500734,1.3430168075
 H,O,3.5978289705,-0.1869120219,-0.9885473835
 H,O,-3.5069093255,1.6197658661,2.5558557681
 H,O,2.4521879145,1.4423580665,1.1194593088
 H,O,0.3222612825,1.540289188,0.3799860939

H,0,1.2671840873,3.1365615182,-1.8622104154
 H,0,3.637677165,2.0249566284,-1.418998497
 H,0,-5.1722879862,-0.0022069227,2.2038994168
 H,0,0.6910601033,-0.9585507834,1.0245230976
 H,0,-0.5251542274,-2.3712346699,-1.4877614827
 O,0,1.2390376996,0.879380658,-4.0103688948
 As,0,2.4965106621,1.9567321812,-3.7381393809
 O,0,3.3609741031,2.2242680365,-5.3225328071
 O,0,1.9972207354,3.4688546647,-3.1755367019
 O,0,3.8012379273,1.3447155299,-2.8197236612
 H,0,0.020993113,0.4656162154,-2.2277795397
 H,0,4.2593170701,1.9920933317,-5.0313222801

LG 2.3 Nuc 2.9

grid1aslg23.6

E(RB+HF-LYP) = -3518.64932848

Zero-point correction= 0.258702
 (Hartree/Particle)
 Thermal correction to Energy= 0.281103
 Thermal correction to Enthalpy= 0.282047
 Thermal correction to Gibbs Free Energy= 0.204661
 Sum of electronic and zero-point Energies= -
 3518.390626
 Sum of electronic and thermal Energies= -
 3518.368225
 Sum of electronic and thermal Enthalpies= -
 3518.367281
 Sum of electronic and thermal Free Energies= -
 3518.444668

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.395	83.347	162.874

C,0,1.0059672361,1.6853036686,-0.4442208946
 C,0,0.7293219797,0.5031789767,-1.3610288719
 O,0,1.6410731892,-0.4031074968,-1.3511279638
 C,0,2.705196644,-0.0968236453,-0.363176039
 C,0,2.5037819625,1.3875233965,0.0362460691
 C,0,2.59361227,-1.1229748014,0.7548596417
 O,0,1.4696221475,-0.9544678763,1.5964790595
 N,0,-0.8641540591,-0.7044501284,-0.2241653427
 C,0,-1.2361112939,-1.8615500045,-0.8530915107
 N,0,-2.4613075769,-2.3217693471,-0.6042280154
 C,0,-2.9579533231,-1.3796102833,0.2645409578
 C,0,-1.9777484087,-0.3844830185,0.4934108511
 N,0,-2.1087206185,0.7080606783,1.3180996933
 C,0,-3.2643429039,0.7829006144,1.8962998987
 N,0,-4.2795167619,-0.1310621337,1.7326154464
 C,0,-4.2355313685,-1.3034887724,0.9159893943
 O,0,-5.2236565983,-2.0404071759,0.883277054
 O,0,3.4873789469,2.2273278186,-0.457201686
 O,0,0.7232855955,2.92393839,-0.9707575133
 H,0,2.6203381438,-2.1352789799,0.3121779644
 H,0,3.4823306453,-1.0237045516,1.3924470981
 H,0,3.6233901233,-0.2121184497,-0.9421870605
 H,0,-3.484732666,1.6119189347,2.5678974235
 H,0,2.5136504702,1.4668164993,1.1305884457
 H,0,0.3604940995,1.5335988509,0.4306466147
 H,0,1.2384858533,3.0979007279,-1.8698880657
 H,0,3.6147453824,2.0064066829,-1.461676379
 H,0,-5.1571897262,-0.0038198298,2.2211871085
 H,0,0.6661977568,-0.9413329071,1.0292092944
 H,0,-0.5494591398,-2.3623642324,-1.5278519465
 O,0,1.2607071461,0.7969937329,-4.1967459743
 As,0,2.4506800829,1.9055858319,-3.8021461426
 O,0,3.3943634361,2.2919162218,-5.3168162636

O,0,1.8735667377,3.3790403964,-3.2017359562
 O,0,3.7349444531,1.3155043615,-2.8376974397
 H,0,0.0837180659,0.5041856742,-2.2320331075
 H,0,4.2858165471,2.1193797967,-4.9685296822

LG 2.3 Nuc 3.1

grid1aslg23.7

E(RB+HF-LYP) = -3518.64822281

Zero-point correction= 0.258326
 (Hartree/Particle)
 Thermal correction to Energy= 0.280844
 Thermal correction to Enthalpy= 0.281788
 Thermal correction to Gibbs Free Energy= 0.202670
 Sum of electronic and zero-point Energies= -
 3518.389897
 Sum of electronic and thermal Energies= -
 3518.367379
 Sum of electronic and thermal Enthalpies= -
 3518.366435
 Sum of electronic and thermal Free Energies= -
 3518.445552

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.232	83.287	166.517

C,0,1.0077553479,1.6877198877,-0.421355796
 C,0,0.7275242917,0.5130180929,-1.3424370105
 O,0,1.6410974228,-0.3888841676,-1.3571275985
 C,0,2.7078913266,-0.0962476245,-0.3656699568
 C,0,2.5132166133,1.3879609005,0.0394207563
 C,0,2.5890258994,-1.1274593926,0.7466860885
 O,0,1.4682963405,-0.9539203654,1.5918665127
 N,0,-0.8736469523,-0.7037136151,-0.2262769875
 C,0,-1.2471387422,-1.8642471742,-0.8479739727
 N,0,-2.4702191017,-2.3242080993,-0.5895161343
 C,0,-2.9633682586,-1.3779180977,0.2768180593
 C,0,-1.9837635269,-0.3803438767,0.4954197206
 N,0,-2.1114549757,0.7164093906,1.3147197671
 C,0,-3.2641975142,0.7930284717,1.8984779027
 N,0,-4.2790234081,-0.1229231117,1.744916722
 C,0,-4.2380075402,-1.2995261245,0.9341322023
 O,0,-5.2252791693,-2.0375551911,0.9098053527
 O,0,3.4860124094,2.2272469837,-0.4707509996
 O,0,0.7256084826,2.9228668082,-0.9520757646
 H,0,2.6066379956,-2.1377391471,0.2993983386
 H,0,3.4798324795,-1.0383830945,1.3827889504
 H,0,3.6239894368,-0.2146527994,-0.947176771
 H,0,-3.4819345841,1.6253680494,2.5667575199
 H,0,2.5379107436,1.4653799844,1.1339617272
 H,0,0.3714018752,1.5361563127,0.4601469693
 H,0,1.2093842215,3.0626324224,-1.8813166404
 H,0,3.5949477152,2.0022967562,-1.4816506134
 H,0,-5.154496885,0.0062862073,2.2369304792
 H,0,0.6629239965,-0.9413827114,1.0279137666
 H,0,-0.563629896,-2.3675464777,-1.5240292251
 O,0,1.3539934204,0.7109037194,-4.3720203133
 As,0,2.4496952809,1.8587103685,-3.8541341942
 O,0,3.4674427202,2.3699094501,-5.2833157281
 O,0,1.7644323285,3.279313238,-3.2335793077
 O,0,3.7104025213,1.3049636577,-2.834554027
 H,0,0.0781991869,0.5246409347,-2.2121129747
 H,0,4.3407829682,2.2465070543,-4.8734206598

LG 2.5 Nuc 1.9

grid1aslg25.1

E(RB+HF-LYP) = -3518.67824072

Zero-point correction= 0.262156
 (Hartree/Particle)
 Thermal correction to Energy= 0.284232
 Thermal correction to Enthalpy= 0.285176
 Thermal correction to Gibbs Free Energy= 0.209059
 Sum of electronic and zero-point Energies= -
 3518.416085
 Sum of electronic and thermal Energies= -
 3518.394009
 Sum of electronic and thermal Enthalpies= -
 3518.393065
 Sum of electronic and thermal Free Energies= -
 3518.469182

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.358	83.000	160.202

C,0,1.0455622813,1.7119323809,-0.5426932901
 C,0,0.7714665083,0.6086390501,-1.5715700187
 O,0,1.543251471,-0.4484564604,-1.3580598207
 C,0,2.6601646565,-0.1359718792,-0.4608056551
 C,0,2.467218541,1.3195161488,0.03235731
 C,0,2.6343983525,-1.1942052027,0.63401152
 O,0,1.5364068842,-1.0810289927,1.5130281096
 N,0,-0.8307909935,-0.6681127519,-0.1388552957
 C,0,-1.1649586891,-1.8019530024,-0.8270657943
 N,0,-2.4121652209,-2.2668227367,-0.701915781
 C,0,-2.9691368457,-1.3604523682,0.1653463508
 C,0,-1.9918940922,-0.3892080158,0.5119697456
 N,0,-2.1833855418,0.6695217442,1.3737073094
 C,0,-3.378413689,0.7303227351,1.8661210688
 N,0,-4.3875119267,-0.1634313867,1.5832592717
 C,0,-4.2910126722,-1.2966068928,0.716694421
 O,0,-5.2859802188,-2.0160283631,0.5751327954
 O,0,3.5394899601,2.1697107189,-0.2776794868
 O,0,0.828048434,3.036086754,-0.904337269
 H,0,2.6720502817,-2.1916651235,0.1563844865
 H,0,3.5467407564,-1.0877812061,1.2385539027
 H,0,3.5678306419,-0.2064805365,-1.0669382466
 H,0,-3.6446695587,1.5297820555,2.5578315121
 H,0,2.3854304917,1.3199937147,1.1243193089
 H,0,0.3229144018,1.4936812712,0.2524436574
 H,0,1.4282861754,3.3186831607,-1.6522352607
 H,0,3.8284970993,1.9967773464,-1.2232073085
 H,0,-5.2989347609,-0.0492639832,2.0088961284
 H,0,0.7231084731,-0.961794853,0.962423465
 H,0,-0.4300582115,-2.2876241125,-1.4616880907
 O,0,1.2639841744,1.2086456703,-3.3057603481
 As,0,2.6906923486,2.1763406729,-3.4724666954
 O,0,3.0235739564,2.0579402492,-5.2445928293
 O,0,2.3799732966,3.7637650443,-3.068619483
 O,0,4.0624111679,1.4574883864,-2.8050676035
 H,0,-0.206039157,0.4082385339,-1.9648080055
 H,0,3.8156956942,1.4944898498,-5.2344479205

LG 2.5 Nuc 2.1

grid1aslg25.2
 E(RB+HF-LYP) = -3518.66829445

Zero-point correction= 0.261283
 (Hartree/Particle)
 Thermal correction to Energy= 0.283455
 Thermal correction to Enthalpy= 0.284399
 Thermal correction to Gibbs Free Energy= 0.208047
 Sum of electronic and zero-point Energies= -
 3518.407012
 Sum of electronic and thermal Energies= -
 3518.384839

Sum of electronic and thermal Enthalpies= -
 3518.383895
 Sum of electronic and thermal Free Energies= -
 3518.460248

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.871	83.138	160.698

C,0,1.0339826689,1.6968924861,-0.5493877037
 C,0,0.7522423103,0.5623996815,-1.5338172274
 O,0,1.5408776012,-0.4633382508,-1.3576287643
 C,0,2.6664846209,-0.1394242962,-0.4585613799
 C,0,2.4672835733,1.3194521058,0.0201541517
 C,0,2.6423214106,-1.1945754223,0.6380885215
 O,0,1.5547888392,-1.0736266406,1.5283876816
 N,0,-0.8454978393,-0.7167420595,-0.0981913575
 C,0,-1.1949699366,-1.8458449261,-0.7864594251
 N,0,-2.4495810784,-2.2889667108,-0.6640132084
 C,0,-2.9947302684,-1.370064297,0.1979775689
 C,0,-2.004626046,-0.4137613378,0.5458058523
 N,0,-2.1820250841,0.6527550988,1.3999935765
 C,0,-3.3792996179,0.7375269862,1.8837198307
 N,0,-4.4013303438,-0.140736477,1.6000513461
 C,0,-4.3192254359,-1.2802802724,0.7404272762
 O,0,-5.3248511644,-1.9829656026,0.5951711929
 O,0,3.5300080822,2.16838926,-0.3020873146
 O,0,0.7985524851,3.0026990114,-0.9435465969
 H,0,2.6721198435,-2.193577973,0.1636197339
 H,0,3.560986491,-1.0892861016,1.2326084649
 H,0,3.5627903097,-0.2119682912,-1.0799772629
 H,0,-3.6361777079,1.5461606057,2.5680178789
 H,0,2.3875021105,1.3259854349,1.1125555696
 H,0,0.3211271049,1.4870830634,0.2595232164
 H,0,1.405089641,3.2850550716,-1.6994847456
 H,0,3.8025638653,2.006592826,-1.2619467432
 H,0,-5.3141404198,-0.0063930347,2.0168014365
 H,0,0.7301579797,-0.977384074,0.9899182139
 H,0,-0.4666606135,-2.3451786927,-1.4182997829
 O,0,1.2901317271,1.1745835519,-3.4692510936
 As,0,2.6826328242,2.1728595494,-3.5225320399
 O,0,3.1647921436,2.1687052805,-5.2692588706
 O,0,2.3340765384,3.739162206,-3.049677832
 O,0,4.0452485261,1.470809541,-2.8044089629
 H,0,-0.1813883299,0.387185548,-2.0318346269
 H,0,4.0109876592,1.6944847722,-5.202790414

LG 2.5 Nuc 2.3

grid1aslg25.3
 E(RB+HF-LYP) = -3518.66111441

Zero-point correction= 0.260368
 (Hartree/Particle)
 Thermal correction to Energy= 0.282667
 Thermal correction to Enthalpy= 0.283611
 Thermal correction to Gibbs Free Energy= 0.206755
 Sum of electronic and zero-point Energies= -
 3518.400747
 Sum of electronic and thermal Energies= -
 3518.378447
 Sum of electronic and thermal Enthalpies= -
 3518.377503
 Sum of electronic and thermal Free Energies= -
 3518.454359

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.376	83.330	161.757

C,0,1.0167571605,1.6831932045,-0.5512518665
 C,0,0.7393304214,0.5276286113,-1.5047812112
 O,0,1.5531483708,-0.4661295683,-1.3659641588
 C,0,2.6732994415,-0.1347165157,-0.4515224726
 C,0,2.4597332812,1.326178441,0.0165172423
 C,0,2.6445749087,-1.1896584172,0.6448349039
 O,0,1.5553402554,-1.0716600366,1.5336324652
 N,0,-0.8572683515,-0.7638039518,-0.0789231416
 C,0,-1.2289569864,-1.8837424766,-0.7705470069
 N,0,-2.4908666016,-2.3022882031,-0.6447275129
 C,0,-3.0163551388,-1.3737509545,0.2197053919
 C,0,-2.0090373036,-0.4367555609,0.5667067629
 N,0,-2.1632698381,0.6327903832,1.4208030535
 C,0,-3.3582761489,0.7412256236,1.9057874086
 N,0,-4.3969781912,-0.1173631925,1.6239893563
 C,0,-4.3381857584,-1.258894652,0.7649927177
 O,0,-5.3562650427,-1.9427997895,0.6216292862
 O,0,3.5079369931,2.1807424038,-0.3183792452
 O,0,0.764670167,2.9726689913,-0.9757740287
 H,0,2.6799231524,-2.1890753316,0.1721319723
 H,0,3.5611067646,-1.0799748011,1.2412589183
 H,0,3.566764963,-0.2037925647,-1.0766733591
 H,0,-3.5984238284,1.5553849714,2.589372919
 H,0,2.3811670788,1.3367093426,1.1092719533
 H,0,0.3098278952,1.4793235994,0.2665149875
 H,0,1.3703715384,3.2480825476,-1.748496131
 H,0,3.7661937978,2.021123287,-1.2893686826
 H,0,-5.3065082291,0.0350419256,2.0417611568
 H,0,0.7261956398,-1.0000838519,0.9986270045
 H,0,-0.5122876825,-2.3956526554,-1.4058264147
 O,0,1.3180989266,1.1171689486,-3.651282193
 As,0,2.6688261597,2.1463244294,-3.5739860759
 O,0,3.3035219312,2.2600241154,-5.2724049472
 O,0,2.2678299238,3.6873819368,-3.0438290429
 O,0,4.013393091,1.4648582188,-2.7913132788
 H,0,-0.140632286,0.3784600608,-2.1015410138
 H,0,4.187543995,1.8804991012,-5.1312795565

LG 2.5 Nuc 2.5

grid1aslg25.4

E(RB+HF-LYP) = -3518.65645001

Zero-point correction= 0.259715
 (Hartree/Particle)
 Thermal correction to Energy= 0.282038
 Thermal correction to Enthalpy= 0.282982
 Thermal correction to Gibbs Free Energy= 0.206111
 Sum of electronic and zero-point Energies= -
 3518.396735
 Sum of electronic and thermal Energies= -
 3518.374412
 Sum of electronic and thermal Enthalpies= -
 3518.373468
 Sum of electronic and thermal Free Energies= -
 3518.450339

	E (Thermal)	CV	S
Total	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
	176.981	83.393	161.788

C,0,1.0146814101,1.6928064616,-0.5358140801
 C,0,0.7334094925,0.5325763986,-1.4775418526
 O,0,1.5673221409,-0.4379670356,-1.3857615923
 C,0,2.6759236715,-0.1241812996,-0.441137137
 C,0,2.4670741469,1.3392922636,0.0205790848
 C,0,2.6211922046,-1.1824742043,0.6503712327
 O,0,1.5369970706,-1.0484511375,1.5425739847
 N,0,-0.8680437514,-0.7803807422,-0.0770088955
 C,0,-1.246410414,-1.8979105212,-0.7693032268

N,0,-2.5076313942,-2.3131500577,-0.6336726592
 C,0,-3.0250393071,-1.3836249536,0.2350513981
 C,0,-2.0151602654,-0.448113441,0.5750045647
 N,0,-2.1605283064,0.621452667,1.4299111151
 C,0,-3.3518822694,0.7316878965,1.9237653275
 N,0,-4.393386676,-0.1257203828,1.6501659147
 C,0,-4.3424893798,-1.2678766655,0.7914469367
 O,0,-5.3612293402,-1.9517683013,0.6569043935
 O,0,3.5060777846,2.1896119056,-0.339244424
 O,0,0.7641945511,2.9698677822,-0.9900290466
 H,0,2.6395973675,-2.1808064693,0.1748400032
 H,0,3.5404310674,-1.0908070246,1.2455618222
 H,0,3.5720211174,-0.2018642943,-1.0605052647
 H,0,-3.5856459186,1.5465422952,2.6085537531
 H,0,2.4004261436,1.3558685524,1.1142587456
 H,0,0.3143171499,1.5015761049,0.2912664345
 H,0,1.3698995592,3.2272861257,-1.784427801
 H,0,3.7365598652,2.0178453939,-1.3210414598
 H,0,-5.299213608,0.0273271153,2.0757359377
 H,0,0.7045402515,-0.9902114914,1.0112093545
 H,0,-0.5355537927,-2.4104345402,-1.4105329796
 O,0,1.3163543286,1.0878199752,-3.8443714221
 As,0,2.6471895623,2.1053784129,-3.6323425819
 O,0,3.4276634677,2.3107102307,-5.2636044277
 O,0,2.2273105785,3.6298831073,-3.0545539521
 O,0,3.944818989,1.4071435809,-2.7775264682
 H,0,-0.0881846632,0.42803744,-2.1647116948
 H,0,4.3146416356,1.9776964724,-5.0444028771

LG 2.5 Nuc 2.7

grid1aslg25.5

E(RB+HF-LYP) = -3518.65364310

C,0,1.02139284,1.6949772532,-0.5100840698
 C,0,0.7514530884,0.534882834,-1.4476323274
 O,0,1.6072860474,-0.4122684332,-1.3871722904
 C,0,2.6922455475,-0.1121115228,-0.4093000226
 C,0,2.4851245366,1.3574767477,0.0354263105
 C,0,2.5973642739,-1.1673448611,0.6832792446
 O,0,1.4955113769,-1.016419286,1.5504985604
 N,0,-0.882984121,-0.8019269765,-0.1091458095
 C,0,-1.2849507227,-1.90228583,-0.8154635696
 N,0,-2.5485363636,-2.3035574356,-0.6656733786
 C,0,-3.0411278761,-1.3812680317,0.2253263259
 C,0,-2.0162314149,-0.4628325522,0.5636443403
 N,0,-2.1342184292,0.5948160092,1.4368754428
 C,0,-3.3161598758,0.7112367349,1.9516372067
 N,0,-4.3714374034,-0.1301897765,1.6824673638
 C,0,-4.34781365,-1.2598363787,0.8062015103
 O,0,-5.3755517225,-1.9308443839,0.6789203163
 O,0,3.5089358255,2.2039096572,-0.3609815592
 O,0,0.762433117,2.9601325519,-0.9852977063
 H,0,2.6139906198,-2.1668650937,0.210841955
 H,0,3.503291609,-1.0860035049,1.2996267368
 H,0,3.6000567277,-0.2041087946,-1.0086592184
 H,0,-3.5290188114,1.5181621352,2.6523145835
 H,0,2.4338119146,1.3907840762,1.129850947
 H,0,0.3299204363,1.5050696129,0.3253909899
 H,0,1.3450054096,3.1920361757,-1.8187594264
 H,0,3.7011398295,2.0201046048,-1.3550704495
 H,0,-5.2682196752,0.0263059675,2.1256159131
 H,0,0.6726430439,-0.9864305637,1.0029067763
 H,0,-0.5906694066,-2.4128818925,-1.4760177432
 O,0,1.3363632409,1.0084440564,-4.0406252153
 As,0,2.6093177858,2.0494290758,-3.6958958317
 O,0,3.5091694898,2.3587428714,-5.2501399778
 O,0,2.1257454064,3.5487466698,-3.0884137469
 O,0,3.8750558115,1.3697158471,-2.773337736
 H,0,-0.0038035285,0.4702005845,-2.2159320449

H,0,4.3957094932,2.0866694719,-4.9575562398

LG 2.5 Nuc 2.7 (b)

gridaslg25.1

E(RB+HF-LYP) = -3518.65364310

Zero-point correction= 0.258945
(Hartree/Particle)
Thermal correction to Energy= 0.281356
Thermal correction to Enthalpy= 0.282300
Thermal correction to Gibbs Free Energy= 0.205021
Sum of electronic and zero-point Energies= -
3518.394698
Sum of electronic and thermal Energies= -
3518.372287
Sum of electronic and thermal Enthalpies= -
3518.371343
Sum of electronic and thermal Free Energies= -
3518.448622

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.554	83.482	162.648

C,0,1.02139284,1.6949772532,-0.5100840698
C,0,0.7514530884,0.534882834,-1.4476323274
O,0,1.6072860474,-0.4122684332,-1.3871722904
C,0,2.6922455475,-0.1121115228,-0.4093000226
C,0,2.4851245366,1.3574767477,0.0354263105
C,0,2.5973642739,-1.1673448611,0.6832792446
O,0,1.4955113769,-1.016419286,1.5504985604
N,0,-0.882984121,-0.8019269765,-0.1091458095
C,0,-1.2849507227,-1.90228583,-0.8154635696
N,0,-2.5485363636,-2.3035574356,-0.6656733786
C,0,-3.0411278761,-1.3812680317,0.2253263259
C,0,-2.0162314149,-0.4628325522,0.5636443403
N,0,-2.1342184292,0.5948160092,1.4368754428
C,0,-3.3161598758,0.7112367349,1.9516372067
N,0,-4.3714374034,-0.1301897765,1.6824673638
C,0,-4.34781365,-1.2598363787,0.8062015103
O,0,-5.3755517225,-1.9308443839,0.6789203163
O,0,3.5089358255,2.2039096572,-0.3609815592
O,0,0.762433117,2.9601325519,-0.9852977063
H,0,2.6139906198,-2.1668650937,0.210841955
H,0,3.503291609,-1.0860035049,1.2996267368
H,0,3.6000567277,-0.2041087946,-1.0086592184
H,0,-3.5290188114,1.5181621352,2.6523145835
H,0,2.4338119146,1.3907840762,1.129850947
H,0,0.3299204363,1.5050696129,0.3253909899
H,0,1.3450054096,3.1920361757,-1.8187594264
H,0,3.7011398295,2.0201046048,-1.3550704495
H,0,-5.2682196752,0.0263059675,2.1256159131
H,0,0.6726430439,-0.9864305637,1.0029067763
H,0,-0.5906694066,-2.4128818925,-1.4760177432
O,0,1.3363632409,1.0084440564,-4.0406252153
As,0,2.6093177858,2.0494290758,-3.6958958317
O,0,3.5091694898,2.3587428714,-5.2501399778
O,0,2.1257454064,3.5487466698,-3.0884137469
O,0,3.8750558115,1.3697158471,-2.773337736
H,0,-0.0038035285,0.4702005845,-2.2159320449
H,0,4.3957094932,2.0866694719,-4.9575562398

LG 2.5 Nuc 2.9

gridaslg25.2

E(RB+HF-LYP) = -3518.65167829

Zero-point correction= 0.258268
(Hartree/Particle)
Thermal correction to Energy= 0.280756

Thermal correction to Enthalpy= 0.281701
Thermal correction to Gibbs Free Energy= 0.203842
Sum of electronic and zero-point Energies= -
3518.393410
Sum of electronic and thermal Energies= -
3518.370922
Sum of electronic and thermal Enthalpies= -
3518.369978
Sum of electronic and thermal Free Energies= -
3518.447836

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.177	83.440	163.867

C,0,1.0420703678,1.6880629007,-0.4652036952
C,0,0.7770194026,0.5376765258,-1.4100744893
O,0,1.6449093171,-0.3968145224,-1.3801829552
C,0,2.7153468104,-0.1158799479,-0.3797096277
C,0,2.5224630693,1.3609260298,0.050044095
C,0,2.5824902415,-1.1652333063,0.7151295278
O,0,1.4718623416,-0.9889857102,1.5658351799
N,0,-0.8857157801,-0.8160380257,-0.1244739079
C,0,-1.2987371791,-1.9097098246,-0.8348474932
N,0,-2.5649097868,-2.3000893809,-0.6817453485
C,0,-3.0469824736,-1.3763777536,0.2138597266
C,0,-2.0142216335,-0.4676634662,0.5521785311
N,0,-2.1195695881,0.5876277197,1.4293469298
C,0,-3.2989252601,0.7127420524,1.9480801815
N,0,-4.3619533884,-0.1187876546,1.6795727295
C,0,-4.3508956005,-1.2457781429,0.7995742126
O,0,-5.3842655054,-1.9078634632,0.6736060969
O,0,3.529287948,2.1994515355,-0.3937104846
O,0,0.7698351834,2.9459270038,-0.9449038011
H,0,2.5868035201,-2.1667150909,0.2469767113
H,0,3.4808177546,-1.0991665266,1.3442387154
H,0,3.6311210682,-0.2291777078,-0.9625658607
H,0,-3.502472566,1.5192909041,2.6518535081
H,0,2.5002626471,1.4110744771,1.1451498683
H,0,0.3700848139,1.4911167626,0.3842908688
H,0,1.3103194313,3.1527618138,-1.8257907198
H,0,3.6729105876,2.0074366945,-1.4012037885
H,0,-5.2561590055,0.0444599591,2.1255139362
H,0,0.6545536602,-0.9752914951,1.0094018679
H,0,-0.6112229974,-2.4231391161,-1.500119067
O,0,1.347751531,0.936837464,-4.2252007363
As,0,2.5508371215,2.0049371608,-3.7613113973
O,0,3.5337957887,2.4303319359,-5.2376396409
O,0,1.989526237,3.4657579329,-3.1162618046
O,0,3.796171369,1.3460779922,-2.7919478188
H,0,0.0640837877,0.5070990529,-2.2252199265
H,0,4.4139512348,2.2177828378,-4.8828739637

LG 2.5 Nuc 3.1

gridaslg25.3

E(RB+HF-LYP) = -3518.65001404

Zero-point correction= 0.257889
(Hartree/Particle)
Thermal correction to Energy= 0.280479
Thermal correction to Enthalpy= 0.281424
Thermal correction to Gibbs Free Energy= 0.202303
Sum of electronic and zero-point Energies= -
3518.392125
Sum of electronic and thermal Energies= -
3518.369535
Sum of electronic and thermal Enthalpies= -
3518.368590

Sum of electronic and thermal Free Energies= -
3518.447711

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	176.003	83.365	166.523

C,0,1.0454255859,1.6851383463,-0.4277330713
 C,0,0.7886326949,0.5489624133,-1.3863282228
 O,0,1.6639784529,-0.3774644817,-1.3806630978
 C,0,2.7272128206,-0.111703734,-0.3680551958
 C,0,2.5373379213,1.3650800139,0.0646066725
 C,0,2.5777909016,-1.1658546614,0.7199811433
 O,0,1.4587193585,-0.9883555121,1.5596661863
 N,0,-0.8922376329,-0.8260013036,-0.147723891
 C,0,-1.3202534367,-1.9157296915,-0.8552070635
 N,0,-2.5877788634,-2.2957295294,-0.6895908574
 C,0,-3.0540832543,-1.3681841918,0.2106299876
 C,0,-2.0116029063,-0.4675869426,0.5391819812
 N,0,-2.0995790316,0.5885182229,1.4168630322
 C,0,-3.2729656212,0.7234939234,1.9466963336
 N,0,-4.3448927206,-0.0996000457,1.6885773069
 C,0,-4.3513919191,-1.2269723292,0.8087626616
 O,0,-5.3912302742,-1.8802447771,0.6922546164
 O,0,3.5268564412,2.2069584476,-0.4052841343
 O,0,0.7666431542,2.9410859131,-0.9037203087
 H,0,2.5829322414,-2.1652189803,0.2477947998
 H,0,3.4693079272,-1.1065502528,1.3592584764
 H,0,3.6461330146,-0.2285358302,-0.9451828579
 H,0,-3.4632144845,1.532066038,2.6517690645
 H,0,2.5352155028,1.4179641532,1.1600716368
 H,0,0.3853310241,1.4778187414,0.4282983819
 H,0,1.255613053,1.054703172,-1.8297309209
 H,0,3.644690578,2.0099939021,-1.4200196369
 H,0,-5.2336386851,0.0713089323,2.142512593
 H,0,0.646064061,-0.9828749424,0.9968597904
 H,0,-0.6433459887,-2.434278129,-1.5272491075
 O,0,1.4478269685,0.8080188747,-4.4043308244
 As,0,2.5277711809,1.9364103013,-3.8160063735
 O,0,3.5765032738,2.5047980136,-5.1978948244
 O,0,1.8245814353,3.3331760359,-3.1602026232
 O,0,3.7602725499,1.3424222785,-2.7860949222
 H,0,0.0920713422,0.5375668127,-2.2184458378
 H,0,4.4415478078,2.3693012733,-4.774654733

LG 2.7 Nuc 1.9

grid1aslg27.1

E(RB+HF-LYP) = -3518.68751716

Zero-point correction=	0.262055
(Hartree/Particle)	
Thermal correction to Energy=	0.284146
Thermal correction to Enthalpy=	0.285091
Thermal correction to Gibbs Free Energy=	0.208997
Sum of electronic and zero-point Energies=	-
3518.425462	
Sum of electronic and thermal Energies=	-
3518.403371	
Sum of electronic and thermal Enthalpies=	-
3518.402426	
Sum of electronic and thermal Free Energies=	-
3518.478520	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.305	82.907	160.152

C,0,1.1165413684,1.7561740927,-0.596893223
 C,0,0.8358918424,0.6532160101,-1.6204270933

O,0,1.5628727769,-0.4241601187,-1.3592378557
 C,0,2.6791319625,-0.1246529474,-0.4545458008
 C,0,2.5227791567,1.3468276977,0.0009218159
 C,0,2.6036255431,-1.1561114974,0.6641544988
 O,0,1.5085352119,-0.9800138469,1.5332457752
 N,0,-0.8947383734,-0.7047700641,-0.0549272728
 C,0,-1.2386922102,-1.7908425516,-0.8088445744
 N,0,-2.497476118,-2.2355045904,-0.7271159831
 C,0,-3.0496148349,-1.3643731251,0.1781822082
 C,0,-2.0588676959,-0.432564348,0.5903485573
 N,0,-2.2442353304,0.5863339494,1.5004489884
 C,0,-3.4463131108,0.646628216,1.9756103504
 N,0,-4.4677588373,-0.2114259923,1.632460275
 C,0,-4.3788483572,-1.3014089567,0.7114571171
 O,0,-5.385469963,-1.9921704233,0.5182019929
 O,0,3.6183381681,2.1616496096,-0.3216737878
 O,0,0.9153188014,3.0814806623,-0.9600817212
 H,0,2.6068656185,-2.1643791458,0.2079571738
 H,0,3.5167843925,-1.0709757376,1.2710858517
 H,0,3.5921357723,-0.2385900031,-1.0459160666
 H,0,-3.7092860288,1.4163784639,2.7015780352
 H,0,2.4318559719,1.3774661596,1.0914836572
 H,0,0.379904838,1.5360785828,0.1879533865
 H,0,1.5190073363,3.3486857108,-1.7124666313
 H,0,3.90107057,1.9698946519,-1.2650354963
 H,0,-5.3839536496,-0.1002327563,2.0485347782
 H,0,0.6890668076,-0.8919938714,0.9813969616
 H,0,-0.5033162686,-2.2587814747,-1.4562138318
 O,0,1.3294509031,1.1939018744,-3.3737258987
 As,0,2.768217335,2.1514590275,-3.5250779498
 O,0,3.1079582596,2.0273524487,-5.2939689113
 O,0,2.46817828,3.7424666657,-3.1282370393
 O,0,4.1219073642,1.4151959441,-2.8435568558
 H,0,-0.16078541,0.4515790702,-1.9739135392
 H,0,3.8861623777,1.4448502335,-5.2834957313

LG 2.7 Nuc 2.1

grid1aslg27.2

E(RB+HF-LYP) = -3518.67572307

Zero-point correction=	0.261205
(Hartree/Particle)	
Thermal correction to Energy=	0.283390
Thermal correction to Enthalpy=	0.284334
Thermal correction to Gibbs Free Energy=	0.207839
Sum of electronic and zero-point Energies=	-
3518.414519	
Sum of electronic and thermal Energies=	-
3518.392333	
Sum of electronic and thermal Enthalpies=	-
3518.391389	
Sum of electronic and thermal Free Energies=	-
3518.467884	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.830	83.067	160.999

C,0,1.1063719625,1.7474401407,-0.6010983311
 C,0,0.8101475127,0.6178883985,-1.5808841478
 O,0,1.5486965681,-0.4343292923,-1.3578324765
 C,0,2.679313966,-0.1291796069,-0.4568242232
 C,0,2.5225376552,1.3451615164,-0.0114258503
 C,0,2.6077573094,-1.1589805114,0.6630318794
 O,0,1.5255964347,-0.9746966743,1.5459387801
 N,0,-0.9037467134,-0.7535423608,-0.0087073854
 C,0,-1.2580039159,-1.8398670548,-0.7578858624
 N,0,-2.5232839313,-2.2646992272,-0.6811458633
 C,0,-3.0686919286,-1.3779334293,0.2131078412

C,0,-2.0683911901,-0.4576670503,0.6255448956
 N,0,-2.2451803725,0.5730355301,1.5234118827
 C,0,-3.4508710248,0.657488271,1.9859991124
 N,0,-4.4821316485,-0.1880872459,1.642166589
 C,0,-4.4020658498,-1.2886769006,0.7330325396
 O,0,-5.4168841437,-1.9653908771,0.5362709998
 O,0,3.6104718132,2.1566073499,-0.3455838463
 O,0,0.8949506952,3.0575632603,-0.9920428146
 H,0,2.6010525413,-2.168165463,0.2096048477
 H,0,3.5288333425,-1.0762147619,1.2575394863
 H,0,3.5775514187,-0.2459872459,-1.0684761582
 H,0,-3.7084928273,1.4393265131,2.7006724175
 H,0,2.435380577,1.3785902186,1.0795755856
 H,0,0.377678516,1.5368258384,0.1973506096
 H,0,1.5023267264,3.3193888755,-1.7553198773
 H,0,3.8755865,1.9755833335,-1.3026555227
 H,0,-5.4008978077,-0.0565571594,2.0465315138
 H,0,0.6931154486,-0.9087612696,1.010117895
 H,0,-0.5262415102,-2.3236249499,-1.3979143022
 O,0,1.3492578173,1.1700799449,-3.5339437552
 As,0,2.7603232463,2.1482660749,-3.5733519146
 O,0,3.2450659436,2.1340130362,-5.3178294093
 O,0,2.4339236559,3.7206675827,-3.1063564357
 O,0,4.1023732877,1.4196687484,-2.8466288394
 H,0,-0.1506351936,0.4402044268,-2.0312356233
 H,0,4.0794495894,1.6392296405,-5.2530880768

LG 2.7 Nuc 2.3

grid1aslg27.3
 E(RB+HF-LYP) = -3518.66688523

Zero-point correction= 0.260354
 (Hartree/Particle)
 Thermal correction to Energy= 0.282657
 Thermal correction to Enthalpy= 0.283601
 Thermal correction to Gibbs Free Energy= 0.206562
 Sum of electronic and zero-point Energies= -
 3518.406532
 Sum of electronic and thermal Energies= -
 3518.384228
 Sum of electronic and thermal Enthalpies= -
 3518.383284
 Sum of electronic and thermal Free Energies= -
 3518.460323

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.370	83.262	162.142

C,0,1.0706504046,1.7354296889,-0.6183715811
 C,0,0.788456289,0.5865252313,-1.5714932538
 O,0,1.5492055,-0.4373526983,-1.3780947842
 C,0,2.6719809156,-0.1212250125,-0.4567166328
 C,0,2.4902106762,1.3513026801,-0.0148863327
 C,0,2.603565743,-1.1581212976,0.6558127522
 O,0,1.5238635135,-0.9871620748,1.5439342014
 N,0,-0.9104085815,-0.8005412404,0.0032774964
 C,0,-1.2892768821,-1.8834537424,-0.7388938488
 N,0,-2.5606784221,-2.2852427334,-0.6492331539
 C,0,-3.0831656592,-1.3841942764,0.2447754031
 C,0,-2.0648270784,-0.4793627072,0.6442999808
 N,0,-2.215374784,0.559787624,1.5366014769
 C,0,-3.4157297272,0.6684448804,2.0082437537
 N,0,-4.4637671851,-0.1615868811,1.6786002298
 C,0,-4.4105236137,-1.2691026626,0.7758055853
 O,0,-5.4376029499,-1.9299350445,0.5919814037
 O,0,3.5663185463,2.1736325539,-0.3434936309
 O,0,0.8473487622,3.030281375,-1.0389329532
 H,0,2.6043148363,-2.1646139971,0.1967744567

H,0,3.5259814342,-1.0716036026,1.2473613334
 H,0,3.5681051729,-0.224629904,-1.0730145547
 H,0,-3.6537349443,1.4595931653,2.7192632991
 H,0,2.3908474503,1.3819388537,1.0753115963
 H,0,0.3380252901,1.5276935767,0.1795097753
 H,0,1.464532908,3.2864754844,-1.8101980777
 H,0,3.8290083726,1.9981723535,-1.3083177134
 H,0,-5.3767082473,-0.0114357596,2.0896637818
 H,0,0.6856826653,-0.9387689468,1.0149801559
 H,0,-0.5718229623,-2.3836112091,-1.3827653282
 O,0,1.3858151124,1.1262380187,-3.7259933926
 As,0,2.7606266321,2.1253122189,-3.6164364087
 O,0,3.4235691576,2.2204572443,-5.3033318957
 O,0,2.3852302736,3.6765276245,-3.0984955195
 O,0,4.0684209911,1.409187534,-2.8063851684
 H,0,-0.1184110462,0.4285664579,-2.1286436867
 H,0,4.2925159062,1.8110448451,-5.1528326046

LG 2.7 Nuc 2.5

grid1aslg27.4
 E(RB+HF-LYP) = -3518.66081448

Zero-point correction= 0.259626
 (Hartree/Particle)
 Thermal correction to Energy= 0.281974
 Thermal correction to Enthalpy= 0.282918
 Thermal correction to Gibbs Free Energy= 0.205711
 Sum of electronic and zero-point Energies= -
 3518.401188
 Sum of electronic and thermal Energies= -
 3518.378841
 Sum of electronic and thermal Enthalpies= -
 3518.377896
 Sum of electronic and thermal Free Energies= -
 3518.455103

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.941	83.366	162.496

C,0,1.0550103814,1.7361995958,-0.6163637279
 C,0,0.777360836,0.579965957,-1.5543431303
 O,0,1.5585101174,-0.4222921903,-1.3977511154
 C,0,2.669741476,-0.1121575661,-0.4496084628
 C,0,2.4816110401,1.3612942324,-0.0137253169
 C,0,2.5860147416,-1.152542347,0.6580111589
 O,0,1.5084649613,-0.9756947171,1.546719399
 N,0,-0.9178081195,-0.83019729,0.0038104968
 C,0,-1.3121519898,-1.9112049005,-0.7334402144
 N,0,-2.5856529664,-2.3012887013,-0.6309126123
 C,0,-3.0925663645,-1.3929692337,0.2650556209
 C,0,-2.0642733092,-0.4953402666,0.652612307
 N,0,-2.197324314,0.5481549632,1.5421422607
 C,0,-3.3924990209,0.6685694466,2.0242282652
 N,0,-4.4497633798,-0.1544686477,1.7077521049
 C,0,-4.4139363322,-1.2659280658,0.8088594909
 O,0,-5.4472071807,-1.9196418285,0.6372859318
 O,0,3.5482859417,2.1839972469,-0.3562918345
 O,0,0.8280890221,3.0188321871,-1.0621190008
 H,0,2.5804795102,-2.1574846376,0.1960882101
 H,0,3.5086808737,-1.0744933675,1.2501145571
 H,0,3.5674968373,-0.2160055031,-1.0627579154
 H,0,-3.6173809523,1.4645613053,2.7339541894
 H,0,2.384674267,1.3952768216,1.0767778106
 H,0,0.3250857784,1.5337963125,0.1869046623
 H,0,1.4475029443,3.2605417777,-1.851759058
 H,0,3.7928716465,2.0013668638,-1.3308973916
 H,0,-5.3575308064,0.0045469859,2.1269010494
 H,0,0.6685881026,-0.9418928603,1.0192984875

H,0,-0.6049608641,-2.419493438,-1.3823580621
 O,0,1.4047540978,1.0929119081,-3.919351622
 As,0,2.7467134646,2.0910801801,-3.6671193677
 O,0,3.5624750689,2.2858263406,-5.2803878082
 O,0,2.3369353924,3.6227228845,-3.1018833676
 O,0,4.008134766,1.3676101944,-2.7826666392
 H,0,-0.0716404074,0.45435245,-2.2054084688
 H,0,4.43945921,1.9361555278,-5.0477047269

LG 2.7 Nuc 2.7

grid1aslg27.5
 E(RB+HF-LYP) = -3518.65680718

Zero-point correction= 0.258692
 (Hartree/Particle)
 Thermal correction to Energy= 0.281148
 Thermal correction to Enthalpy= 0.282093
 Thermal correction to Gibbs Free Energy= 0.204382
 Sum of electronic and zero-point Energies= -
 3518.398115
 Sum of electronic and thermal Energies= -
 3518.375659
 Sum of electronic and thermal Enthalpies= -
 3518.374715
 Sum of electronic and thermal Free Energies= -
 3518.452425

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	176.423	83.501	163.556

C,0,1.0578201869,1.7299574804,-0.5871833839
 C,0,0.7881997327,0.5746283678,-1.5209261706
 O,0,1.590643358,-0.4079203797,-1.4016544467
 C,0,2.6852810414,-0.1086701423,-0.4255087105
 C,0,2.4993999007,1.3691703528,-0.0013995933
 C,0,2.572853991,-1.1481465251,0.6808720737
 O,0,1.4896543768,-0.9573170145,1.5591752188
 N,0,-0.9208689214,-0.8611950619,-0.0018849967
 C,0,-1.3332442513,-1.9315711678,-0.7449766605
 N,0,-2.6117538555,-2.3025426428,-0.6397964714
 C,0,-3.1023133628,-1.3910738605,0.2623732592
 C,0,-2.0604559489,-0.5108109551,0.6512779987
 N,0,-2.1740895739,0.530011225,1.5461790345
 C,0,-3.3657839465,0.6660293478,2.0328890088
 N,0,-4.4358392868,-0.1399366051,1.716414126
 C,0,-4.419893955,-1.2473606122,0.8118689438
 O,0,-5.4626917665,-1.8854254915,0.641340533
 O,0,3.5500453187,2.1905730517,-0.3801227029
 O,0,0.8186968668,3.0014444012,-1.049548737
 H,0,2.5600301319,-2.1528552553,0.2190831779
 H,0,3.490681248,-1.0816108951,1.281702622
 H,0,3.5892257566,-0.2231752092,-1.0269744856
 H,0,-3.5762229843,1.4619541366,2.7469802063
 H,0,2.4210492878,1.4147726208,1.0903935615
 H,0,0.3407609982,1.5250382413,0.2277368119
 H,0,1.4171897655,3.2269286547,-1.8763690082
 H,0,3.7562737744,2.0015632745,-1.3688272658
 H,0,-5.339791897,0.0309074414,2.1391668419
 H,0,0.6513904891,-0.9476953877,1.0280366062
 H,0,-0.6362063881,-2.4465758441,-1.399548528
 O,0,1.419062669,1.0330184545,-4.1058596194
 As,0,2.7022136492,2.0527589065,-3.7276953911
 O,0,3.6312927122,2.3565883301,-5.2636226703
 O,0,2.2291890067,3.5565441688,-3.1231600171
 O,0,3.9353861295,1.3436670119,-2.7861849545
 H,0,-0.0024257691,0.4829221115,-2.2508243308
 H,0,4.5074859861,2.0600730905,-4.9637557198

LG 2.7 Nuc 2.9

grid1aslg27.6
 E(RB+HF-LYP) = -3518.65403508

Zero-point correction= 0.257869
 (Hartree/Particle)
 Thermal correction to Energy= 0.280442
 Thermal correction to Enthalpy= 0.281386
 Thermal correction to Gibbs Free Energy= 0.202934
 Sum of electronic and zero-point Energies= -
 3518.396166
 Sum of electronic and thermal Energies= -
 3518.373594
 Sum of electronic and thermal Enthalpies= -
 3518.372649
 Sum of electronic and thermal Free Energies= -
 3518.451101

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	175.980	83.535	165.115

C,0,1.0889436298,1.719836513,-0.5242636532
 C,0,0.8209864818,0.5800990392,-1.4694294314
 O,0,1.6360568508,-0.3921512377,-1.3893470168
 C,0,2.7169390864,-0.1170630506,-0.39006999
 C,0,2.5520626714,1.3682605206,0.0202042286
 C,0,2.5630140982,-1.1498555174,0.7183950821
 O,0,1.4703502392,-0.9317753065,1.5775792426
 N,0,-0.913854041,-0.8878392778,-0.0115241836
 C,0,-1.3371059094,-1.9537228443,-0.7551141112
 N,0,-2.6206916892,-2.3065989469,-0.6541042425
 C,0,-3.1029149918,-1.3861160643,0.2436938899
 C,0,-2.0516628972,-0.5190798346,0.6351251108
 N,0,-2.1539070235,0.5251076088,1.5269931302
 C,0,-3.3459396467,0.6796241017,2.0075004134
 N,0,-4.4254575902,-0.1121607118,1.6881619064
 C,0,-4.4209346764,-1.2226681896,0.7870535893
 O,0,-5.4714588874,-1.8466959703,0.6136941645
 O,0,3.5827457061,2.1800113014,-0.4174362049
 O,0,0.8316256955,2.9873188498,-0.9795678515
 H,0,2.5370072095,-2.1561429235,0.2610495849
 H,0,3.4724205025,-1.0997997027,1.3335288434
 H,0,3.6280077595,-0.2567177558,-0.9747415086
 H,0,-3.548348623,1.4806403907,2.7181037382
 H,0,2.5131990808,1.4311987872,1.113590981
 H,0,0.3969507411,1.4997526496,0.3081450581
 H,0,1.3718418181,3.1875846058,-1.86480998
 H,0,3.7244883171,1.986383089,-1.4239124666
 H,0,-5.3291538916,0.0733468136,2.1052649894
 H,0,0.6375883311,-0.9434560477,1.0370940954
 H,0,-0.6448610527,-2.4787934962,-1.4066504177
 O,0,1.4018267946,0.9571551835,-4.2855356603
 As,0,2.6108481559,2.0079245795,-3.7948557468
 O,0,3.6163428205,2.4351573714,-5.2533779853
 O,0,2.057712613,3.4712315626,-3.1474090737
 O,0,3.8308350719,1.3214087877,-2.8144880676
 H,0,0.0771579806,0.5298216806,-2.2553591551
 H,0,4.4895837345,2.203441062,-4.8935151413

LG 2.7 Nuc 3.1

grid1aslg27.7
 E(RB+HF-LYP) = -3518.65195764

Zero-point correction= 0.257489
 (Hartree/Particle)
 Thermal correction to Energy= 0.280145
 Thermal correction to Enthalpy= 0.281090
 Thermal correction to Gibbs Free Energy= 0.201864

Sum of electronic and zero-point Energies= -
 3518.394469
 Sum of electronic and thermal Energies= -
 3518.371812
 Sum of electronic and thermal Enthalpies= -
 3518.370868
 Sum of electronic and thermal Free Energies= -
 3518.450093

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.794	83.456	166.743

C,0,1.0969011594,1.7062316478,-0.4781361816
 C,0,0.8426266514,0.5848175668,-1.4426523642
 O,0,1.6656762944,-0.3804833871,-1.3869628052
 C,0,2.7358153097,-0.1210846196,-0.3717224143
 C,0,2.5740447671,1.3650028251,0.0397067292
 C,0,2.5623551166,-1.1578644486,0.7303664324
 O,0,1.4614084731,-0.9360058481,1.5777133576
 N,0,-0.9073316512,-0.9096989994,-0.0305408119
 C,0,-1.3459618028,-1.9782480833,-0.7615647936
 N,0,-2.6330420412,-2.3143158686,-0.6517922126
 C,0,-3.1010088488,-1.3782919545,0.2377257989
 C,0,-2.0384961661,-0.5198301095,0.6158952517
 N,0,-2.1241087873,0.5348113626,1.4967800672
 C,0,-3.3124610497,0.7097266356,1.9795254679
 N,0,-4.4026349923,-0.072049255,1.6724700606
 C,0,-4.415024424,-1.192684096,0.7838950638
 O,0,-5.473436096,-1.8059219793,0.6214565014
 O,0,3.5844130732,2.1803144832,-0.4301394989
 O,0,0.8253104467,2.9742824028,-0.9184159458
 H,0,2.5352724437,-2.1619922729,0.2687555266
 H,0,3.4651641507,-1.1162393437,1.3557740611
 H,0,3.6517178152,-0.2662815335,-0.9472629551
 H,0,-3.5022523742,1.5210850111,2.681721426
 H,0,2.5584214204,1.4316486167,1.1337195658
 H,0,0.4198081421,1.4664668545,0.3605372177
 H,0,1.3035925079,3.1419644598,-1.8499591898
 H,0,3.6869110664,1.986146821,-1.4474598683
 H,0,-5.3026190663,0.1296662027,2.0900874672
 H,0,0.6336478047,-0.9577688795,1.0296435488
 H,0,-0.662812504,-2.5181147181,-1.4105620038
 O,0,1.4639043784,0.8506324144,-4.4681019187
 As,0,2.5538855109,1.9535234984,-3.8494952134
 O,0,3.6277194585,2.5273434902,-5.2076690269
 O,0,1.8639969026,3.3513012437,-3.1811680675
 O,0,3.7600172512,1.3189479879,-2.8135966972
 H,0,0.1249081312,0.5573824114,-2.2572074795
 H,0,4.4859159984,2.360247081,-4.7816979355

LG 2.9 Nuc 1.9

grid1aslg29.2
 E(RB+HF-LYP) = -3518.69307011

Zero-point correction=	0.261832
(Hartree/Particle)	
Thermal correction to Energy=	0.284001
Thermal correction to Enthalpy=	0.284945
Thermal correction to Gibbs Free Energy=	0.208180
Sum of electronic and zero-point Energies=	-
3518.431238	
Sum of electronic and thermal Energies=	-
3518.409069	
Sum of electronic and thermal Enthalpies=	-
3518.408125	
Sum of electronic and thermal Free Energies=	-
3518.484890	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.214	82.890	161.566

C,0,1.1740335441,1.806115594,-0.6489447688
 C,0,0.8846091511,0.7022310862,-1.6667747955
 O,0,1.5685429963,-0.3924630365,-1.3656751272
 C,0,2.6872135808,-0.105290283,-0.4572099871
 C,0,2.5655301415,1.3781806831,-0.0320338247
 C,0,2.5769152648,-1.113689978,0.6803969767
 O,0,1.4951160676,-0.88443916,1.5512534571
 N,0,-0.949745276,-0.7552040526,0.0423236399
 C,0,-1.2956723076,-1.7937137957,-0.7725352564
 N,0,-2.5640698252,-2.2178197065,-0.7376646003
 C,0,-3.1190468264,-1.3814916281,0.1978881109
 C,0,-2.1207088505,-0.4895210179,0.6759185889
 N,0,-2.3078101514,0.4900021526,1.628126611
 C,0,-3.5190664976,0.5507311793,2.0794351358
 N,0,-4.5477630131,-0.2712088417,1.6750517713
 C,0,-4.4586270147,-1.3174108858,0.7046722759
 O,0,-5.4734474119,-1.9782090603,0.4571728486
 O,0,3.6816667218,2.1600495787,-0.363848594
 O,0,0.9939874959,3.1318156262,-1.0186000562
 H,0,2.5441963387,-2.1287063679,0.2407412184
 H,0,3.4960508858,-1.049718522,1.2811535804
 H,0,3.6011505196,-0.2553101591,-1.0394924601
 H,0,-3.7847268785,1.2911621585,2.8344417663
 H,0,2.4677675858,1.4332874658,1.0568134611
 H,0,0.4252786925,1.5933528255,0.1289883311
 H,0,1.6061621413,3.3825412358,-1.7709200111
 H,0,3.9644878558,1.9482947019,-1.3028569483
 H,0,-5.4713135175,-0.1609296076,2.074803634
 H,0,0.6620523444,-0.8344911609,1.0112983087
 H,0,-0.5551271086,-2.2426183545,-1.4274402995
 O,0,1.3992098347,1.1905895395,-3.4293546996
 As,0,2.8485679569,2.13664398,-3.5709737525
 O,0,3.1967536489,2.0024460652,-5.3363535261
 O,0,2.5604223288,3.7320896979,-3.1838069081
 O,0,4.1858898072,1.3848515803,-2.8759046064
 H,0,-0.1219168749,0.5146791714,-2.0092778754
 H,0,3.9656811196,1.4078389164,-5.3211454587

LG 2.9 Nuc 2.1

grid1aslg29.3
 E(RB+HF-LYP) = -3518.68027892

Zero-point correction=	0.260990
(Hartree/Particle)	
Thermal correction to Energy=	0.283255
Thermal correction to Enthalpy=	0.284200
Thermal correction to Gibbs Free Energy=	0.206954
Sum of electronic and zero-point Energies=	-
3518.419289	
Sum of electronic and thermal Energies=	-
3518.397024	
Sum of electronic and thermal Enthalpies=	-
3518.396079	
Sum of electronic and thermal Free Energies=	-
3518.473325	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.745	83.053	162.576

C,0,1.1573408835,1.7978666663,-0.6602531183
 C,0,0.8568321737,0.6686331894,-1.6367430733
 O,0,1.5522260948,-0.4023320318,-1.3694383827
 C,0,2.6816857146,-0.1088663923,-0.4600322535
 C,0,2.5560956342,1.3768465612,-0.0446411721

C,0,2.5745979684,-1.1164195599,0.6781468994
 O,0,1.504265883,-0.8816995358,1.5608657762
 N,0,-0.9567187153,-0.8006975786,0.0843311873
 C,0,-1.3142210301,-1.8387408279,-0.7266351829
 N,0,-2.5884841499,-2.2436355919,-0.6943015412
 C,0,-3.1349652678,-1.3932005669,0.2334267831
 C,0,-2.1266278746,-0.5130348213,0.7106494268
 N,0,-2.3034576816,0.4764781166,1.6541238236
 C,0,-3.5166115295,0.5599247109,2.0969907951
 N,0,-4.5552760373,-0.2491893269,1.6929109959
 C,0,-4.4766928928,-1.304513123,0.7314952835
 O,0,-5.4995578476,-1.9512136129,0.4820728789
 O,0,3.6656313136,2.1568170529,-0.3819107773
 O,0,0.968171487,3.1088402865,-1.0567502092
 H,0,2.534943408,-2.1319333861,0.2408515125
 H,0,3.5006931541,-1.0535024638,1.2675882457
 H,0,3.5828373815,-0.2599032246,-1.0600355908
 H,0,-3.7752862112,1.3107350384,2.8439720106
 H,0,2.4565506384,1.4340443497,1.0440768135
 H,0,0.4127100515,1.5925383831,0.1273803649
 H,0,1.5858194952,3.3541002366,-1.8186538543
 H,0,3.9356257414,1.9560484617,-1.333647661
 H,0,-5.4798088208,-0.1199787186,2.0846822851
 H,0,0.6594351502,-0.8544319413,1.0370477115
 H,0,-0.578863625,-2.3027647665,-1.3770068299
 O,0,1.4237652763,1.1689550456,-3.5958914467
 As,0,2.8476250829,2.1326261831,-3.6170237943
 O,0,3.3507423914,2.1058080969,-5.3547772247
 O,0,2.5322155628,3.7108235513,-3.1630231968
 O,0,4.1675864754,1.3874738144,-2.8692822051
 H,0,-0.1122508208,0.4989036441,-2.0781921203
 H,0,4.1736700123,1.5932617014,-5.2827069991

LG 2.9 Nuc 2.3

grid1aslg29.4

E(RB+HF-LYP) = -3518.67058101

Zero-point correction=	0.260145
(Hartree/Particle)	
Thermal correction to Energy=	0.282508
Thermal correction to Enthalpy=	0.283452
Thermal correction to Gibbs Free Energy=	0.205876
Sum of electronic and zero-point Energies=	-
3518.410436	
Sum of electronic and thermal Energies=	-
3518.388073	
Sum of electronic and thermal Enthalpies=	-
3518.387129	
Sum of electronic and thermal Free Energies=	-
3518.464705	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.276	83.253	163.273

C,0,1.1032150955,1.7857400516,-0.6973161234
 C,0,0.8297853982,0.6351556884,-1.6478962777
 O,0,1.546404831,-0.4076099343,-1.3999784307
 C,0,2.6625123228,-0.0965955551,-0.4639595819
 C,0,2.4983174033,1.3854386534,-0.0485013854
 C,0,2.5638198513,-1.1161876333,0.6625094632
 O,0,1.4939430859,-0.9045278326,1.5504672389
 N,0,-0.9633948446,-0.848443978,0.0822572659
 C,0,-1.3536306756,-1.8827911263,-0.7184257269
 N,0,-2.6342981295,-2.2629387087,-0.6628362276
 C,0,-3.1489868257,-1.3982733356,0.2701478044
 C,0,-2.1173836938,-0.5349557114,0.7258909757
 N,0,-2.258478688,0.4621647268,1.6669287923
 C,0,-3.4617042215,0.56975378,2.1312965834

N,0,-4.5214572165,-0.2227754774,1.750532636
 C,0,-4.4796214688,-1.2838567711,0.7930471099
 O,0,-5.5175101715,-1.9138342909,0.5658713218
 O,0,3.5980328078,2.1827922627,-0.360615697
 O,0,0.9059876958,3.0801088639,-1.127943154
 H,0,2.5380956227,-2.1277184091,0.2152922199
 H,0,3.4908314391,-1.0460397711,1.2493449677
 H,0,3.5643424108,-0.224102914,-1.0673587109
 H,0,-3.6929998358,1.3289346093,2.8786296306
 H,0,2.3697051924,1.4345548974,1.037637868
 H,0,0.345123686,1.5818374709,0.0807450254
 H,0,1.546511271,3.3208250007,-1.8871914972
 H,0,3.8785066818,1.9916623541,-1.3169223965
 H,0,-5.435935682,-0.0755762404,2.1592188385
 H,0,0.6466598454,-0.8873667624,1.0301050368
 O,0,-0.6385015166,-2.3651524519,-1.3782693723
 O,0,1.4818185585,1.1299676833,-3.797317184
 As,0,2.8679669717,2.1120026281,-3.6519161669
 O,0,3.5753577972,2.189899977,-5.3201386121
 O,0,2.4971160119,3.6709457108,-3.1551041094
 O,0,4.1381494504,1.378947738,-2.8005890675
 H,0,-0.0801619645,0.4770300392,-2.2040437588
 H,0,4.4241059737,1.745652388,-5.1539331382

LG 2.9 Nuc 2.5

grid1aslg29.5

E(RB+HF-LYP) = -3518.66377757

Zero-point correction=	0.259433
(Hartree/Particle)	
Thermal correction to Energy=	0.281831
Thermal correction to Enthalpy=	0.282775
Thermal correction to Gibbs Free Energy=	0.205092
Sum of electronic and zero-point Energies=	-
3518.404344	
Sum of electronic and thermal Energies=	-
3518.381946	
Sum of electronic and thermal Enthalpies=	-
3518.381002	
Sum of electronic and thermal Free Energies=	-
3518.458685	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	176.852	83.370	163.498

C,0,1.0784443334,1.7805975923,-0.7064791259
 C,0,0.8129375356,0.6232632675,-1.6417687709
 O,0,1.5452909458,-0.4022944892,-1.4227611689
 C,0,2.652269775,-0.0926963223,-0.4643174904
 C,0,2.4756294191,1.3882615596,-0.0493438852
 C,0,2.5497045498,-1.1198260899,0.6544802563
 O,0,1.4838693561,-0.9134599064,1.5480081128
 N,0,-0.9694984588,-0.8765179158,0.0855322112
 C,0,-1.3761066343,-1.9140873869,-0.7032732529
 N,0,-2.658876014,-2.2826299367,-0.6313888441
 C,0,-3.1570386862,-1.4056071935,0.2992633288
 C,0,-2.114681866,-0.5470225658,0.7372455961
 N,0,-2.2373758323,0.4596891751,1.6702564305
 C,0,-3.4349056791,0.5813517049,2.1459893711
 N,0,-4.5044954643,-0.206264911,1.78368782
 C,0,-4.4812760007,-1.2762136963,0.8353597006
 O,0,-5.5257404914,-1.9004342892,0.6249662145
 O,0,3.5673099647,2.1898901928,-0.3623931877
 O,0,0.8786171051,3.0643868793,-1.1569263328
 H,0,2.5235089667,-2.1285326994,0.2014067898
 H,0,3.4787232727,-1.0531335672,1.2382350465
 H,0,3.5534208086,-0.212748619,-1.069901595
 H,0,-3.6522070661,1.3493517966,2.8883516457

H,0,2.3411522597,1.4351240796,1.0362583963
H,0,0.3170491698,1.5777350003,0.0709971568
H,0,1.5227447314,3.2932767186,-1.9320475918
H,0,3.8382932624,1.9998849712,-1.3272175884
H,0,-5.4133849026,-0.0480675502,2.200680213
H,0,0.6327822249,-0.9059900369,1.0335990755
H,0,-0.6720455304,-2.4086376204,-1.3661245241
O,0,1.5232209779,1.0946433401,-3.9919368161
As,0,2.8644967669,2.0847931366,-3.6986291948
O,0,3.7283051181,2.2650953828,-5.2870913013
O,0,2.4478690428,3.6229636591,-3.1571894656
O,0,4.0884269233,1.3529032419,-2.7719425804
H,0,-0.0375399012,0.4934234565,-2.292631491
H,0,4.5933504876,1.9021972612,-5.0312866944

LG 2.9 Nuc 2.7

grid1aslg29.6

E(RB+HF-LYP) = -3518.65912855

Zero-point correction=	0.258406
(Hartree/Particle)	
Thermal correction to Energy=	0.280908
Thermal correction to Enthalpy=	0.281852
Thermal correction to Gibbs Free Energy=	0.203590
Sum of electronic and zero-point Energies=	-
3518.400722	
Sum of electronic and thermal Energies=	-
3518.378221	
Sum of electronic and thermal Enthalpies=	-
3518.377277	
Sum of electronic and thermal Free Energies=	-
3518.455539	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	176.272	83.506	164.716

C,0,1.1028006082,1.7763271042,-0.6470460392
C,0,0.8244602887,0.6304261297,-1.5833723506
O,0,1.5747050389,-0.3845854814,-1.4195886638
C,0,2.676927413,-0.1002042382,-0.4413526771
C,0,2.523425565,1.3854716549,-0.0322872248
C,0,2.5404145798,-1.125877416,0.6757112261
O,0,1.4743771242,-0.8932137492,1.5615044735
N,0,-0.9629119024,-0.9221711153,0.0913632306
C,0,-1.3762863581,-1.9714615351,-0.6784964714
N,0,-2.6634175294,-2.3228791483,-0.6071890803
C,0,-3.1575368632,-1.4195307483,0.3004363917
C,0,-2.1087298004,-0.5641227322,0.7271773831
N,0,-2.2248662729,0.4643725337,1.6365426229
C,0,-3.4244192821,0.6120130095,2.099945533
N,0,-4.5008496451,-0.1702999138,1.7471420364
C,0,-4.4841032551,-1.261814388,0.823391637
O,0,-5.5341521216,-1.8782307859,0.6194818292
O,0,3.6005093462,2.1767070628,-0.3996102082
O,0,0.8884517613,0.0550506025,-1.095359657
H,0,2.4942940033,-2.1337398951,0.2230218846
H,0,3.4673126229,-1.0804805801,1.2649194719
H,0,3.5776916553,-0.2409789583,-1.0422428597
H,0,-3.6373938599,1.3994440719,2.8228099503
H,0,2.4269775341,1.4420300113,1.0571632627
H,0,0.3654101954,1.5630854582,0.1520373986
H,0,1.4971699138,3.2703277312,-1.9200733969
H,0,3.8122449386,1.9829646759,-1.385937286
H,0,-5.4110094183,0.0094507079,2.1524900187
H,0,0.6226747767,-0.9118704996,1.0471258471
H,0,-0.674485895,-2.4874323278,-1.3272905759
O,0,1.491757394,1.0633253108,-4.1635486612
As,0,2.7841328381,2.0626708245,-3.7580712418

O,0,3.7385706634,2.3624392135,-5.2776848381
O,0,2.3236939333,3.5708255238,-3.1543559185
O,0,3.9890958095,1.3259763365,-2.8031338925
H,0,0.0221718775,0.5432786813,-2.3023210549
H,0,4.6031367918,2.0373744883,-4.9736359396

LG 2.9 Nuc 2.9

grid1aslg29.7

E(RB+HF-LYP) = -3518.65590172

Zero-point correction=	0.257364
(Hartree/Particle)	
Thermal correction to Energy=	0.279996
Thermal correction to Enthalpy=	0.280940
Thermal correction to Gibbs Free Energy=	0.201879
Sum of electronic and zero-point Energies=	-
3518.398538	
Sum of electronic and thermal Energies=	-
3518.375906	
Sum of electronic and thermal Enthalpies=	-
3518.374961	
Sum of electronic and thermal Free Energies=	-
3518.454023	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	175.700	83.575	166.398

C,0,1.148468908,1.7637854846,-0.5754751823
C,0,0.8606751559,0.6361460015,-1.5225213344
O,0,1.6197801361,-0.3750101534,-1.4050935343
C,0,2.7131725164,-0.1209712803,-0.4046806791
C,0,2.5951726285,1.3731475035,-0.0148043378
C,0,2.5294199536,-1.133481324,0.7185214636
O,0,1.4657025262,-0.8557937128,1.5924962984
N,0,-0.9457283587,-0.9359346824,0.1131620851
C,0,-1.3537541547,-1.9833238743,-0.6627233773
N,0,-2.6450261375,-2.3216325045,-0.6154068172
C,0,-3.1483143004,-1.4104090556,0.27937599
C,0,-2.1005336539,-0.5639659194,0.7246206826
N,0,-2.2236785968,0.4669170708,1.630066453
C,0,-3.4308659475,0.6281468953,2.068575184
N,0,-4.5078370183,-0.1438277929,1.6956366303
C,0,-4.4834326113,-1.2385574449,0.7758149332
O,0,-5.5347574251,-1.8458256999,0.5531762344
O,0,3.6536170884,2.145730406,-0.4551934742
O,0,0.9187131117,3.0405592954,-1.0102341709
H,0,2.451702621,-2.1423969798,0.2730784034
H,0,3.4534621234,-1.1166063648,1.3140700752
H,0,3.617374364,-0.2990007398,-0.9899205404
H,0,-3.6501942336,1.4193601752,2.7853194288
H,0,2.5499018691,1.4512289431,1.0769739067
H,0,0.4425278344,1.535139302,0.2470912053
H,0,1.4632196006,3.2352114583,-1.9027621977
H,0,3.7864818989,1.9496639939,-1.4621483417
H,0,-5.4242797489,0.0468740957,2.0813633332
H,0,0.6138714153,-0.8937455208,1.0771796461
H,0,-0.6449427915,-2.5070528378,-1.2974125108
O,0,1.4323850094,1.0135518463,-4.3404468759
As,0,2.6693399131,2.0229985416,-3.8320315557
O,0,3.6880640727,2.4441825672,-5.2807160022
O,0,2.1531835437,3.4939712113,-3.1683689581
O,0,3.8608497603,1.2886039616,-2.853623287
H,0,0.1107991889,0.5954894971,-2.3040556763
H,0,4.5577042086,2.2014952572,-4.9192369401

LG 2.9 Nuc 3.1

grid1aslg29.8

E(RB+HF-LYP) = -3518.65365135

Zero-point correction= 0.257024
 (Hartree/Particle)
 Thermal correction to Energy= 0.279762
 Thermal correction to Enthalpy= 0.280706
 Thermal correction to Gibbs Free Energy= 0.200499
 Sum of electronic and zero-point Energies= -
 3518.396627
 Sum of electronic and thermal Energies= -
 3518.373889
 Sum of electronic and thermal Enthalpies= -
 3518.372945
 Sum of electronic and thermal Free Energies= -
 3518.453152

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.553	83.497	168.810

C,0,1.1806166604,1.7426563406,-0.5288955545
 C,0,0.9107444847,0.6335637781,-1.4958393233
 O,0,1.6639807174,-0.381032093,-1.3829976757
 C,0,2.7406548957,-0.1415025678,-0.3647162242
 C,0,2.6385368126,1.3594538118,0.0096842175
 C,0,2.5271042062,-1.1440129637,0.7629078393
 O,0,1.4525066789,-0.847248524,1.6167604947
 N,0,-0.926735583,-0.9512289056,0.0922722207
 C,0,-1.3439097374,-2.0033351317,-0.6723023425
 N,0,-2.6383723211,-2.3281983417,-0.6228444325
 C,0,-3.1341402536,-1.4014942572,0.2603562852
 C,0,-2.0790036249,-0.5604562225,0.6973426689
 N,0,-2.1925393915,0.4827822991,1.5894564919
 C,0,-3.3988997678,0.662703821,2.023100665
 N,0,-4.4829229657,-0.1027813465,1.6577745633
 C,0,-4.4682549833,-1.2098901014,0.7524478825
 O,0,-5.5251573049,-1.8095475607,0.5363885128
 O,0,3.6806946483,2.1225673279,-0.4780613471
 O,0,0.9340948306,3.0228196815,-0.9367287965
 H,0,2.4451889395,-2.1551954295,0.3236164233
 H,0,3.4414067441,-1.1334005823,1.3733943657
 H,0,3.6516340598,-0.3386518078,-0.9329546953
 H,0,-3.611277645,1.4658073038,2.7285346582
 H,0,2.6208513575,1.4553071132,1.1008788882
 H,0,0.4880504044,1.4845651592,0.2965136715
 H,0,1.4049423481,3.2031605672,-1.8769074205
 H,0,3.7373813662,1.9331890826,-1.4979374878
 H,0,-5.3981670404,0.1027443506,2.038713579
 H,0,0.6080045866,-0.8979550375,1.0898411559
 H,0,-0.6397438363,-2.5412498948,-1.3002427334
 O,0,1.3940878707,0.9852655735,-4.5376615004
 As,0,2.5515424183,2.0024163437,-3.8941887522
 O,0,3.6613118658,2.5351405576,-5.2377856068
 O,0,1.9543218202,3.4278698169,-3.1938440615
 O,0,3.7034640683,1.2635926955,-2.8675905264
 H,0,0.2022699953,0.6202052396,-2.3208578937
 H,0,4.5079771453,2.3060375245,-4.8179620497

LG 3.1 Nuc 1.9

lg31.1
 E(RB+HF-LYP) = -3518.69630863

Zero-point correction= 0.261505
 (Hartree/Particle)
 Thermal correction to Energy= 0.283786
 Thermal correction to Enthalpy= 0.284730
 Thermal correction to Gibbs Free Energy= 0.206900
 Sum of electronic and zero-point Energies= -
 3518.434804

Sum of electronic and thermal Energies= -
 3518.412523
 Sum of electronic and thermal Enthalpies= -
 3518.411578
 Sum of electronic and thermal Free Energies= -
 3518.489408

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.078	82.958	163.807

C,0,1.2304429276,1.8424868839,-0.669297612
 C,0,0.9234224872,0.7532903762,-1.6986966551
 O,0,1.569853827,-0.3614517638,-1.3882248885
 C,0,2.6917211888,-0.1067441477,-0.4732338021
 C,0,2.6075313686,1.3788142271,-0.0463997917
 C,0,2.5523518098,-1.1121662156,0.6655604685
 O,0,1.4942365358,-0.8438482618,1.5522013725
 N,0,-0.9928778239,-0.8335155344,0.1505831812
 C,0,-1.3443514908,-1.8135166955,-0.7296550703
 N,0,-2.6285047042,-2.1891074671,-0.7620433265
 C,0,-3.1869020331,-1.3790305056,0.1938124585
 C,0,-2.1752420708,-0.5504214543,0.7527125103
 N,0,-2.362905788,0.3888613851,1.7447110911
 C,0,-3.5881122151,0.4751194416,2.1522568599
 N,0,-4.6299807456,-0.2858076141,1.6698424978
 C,0,-4.541846244,-1.2874506207,0.6532053911
 O,0,-5.5701655532,-1.8953394811,0.3359262797
 O,0,3.7439641876,2.133532706,-0.3720009922
 O,0,1.0803871188,3.1742404499,-1.0288942313
 H,0,2.4765304342,-2.1242910097,0.2247807421
 H,0,3.4818081083,-1.0836524307,1.253177568
 H,0,3.6035391736,-0.2805718828,-1.0520833028
 H,0,-3.8558832075,1.1887404156,2.932004672
 H,0,2.505285569,1.4346544682,1.0416785488
 H,0,0.4727321488,1.6373386671,0.1033135263
 H,0,1.704163299,3.415894451,-1.7752740612
 H,0,4.0239440137,1.9174698779,-3.3105542921
 H,0,-5.5640444323,-0.157682658,2.0386219559
 H,0,0.6414357733,-0.8234112008,1.038527281
 H,0,-0.5967951574,-2.2571487733,-1.3800655867
 O,0,1.4485690482,1.2443838581,-3.4574026213
 As,0,2.9267224736,2.15054491,-3.5804369532
 O,0,3.276250491,2.0274500607,-5.3456038182
 O,0,2.6784230658,3.7485808961,-3.1771151651
 O,0,4.2369511172,1.3538067707,-2.8857226984
 H,0,-0.0886660956,0.5850953928,-2.0410888004
 H,0,4.0182558645,1.3995200988,-5.3394565754

LG 3.1 Nuc 2.1

lg31.2
 E(RB+HF-LYP) = -3518.68296100

Zero-point correction= 0.260641
 (Hartree/Particle)
 Thermal correction to Energy= 0.283028
 Thermal correction to Enthalpy= 0.283972
 Thermal correction to Gibbs Free Energy= 0.205418
 Sum of electronic and zero-point Energies= -
 3518.422320
 Sum of electronic and thermal Energies= -
 3518.399933
 Sum of electronic and thermal Enthalpies= -
 3518.398989
 Sum of electronic and thermal Free Energies= -
 3518.477543

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
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Total 177.603 83.119 165.331

C,0,1.2248801326,1.8626642715,-0.6944439379
 C,0,0.8897003628,0.7497044648,-1.6781943587
 O,0,1.5235984887,-0.3529212736,-1.3894372199
 C,0,2.6654344751,-0.1048580189,-0.4796258298
 C,0,2.5985037566,1.3848435789,-0.0653970453
 C,0,2.5231847883,-1.1063001086,0.6610154387
 O,0,1.4790550644,-0.8223081724,1.5584397672
 N,0,-1.0149979939,-0.8439275687,0.1771914101
 C,0,-1.3699310207,-1.8232696095,-0.7032370612
 N,0,-2.6526258884,-2.2024831428,-0.7269963029
 C,0,-3.2066112835,-1.3963849663,0.2346486441
 C,0,-2.1943841493,-0.5661370597,0.7885677463
 N,0,-2.3778797278,0.3703103859,1.7838802368
 C,0,-3.6008251065,0.452244473,2.1993646545
 N,0,-4.6435317364,-0.3104008967,1.7219855419
 C,0,-4.5591298256,-1.3096971336,0.7029004485
 O,0,-5.5870410766,-1.9199208766,0.3902912057
 O,0,3.7416035722,2.1190635772,-0.39246913
 O,0,1.0884603,3.1811582007,-1.0849546505
 H,0,2.4321373959,-2.1188729293,0.224957165
 H,0,3.460109058,-1.0851125712,1.2364115085
 H,0,3.5585038916,-0.2908466652,-1.0820576306
 H,0,-3.8655277003,1.1634717235,2.9822217478
 H,0,2.4905497396,1.446139254,1.0220683483
 H,0,0.4646948219,1.6785302318,0.0853513869
 H,0,1.7226333088,3.4033141575,-1.8413198857
 H,0,4.0125442761,1.9072016847,-1.3411743677
 H,0,-5.5756409805,-0.1854094911,2.0967932571
 H,0,0.6166408253,-0.8157574713,1.0596410713
 H,0,-0.6268435074,-2.2631045289,-1.3614170237
 O,0,1.4964071091,1.2180050075,-3.6333408998
 As,0,2.955361433,2.130153342,-3.6329931658
 O,0,3.4725373599,2.0935246763,-5.3656261434
 O,0,2.691026775,3.716439355,-3.17453302
 O,0,4.2379731202,1.3328104256,-2.8755152275
 H,0,-0.0855386318,0.6195608974,-2.1234561642
 H,0,4.2772130436,1.5532403972,-5.2898743543

LG 3.1 Nuc 2.3

lg31.3

E(RB+HF-LYP) = -3518.67284699

Zero-point correction= 0.259869
 (Hartree/Particle)
 Thermal correction to Energy= 0.282332
 Thermal correction to Enthalpy= 0.283276
 Thermal correction to Gibbs Free Energy= 0.204760
 Sum of electronic and zero-point Energies= -
 3518.412978
 Sum of electronic and thermal Energies= -
 3518.390515
 Sum of electronic and thermal Enthalpies= -
 3518.389571
 Sum of electronic and thermal Free Energies= -
 3518.468087

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.166	83.320	165.252

C,0,1.1304684915,1.8391526314,-0.7751904673
 C,0,0.8563683683,0.6990733556,-1.7355536588
 O,0,1.5079985986,-0.37276665,-1.4398584202
 C,0,2.6252715444,-0.088126361,-0.4944581681
 C,0,2.4844755623,1.3948120421,-0.0723919463
 C,0,2.5121522553,-1.1135866778,0.6259005198
 O,0,1.4594103617,-0.8873518786,1.5289090203

N,0,-1.0309919763,-0.8846160912,0.1458794416
 C,0,-1.4379423485,-1.8597552598,-0.7167756009
 N,0,-2.7276211127,-2.2132677884,-0.6905622692
 C,0,-3.228761816,-1.393780578,0.2889278191
 C,0,-2.1810425936,-0.5816421971,0.8001125206
 N,0,-2.3066255266,0.3615249185,1.7976799236
 C,0,-3.5100681833,0.4672801418,2.261855747
 N,0,-4.5845363615,-0.2777761656,1.8297267902
 C,0,-4.5596441094,-1.2814263746,0.8116209421
 O,0,-5.6096847294,-1.8737871297,0.5426801146
 O,0,3.6167728396,2.1642786018,-0.3330438439
 O,0,0.9858189672,3.1405806909,-1.2030036417
 H,0,2.4617909821,-2.1207323891,0.1710218452
 H,0,3.4476443641,-1.0665739561,1.2014682387
 H,0,3.5263769368,-0.2240319839,-1.0981120802
 H,0,-3.7297259894,1.1857562518,3.0518501831
 H,0,2.3130210052,1.4386244384,1.0076998691
 H,0,0.3345676675,1.6498274037,-0.0294520296
 H,0,1.6561678628,3.3602185671,-1.9427017177
 H,0,3.934919852,1.9701323521,-1.2760497825
 H,0,-5.4979538613,-0.1355620042,2.2425175627
 H,0,0.5983539215,-0.8824496755,1.0285870015
 H,0,-0.7294677925,-2.3193570092,-1.3995986785
 O,0,1.6298309374,1.1419233143,-3.8558445651
 As,0,3.0218679611,2.1065979962,-3.6538375869
 O,0,3.7898170495,2.1681860727,-5.2950872978
 O,0,2.6548540911,3.6723284409,-3.1758263161
 O,0,4.2492636015,1.359531355,-2.7539242995
 H,0,-0.0436071633,0.5713930086,-2.3178050808
 H,0,4.6427048121,1.7500362068,-5.087693928

LG 3.1 Nuc 2.5

lg31.4

E(RB+HF-LYP) = -3518.66562041

Zero-point correction= 0.259065
 (Hartree/Particle)
 Thermal correction to Energy= 0.281559
 Thermal correction to Enthalpy= 0.282503
 Thermal correction to Gibbs Free Energy= 0.203853
 Sum of electronic and zero-point Energies= -
 3518.406555
 Sum of electronic and thermal Energies= -
 3518.384061
 Sum of electronic and thermal Enthalpies= -
 3518.383117
 Sum of electronic and thermal Free Energies= -
 3518.461767

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.681	83.427	165.534

C,0,1.1150088467,1.8342283082,-0.781221128
 C,0,0.8452498542,0.6872021536,-1.7251191873
 O,0,1.5138141972,-0.3700099382,-1.4596592406
 C,0,2.6204078127,-0.0871179866,-0.4870274509
 C,0,2.474063102,1.3974014151,-0.0738368349
 C,0,2.4921564949,-1.1141981497,0.6294669691
 O,0,1.4424576577,-0.8813037592,1.5330463522
 N,0,-1.0366113213,-0.9076870207,0.1523583612
 C,0,-1.457151373,-1.8810516865,-0.7062346934
 N,0,-2.7490671617,-2.223766337,-0.6702709515
 C,0,-3.2369547655,-1.3982242731,0.3109343269
 C,0,-2.1799994155,-0.5937346164,0.8136101725
 N,0,-2.2905892171,0.3523722374,1.8098533909
 C,0,-3.4899431294,0.4686724081,2.2822267687
 N,0,-4.5730906206,-0.268695991,1.8591428327
 C,0,-4.5634283451,-1.2743727456,0.8427040574

O,0,-5.6193062673,-1.8595641364,0.5825334508
 O,0,3.6002309718,2.1660518892,-0.3444389685
 O,0,0.9653056977,3.1239762033,-1.2296811911
 H,0,2.4351310645,-2.1198621532,0.1724563832
 H,0,3.4286691403,-1.0755377606,1.2039861423
 H,0,3.5224864445,-0.2251569942,-1.0882336586
 H,0,-3.698200257,1.1904634795,3.0721757851
 H,0,2.3011143401,1.4454806169,1.0058977829
 H,0,0.3203800891,1.6445822502,-0.031534348
 H,0,1.6405357603,3.3357161476,-1.985472492
 H,0,3.9014599368,1.9731860302,-1.2990553749
 H,0,-5.4824028816,-0.1183035256,2.2780864603
 H,0,0.5791979328,-0.8908733041,1.035677712
 H,0,-0.7576419792,-2.347916803,-1.3934872292
 O,0,1.6677617873,1.1199054546,-4.0459462247
 As,0,3.0152672226,2.0877181628,-3.7055659469
 O,0,3.9308579233,2.2553247193,-5.2648904981
 O,0,2.6046680219,3.6322432779,-3.1776022294
 O,0,4.1936077139,1.3327607776,-2.740289749
 H,0,0.0073572185,0.5838011245,-2.398621947
 H,0,4.7794419735,1.8709581453,-4.9863014441

LG 3.1 Nuc 2.7

lg31.5

E(RB+HF-LYP) = -3518.66057999

Zero-point correction= 0.257924
 (Hartree/Particle)
 Thermal correction to Energy= 0.279598
 Thermal correction to Enthalpy= 0.280543
 Thermal correction to Gibbs Free Energy= 0.204999
 Sum of electronic and zero-point Energies= -
 3518.402656
 Sum of electronic and thermal Energies= -
 3518.380982
 Sum of electronic and thermal Enthalpies= -
 3518.380037
 Sum of electronic and thermal Free Energies= -
 3518.455581

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.451	81.565	158.996

C,0,1.2150828204,1.8534145303,-0.6687560219
 C,0,0.8774317074,0.7314772915,-1.6124330485
 O,0,1.5536129249,-0.3313446472,-1.4301578497
 C,0,2.6706377303,-0.1091690035,-0.4494299203
 C,0,2.6136554226,1.387672205,-0.0581844157
 C,0,2.4651519047,-1.1086071957,0.6822995182
 O,0,1.4261433942,-0.785963307,1.5694027347
 N,0,-1.0281289318,-0.9268070069,0.184488196
 C,0,-1.4193935377,-1.9200810157,-0.6654855032
 N,0,-2.7096576692,-2.2688587825,-0.65755946
 C,0,-3.229027144,-1.4249262946,0.2913024852
 C,0,-2.1911515284,0.6043584361,0.8065815042
 N,0,-2.3341638811,0.3624970862,1.7782970185
 C,0,-3.5477747153,0.4845823895,2.2114842871
 N,0,-4.6149957668,-0.2664207269,1.7727856626
 C,0,-4.571304949,-1.2952234721,0.7805962623
 O,0,-5.6162686709,-1.891270548,0.5028486431
 O,0,3.7327345255,2.1082106451,-0.4425200047
 O,0,1.0576975825,3.1457927034,-1.0951578479
 H,0,2.3435898906,-2.1161690559,0.2438246308
 H,0,3.3984623474,-1.1217954747,1.263480587
 H,0,3.5614975433,-0.3178279866,-1.0452398644
 H,0,-3.7821846724,1.2232316323,2.9780971899
 H,0,2.5276801199,1.4635616945,1.0307875054
 H,0,0.4703310927,1.6558289546,0.1304334251

H,0,1.6678405126,3.3364314974,-1.9281759131
 H,0,3.9181750737,1.9016372254,-1.432348466
 H,0,-5.5373169981,-0.109336381,2.1596310753
 H,0,0.5586195638,-0.8311309506,1.0785782013
 H,0,-0.6995830093,-2.3954162115,-1.3253445705
 O,0,1.5204523142,1.1438847282,-4.2021124822
 As,0,2.8672293487,2.0661634917,-3.7894692957
 O,0,3.8277399839,2.3372580526,-5.3093453377
 O,0,2.4915449168,3.5892727756,-3.1638136336
 O,0,4.0315518716,1.2484122316,-2.8515487444
 H,0,0.0706252309,0.68821154,-2.3313239953
 H,0,4.6757081213,1.9618334417,-5.0168463924

LG 3.1 Nuc 2.9

lg31.6

E(RB+HF-LYP) = -3518.65723045

Zero-point correction= 0.257094
 (Hartree/Particle)
 Thermal correction to Energy= 0.278880
 Thermal correction to Enthalpy= 0.279825
 Thermal correction to Gibbs Free Energy= 0.203745
 Sum of electronic and zero-point Energies= -
 3518.400137
 Sum of electronic and thermal Energies= -
 3518.378350
 Sum of electronic and thermal Enthalpies= -
 3518.377406
 Sum of electronic and thermal Free Energies= -
 3518.453486

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	175.000	81.634	160.124

C,0,1.2544587164,1.8284083664,-0.6017099364
 C,0,0.926160487,0.7296234894,-1.5653402828
 O,0,1.6094893681,-0.3303738441,-1.4188684483
 C,0,2.706040952,-0.134790104,-0.4087850025
 C,0,2.6760565304,1.3683100825,-0.0341475297
 C,0,2.4555754744,-1.1204848799,0.7267316437
 O,0,1.4152576792,-0.7616249174,1.5970421869
 N,0,-1.0075864366,-0.9456337695,0.1851251136
 C,0,-1.3985481022,-1.9495355688,-0.6526769354
 N,0,-2.6917344777,-2.2860886316,-0.6528103005
 C,0,-3.2137368312,-1.4211172657,0.2756054316
 C,0,-2.1745039353,-0.6015205109,0.7884851512
 N,0,-2.3182074719,0.3829532385,1.7418987936
 C,0,-3.5354955385,0.5248900452,2.1585770976
 N,0,-4.6048582388,-0.223253336,1.7206325003
 C,0,-4.5601318742,-1.27024154,0.7475420472
 O,0,-5.6073555042,-1.8614544976,0.4688319642
 O,0,3.7737813163,2.0766213714,-0.4847597872
 O,0,1.0748355462,3.1227050244,-1.0026107373
 H,0,2.3115901929,-2.1274058246,0.2940303388
 H,0,3.3813864274,-1.1558171672,1.3191418167
 H,0,3.6027552111,-0.3741392658,-0.9836122771
 H,0,-3.7711371578,1.2793753471,2.9091312739
 H,0,2.6348088178,1.4616562631,1.056263678
 H,0,0.5340165329,1.5986894509,0.211293855
 H,0,1.6144791887,3.3046942292,-1.8975811306
 H,0,3.8754275836,1.877464973,-1.4952929929
 H,0,-5.5300715366,-0.0497571664,2.0933108428
 H,0,0.5501259925,-0.8233132224,1.1019599822
 H,0,-0.6766310948,-2.4421115805,-1.2974047853
 O,0,1.446449929,1.1137880176,-4.3923012463
 As,0,2.7334951217,2.0452637197,-3.858476994
 O,0,3.784336087,2.4316797797,-5.2931721387
 O,0,2.2973682968,3.5321896778,-3.1743825356

O,0,3.8740920378,1.223951496,-2.8883857887
 H,0,0.189072422,0.7329942114,-2.3621946278
 H,0,4.6311827586,2.1080719291,-4.94142408

LG 3.1 Nuc 3.1

lg31.7nofreq

E(RB+HF-LYP) = -3518.71942448

C,0,1.675989533,1.7336121057,-0.4352498854
 C,0,1.4689577841,0.7375102227,-1.5998772612
 O,0,1.8969964185,-0.4999212507,-1.088430623
 C,0,2.9131903595,-0.2948699931,-0.0786908834
 C,0,3.0373821211,1.2326165862,0.1130712747
 C,0,2.4992547249,-1.0782896253,1.1675381309
 O,0,1.3871749028,-0.5456810666,1.8409943411
 N,0,-0.8061936172,-0.5809360064,0.0418832921
 C,0,-0.9957510511,-1.6248711861,-0.8155898548
 N,0,-2.2334736834,-2.1229709948,-0.9274956113
 C,0,-2.9395398613,-1.3339838733,-0.0556997627
 C,0,-2.0548893364,-0.3918496418,0.5394344581
 N,0,-2.4060945867,0.5546950421,1.4791404601
 C,0,-3.661322358,0.5351627279,1.7931105222
 N,0,-4.5876575304,-0.3378711972,1.2658201616
 C,0,-4.3266012119,-1.3616090495,0.3022911153
 O,0,-5.2662970543,-2.081474447,-0.0574889133
 O,0,4.1481658362,1.7834978414,-0.5923238821
 O,0,1.5953740499,3.1039905406,-0.7302298244
 H,0,2.3335158431,-2.1295485147,0.8630861335
 H,0,3.3422919175,-1.0767030318,1.8770395188
 H,0,3.8707092998,-0.6918359599,-0.4514064149
 H,0,-4.0540144955,1.2432450871,2.523913422

H,0,3.175466935,1.4961219888,1.1659119989
 H,0,0.9050843642,1.5248993356,0.3095493356
 H,0,2.1617360635,3.3412603086,-1.5038048341
 H,0,3.8924110911,1.7484391997,-1.5357837537
 H,0,-5.5545909942,-0.2916201274,1.561937536
 H,0,0.6218813223,-0.5324765449,1.2002656681
 H,0,-0.159076747,-2.0183895561,-1.3822225098
 O,0,0.2459980964,2.1277181559,-4.0861764352
 As,0,1.8558692424,2.3520829901,-3.8221825625
 O,0,2.737961243,1.7555465157,-5.2746947124
 O,0,2.6243272446,3.7296080635,-3.3050719156
 O,0,2.3768545513,1.0600959492,-2.6728192524
 H,0,0.4503125467,0.6537841735,-1.9727153751
 H,0,2.0908415065,1.1456828523,-5.6673669417

D. Grid Energies for Arsenolysis

C-N	C-O	zpe	free	Relative zpe	Relative free
1.7	1.9	-3518.3539		50.75920301	
1.7	2.1	-3518.3730		38.77001606	
1.7	2.3	-3518.3861		30.57537603	
1.7	2.5	-3518.3952		24.87320174	
1.7	2.7	-3518.4013		21.03096414	
1.7	2.9	-3518.4036		19.57702578	
1.7	3.1	-3518.4041		19.2576237	
1.9	1.9	-3518.3660	-3518.4201	43.14814635	43.49139377
1.9	2.1	-3518.3660	-3518.4284	43.14814635	38.2573412
1.9	2.3	-3518.3753	-3518.4353	37.31733272	33.97898484
1.9	2.5	-3518.3819	-3518.4399	33.16698819	31.04287023
1.9	2.7	-3518.3862	-3518.4430	30.4762296	29.0957098
1.9	2.9	-3518.3886	-3518.4441	28.97334555	28.4192551
1.9	3.1	-3518.3908	-3518.4450	27.60537593	27.84822191
2.1	1.9	-3518.3911	-3518.4336	27.4083381	35.04700516
2.1	2.1	-3518.3829	-3518.4336	32.56520706	35.01374718
2.1	2.3	-3518.3829	-3518.4375	32.55014685	32.54324425
2.1	2.5	-3518.3832	-3518.4360	32.39201458	33.51462818
2.1	2.7	-3518.3842	-3518.4398	31.72497251	31.12883896
2.1	2.9	-3518.3860	-3518.4414	30.63122433	30.09658666
2.1	3.1	-3518.3882	-3518.4425	29.26137218	29.44836986

2.3	1.9	-3518.3890	-3518.4562	28.75622743	20.83831887
2.3	2.1	-3518.4018	-3518.4494	20.73038732	25.13487299
2.3	2.3	-3518.3961	-3518.4463	24.28836335	27.06258064
2.3	2.5	-3518.3927	-3518.4446	26.3974211	28.08667533
2.3	2.7	-3518.3911	-3518.4445	27.41586821	28.20903959
2.3	2.9	-3518.3909	-3518.4447	27.5614503	28.07475266
2.3	3.1	-3518.3906	-3518.4456	27.7220926	27.5200347
2.5	1.9	-3518.3899	-3518.4692	28.17954666	12.69199703
2.5	2.1	-3518.4161	-3518.4602	11.74634097	18.29816244
2.5	2.3	-3518.4070	-3518.4544	17.43973013	21.99356294
2.5	2.5	-3518.4007	-3518.4503	21.37107401	24.51614912
2.5	2.7	-3518.3967	-3518.4486	23.88864012	25.59358207
2.5	2.9	-3518.3947	-3518.4478	25.16687595	26.08680415
2.5	3.1	-3518.3934	-3518.4477	25.97510755	26.16524277
2.7	1.9	-3518.4255	-3518.4785	5.862189078	6.832317992
2.7	2.1	-3518.4145	-3518.4679	12.72902007	13.50650372
2.7	2.3	-3518.4065	-3518.4603	17.74093445	18.25109927
2.7	2.5	-3518.4012	-3518.4551	21.09434254	21.52669625
2.7	2.7	-3518.3981	-3518.4524	23.0226777	23.20716535
2.7	2.9	-3518.3962	-3518.4511	24.24569274	24.03798726
2.7	3.1	-3518.3945	-3518.4501	25.31057552	24.67051633
2.9	1.9	-3518.4312	-3518.4849	2.237697094	2.835085662
2.9	2.1	-3518.4193	-3518.4733	9.735802135	10.09222725
2.9	2.3	-3518.4104	-3518.4647	15.29113931	15.50135483
2.9	2.5	-3518.4043	-3518.4587	19.11392414	19.27895901
2.9	2.7	-3518.4007	-3518.4555	21.38676174	21.25310232
2.9	2.9	-3518.3985	-3518.4540	22.75724139	22.20440597
2.9	3.1	-3518.3966	-3518.4532	23.95641109	22.7509663
3.1	1.9	-3518.4348	-3518.4894	0	0
3.1	2.1	-3518.4223	-3518.4775	7.833822356	7.445394285
3.1	2.3	-3518.4130	-3518.4681	13.69601143	13.37911939
3.1	2.5	-3518.4066	-3518.4618	17.72650174	17.34497627
3.1	2.7	-3518.4027	-3518.4556	20.17315933	21.22674694
3.1	2.9	-3518.4001	-3518.4535	21.7538545	22.5413783
3.1	3.1	-3518.4558	-3518.5118	-13.19965182	14.02357113

E. Grid Energies for Phosphorolysis

C-N	C-O	zpe	free	Relative zpe	Relative free
1.7	1.9	-1626.0267	-1626.076352	51.47707331	
1.7	2.1	-1626.0466	-1626.098805	38.98148659	
1.7	2.3	-1626.0600	-1626.111699	30.60800649	
1.7	2.5	-1626.0686	-1626.119759	25.21268411	
1.7	2.7				
1.7	2.9				
1.7	3.1				
1.9	1.9	-1626.0393	-1626.0890	43.576735	45.67073253
1.9	2.1	-1626.0493	-1626.1018	37.26650449	37.59971177
1.9	2.3	-1626.0561	-1626.1087	32.99505073	33.3069227
1.9	2.5	-1626.0602	-1626.1134	30.42414636	30.37520065
1.9	2.7	-1626.0622	-1626.1151	29.20552388	29.28521752

1.9	2.9	-1626.0628	-1626.1163	28.82839097	28.51965654
1.9	3.1	-1626.0647	-1626.1176	27.62043614	27.71707253
2.1	1.9	-1626.0564	-1626.1062	32.81809319	34.85059484
2.1	2.1	-1626.0573	-1626.1117	32.24454996	31.38047007
2.1	2.3	-1626.0586	-1626.1126	31.43694588	30.84771493
2.1	2.5	-1626.0604	-1626.1125	30.32562744	30.91799594
2.1	2.7	-1626.0622	-1626.1145	29.2212116	29.68431325
2.1	2.9	-1626.0628	-1626.1158	28.8516088	28.82211588
2.1	3.1	-1626.0624	-1626.1162	29.08566966	28.60939033
2.3	1.9	-1626.0755	-1626.1249	20.88098948	23.09735127
2.3	2.1	-1626.0703	-1626.1227	24.11830841	24.48979374
2.3	2.3	-1626.0672	-1626.1196	26.07048891	26.47585973
2.3	2.5	-1626.0657	-1626.1180	27.00233978	27.47297153
2.3	2.7	-1626.0652	-1626.1180	27.3248794	27.45916633
2.3	2.9	-1626.0646	-1626.1181	27.71770004	27.40269052
2.3	3.1	-1626.0637	-1626.1158	28.27743807	28.82650844
2.5	1.9	-1626.0899	-1626.1425	11.82917216	12.08394081
2.5	2.1	-1626.0812	-1626.1336	17.27281273	17.65684824
2.5	2.3	-1626.0752	-1626.1276	21.05167193	21.41939221
2.5	2.5	-1626.0714	-1626.1240	23.43934368	23.71670266
2.5	2.7	-1626.0691	-1626.1223	24.85123893	24.75962261
2.5	2.9	-1626.0675	-1626.1214	25.86341094	25.32814577
2.5	3.1	-1626.0662	-1626.1211	26.704273	25.49882822
2.7	1.9	-1626.0993	-1626.1519	5.901722145	6.202926465
2.7	2.1	-1626.0888	-1626.1415	12.48366405	12.72023494
2.7	2.3	-1626.0811	-1626.1340	17.30858075	17.42906248
2.7	2.5	-1626.0759	-1626.1290	20.59484538	20.55029224
2.7	2.7	-1626.0725	-1626.1262	22.70578566	22.33618286
2.7	2.9	-1626.0703	-1626.1245	24.08693297	23.36153256
2.7	3.1	-1626.0688	-1626.1239	25.065847	23.73239038
2.9	1.9	-1626.1051	-1626.1578	2.277230161	2.500623365
2.9	2.1	-1626.0935	-1626.1466	9.527469147	9.542529363
2.9	2.3	-1626.0851	-1626.1386	14.85376554	14.5161657
2.9	2.5	-1626.0791	-1626.1329	18.62070207	18.10865472
2.9	2.7	-1626.0752	-1626.1294	21.03786673	20.29489608
2.9	2.9	-1626.0727	-1626.1273	22.62232696	21.62207761
					-
2.9	3.1	-1626.1250	-1626.1794	-10.2352993	11.06674872
3.1	1.9	-1626.1087	-1626.1618	0	0
3.1	2.1	-1626.0966	-1626.1500	7.606036589	7.395193565
3.1	2.3	-1626.0875	-1626.1413	13.30695585	12.84824678
3.1	2.5	-1626.0812	-1626.1354	17.26026255	16.52544952
3.1	2.7	-1626.0771	-1626.1315	19.84434462	18.96520451
3.1	2.9	-1626.0745	-1626.1298	21.46959293	20.02632223
					-
3.1	3.1	-1626.1315	-1626.1858	14.29088997	15.07276618

F. KIEs for Arsenolysis Grid

Arsenolysis

r(C-N)	r(C-O)	¹ -C KIE	9-N KIE
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1.9	1.9	1.146	1.019
1.9	2.1	1.146	1.019
1.9	2.3	1.119	1.020
1.9	2.5	1.103	1.021
1.9	2.7	1.091	1.021
1.9	2.9	1.078	1.024
1.9	3.1	1.078	1.023
2.1	1.9	1.124	1.023
2.1	2.1	1.125	1.023
2.1	2.3	1.107	1.025
2.1	2.5	1.083	1.028
2.1	2.7	1.065	1.029
2.1	2.9	1.064	1.028
2.1	3.1	1.065	1.027
2.3	1.9	1.099	1.023
2.3	2.1	1.096	1.024
2.3	2.3	1.087	1.026
2.3	2.5	1.072	1.027
2.3	2.7	1.056	1.029
2.3	2.9	1.049	1.030
2.3	3.1	1.050	1.030
2.5	1.9	1.078	1.024
2.5	2.1	1.075	1.024
2.5	2.3	1.068	1.025
2.5	2.5	1.058	1.026
2.5	2.7	1.045	1.027
2.5	2.9	1.038	1.028
2.5	3.1	1.036	1.028
2.7	1.9	1.068	1.024
2.7	2.1	1.068	1.024
2.7	2.3	1.056	1.025
2.7	2.5	1.047	1.025
2.7	2.7	1.037	1.026
2.7	2.9	1.029	1.026
2.7	3.1	1.026	1.026
2.9	1.9	1.066	1.024
2.9	2.1	1.060	1.025
2.9	2.3	1.052	1.025
2.9	2.5	1.042	1.025
2.9	2.7	1.032	1.025
2.9	2.9	1.024	1.025

2.9	3.1	1.020	1.025
3.1	1.9	1.065	1.024
3.1	2.1	1.060	1.025
3.1	2.3	1.051	1.025
3.1	2.5	1.040	1.025
3.1	2.7	1.029	1.025
3.1	2.9	1.021	1.025
3.1	3.1	1.005	1.025

G. KIEs for Phosphorolysis Grid

Phosphorolysis

r(C-N)	r(C-O)	1 ¹ -C KIE	9-N KIE
1.9	1.9	1.144	1.019
1.9	2.1	1.134	1.020
1.9	2.3	1.118	1.020
1.9	2.5	1.103	1.021
1.9	2.7	1.093	1.021
1.9	2.9	1.087	1.021
1.9	3.1	1.079	1.023
2.1	1.9	1.124	1.023
2.1	2.1	1.118	1.024
2.1	2.3	1.106	1.025
2.1	2.5	1.083	1.027
2.1	2.7	1.070	1.028
2.1	2.9	1.066	1.028
2.1	3.1	1.066	1.027
2.3	1.9	1.098	1.023
2.3	2.1	1.095	1.024
2.3	2.3	1.085	1.025
2.3	2.5	1.071	1.027
2.3	2.7	1.057	1.029
2.3	2.9	1.051	1.029
2.3	3.1	1.050	1.029
2.5	1.9	1.077	1.024
2.5	2.1	1.075	1.024
2.5	2.3	1.067	1.025
2.5	2.5	1.056	1.026
2.5	2.7	1.045	1.027
2.5	2.9	1.039	1.027
2.5	3.1	1.037	1.027

2.7	1.9	1.068	1.024
2.7	2.1	1.064	1.024
2.7	2.3	1.057	1.025
2.7	2.5	1.047	1.025
2.7	2.7	1.036	1.025
2.7	2.9	1.029	1.027
2.7	3.1	1.026	1.026
2.9	1.9	1.065	1.025
2.9	2.1	1.060	1.024
2.9	2.3	1.052	1.025
2.9	2.5	1.042	1.025
2.9	2.7	1.030	1.025
2.9	2.9	1.023	1.025
2.9	3.1	1.007	1.025
3.1	1.9	1.065	1.025
3.1	2.1	1.060	1.025
3.1	2.3	1.050	1.025
3.1	2.5	1.039	1.025
3.1	2.7	1.028	1.025
3.1	2.9	1.020	1.025
3.1	3.1	1.006	1.025

3. Transition Structures of Stationary Points

Phosphorolysis Transition Structure 1 B3LYP/6-31G*

E(RB+HF-LYP) = -1626.32403896

Zero-point correction= 0.261525
 (Hartree/Particle)
 Thermal correction to Energy= 0.283529
 Thermal correction to Enthalpy= 0.284473
 Thermal correction to Gibbs Free Energy= 0.208147
 Sum of electronic and zero-point Energies= 1626.062514
 Sum of electronic and thermal Energies= 1626.040510
 Sum of electronic and thermal Enthalpies= 1626.039566
 Sum of electronic and thermal Free Energies= 1626.115892

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.917	82.050	160.642

C,0,5.0282989717,-0.5633981841,-0.3534705126
 C,0,3.6787319256,-0.8008092482,-0.7779686034
 C,0,2.5972433006,-0.1494330348,-0.128557377
 N,0,2.6996290343,0.7367231237,0.9212474894
 C,0,3.9187432277,0.9491165863,1.3045543061

N,0,5.0255611576,0.3624946525,0.7386263654
 N,0,1.4442865042,-0.5452841101,-0.7222154358
 C,0,1.8735966007,-1.4047528621,-1.6857296484
 N,0,3.192475383,-1.6036520263,-1.7777230393
 O,0,6.111198738,-0.9992854056,-0.7522682211
 C,0,-0.7456214646,-0.1374883884,-0.4438030276
 C,0,-0.9028877566,-0.0125259944,1.0679588297
 C,0,-1.5205672651,1.4535597347,1.2250610176
 C,0,-1.1655810373,2.1067309743,-0.1320806528
 O,0,-0.8785411338,0.9927413386,-1.064711215
 O,0,-1.5344468972,-1.0476085073,1.7169478523
 C,0,0.0556141669,3.0148523695,-0.1243777405
 O,0,0.4417681647,3.4175180182,-1.4387654657
 O,0,-2.8586992241,1.5298432034,1.5545897677
 O,0,-3.8245907259,-1.5584173275,0.6794104378
 P,0,-3.9061276612,-0.8534615039,-0.7056983031
 O,0,-3.9973356537,0.6912870634,-0.5650252249
 O,0,-2.8587248211,-1.3235551449,-1.7195381862
 O,0,-5.423907639,-1.3743142095,-1.2590735598
 H,0,0.889846165,2.5212771249,0.3956678781
 H,0,-0.1937936273,3.932698937,0.4221216573
 H,0,-2.0369810969,2.5918590692,-0.5737098201
 H,0,4.1196910187,1.6331000968,2.1283052148
 H,0,-0.9558373921,1.9575172432,2.0254250289
 H,0,0.1224939291,0.0528555468,1.4541267918
 H,0,-2.4836231371,-1.219727136,1.3223241447
 H,0,-3.4074979414,1.1437778047,0.7587018189
 H,0,5.9486402909,0.5789744556,1.0937125802
 H,0,0.5237668529,2.5876835024,-1.9381760683
 H,0,1.1637167232,-1.8998591129,-2.3407552851

H,O,-0.9386668825,-1.0252604265,-1.035526518
 H,O,-5.696683798,-1.9234152231,-0.5073882758

Phosphorolysis Transition Structure 2 B3LYP/6-31G*

E(RB3LYP) = -1626.32464403

Zero-point correction=	0.262118
(Hartree/Particle)	
Thermal correction to Energy=	0.283808
Thermal correction to Enthalpy=	0.284753
Thermal correction to Gibbs Free Energy=	0.209224
Sum of electronic and zero-point Energies=	-
1626.062526	
Sum of electronic and thermal Energies=	-
1626.040836	
Sum of electronic and thermal Enthalpies=	-
1626.039892	
Sum of electronic and thermal Free Energies=	-
1626.115420	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.092	81.279	158.964

C,O,-0.753379066,0.6313907841,0.964818412
 C,O,-0.5212196415,-0.0858238162,-0.3710982076
 O,O,-0.8888327165,0.6237093823,-1.4051866421
 C,O,-1.3405940935,1.9688280498,-1.0120374032
 C,O,-1.5943090012,1.9101777124,0.5163325798
 C,O,-0.3003429622,2.9715982205,-1.4908808095
 O,O,0.9309491638,2.9186685107,-0.7872348456
 O,O,-2.9377510492,1.9106023164,0.8500830865
 O,O,-1.2651266104,-0.1454500736,1.9796100694
 N,O,1.5365667029,-0.0901132665,-0.6559215
 C,O,2.6380165896,-0.2714600824,0.1287922432
 C,O,3.6899323079,-0.7206864973,-0.7031014441
 N,O,3.2442652945,-0.8322758645,-1.9985174195
 C,O,1.9719875861,-0.4571029578,-1.9001471604
 N,O,2.7166598676,-0.0277106961,1.4777112868
 C,O,3.8858219282,-0.2688488336,1.977438895
 N,O,4.967398969,-0.7154150562,1.2542592318
 C,O,4.9910299293,-0.9783185197,-0.1498446747
 O,O,6.042421653,-1.3613864313,-0.6658347979
 O,O,-3.4143909355,-1.3775798704,1.3080690962
 P,O,-3.5926106308,-1.3085464631,-0.2377064664
 O,O,-5.0230661229,-2.2077327652,-0.4431498248
 O,O,-3.918359003,0.1351600015,-0.7140342423
 O,O,-2.4899521415,-2.0035055246,-1.0373521453
 H,O,-0.1440016709,2.8349385393,-2.5761528906
 H,O,-0.6996599592,3.983411994,-1.3419921778
 H,O,-2.2878455013,2.097285632,-1.5407944275
 H,O,4.0639102148,-0.1168725878,3.0412034612
 H,O,-1.1348232962,2.7882252675,0.9906433386
 H,O,0.2261017511,0.9995792702,1.2907138792
 H,O,-2.162898834,-0.5975880021,1.7065871208
 H,O,-3.4063241621,1.1602692874,0.3070984233
 H,O,5.8515412261,-0.881894687,1.7189277833
 H,O,1.2381719161,1.9902037884,-0.8038858851
 H,O,1.2904993675,-0.4381828487,-2.742940771
 H,O,-0.6180835288,-1.1598022068,-0.5114324717
 H,O,-5.2027655406,-2.4393727056,0.4815442999

Phosphorolysis Transition Structure B3LYP/6-31+G** (shown in figure 3a)

E(RB3LYP) = -1626.48768640

Zero-point correction=	0.262571
(Hartree/Particle)	
Thermal correction to Energy=	0.284576
Thermal correction to Enthalpy=	0.285521
Thermal correction to Gibbs Free Energy=	0.208329
Sum of electronic and zero-point Energies=	-
1626.225115	
Sum of electronic and thermal Energies=	-
1626.203110	
Sum of electronic and thermal Enthalpies=	-
1626.202166	
Sum of electronic and thermal Free Energies=	-
1626.279357	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.574	81.985	162.462

C,O,-0.7682989781,-0.2821204319,0.6639079023
 C,O,-0.088756702,-0.676561952,-0.6244477362
 O,O,-0.5228741371,0.030563491,-1.653509701
 C,O,-1.2415766286,1.2400916489,-1.1627585657
 C,O,-1.0412486398,1.2320621805,0.3701786339
 C,O,-0.7151016417,2.43251844,-1.9344528951
 O,O,0.6623448233,2.7370577926,-1.7023464523
 O,O,-2.0922590761,1.839136831,1.0620601229
 O,O,-1.8491618711,-1.1223352245,0.6047580742
 N,O,1.9338778549,-0.2347349494,-0.6089169839
 C,O,2.8881190014,-0.1721481109,0.3594930145
 C,O,4.1493905318,-0.3426239628,-0.2649250929
 N,O,3.9757773042,-0.5216676818,-1.6148620201
 C,O,2.6509166997,-0.4542616727,-1.751304171
 N,O,2.6706938385,0.0304932712,1.699949349
 C,O,3.7582420123,0.0586054387,2.4038745202
 N,O,5.0254696984,-0.0962397144,1.8888512819
 C,O,5.3521911492,-0.3102639183,0.5192100299
 O,O,6.5410453847,-0.4347222082,0.2011048499
 O,O,-4.0640360292,-1.2241979213,-1.0495564315
 P,O,-4.9387006547,-0.2566823147,-0.0281455112
 O,O,-4.5241401263,-0.8959236009,1.4420581399
 O,O,-4.3328476878,1.1559490099,-0.1055957872
 O,O,-6.4082023467,-0.4574052153,-0.2754889602
 H,O,-0.8869758198,2.2697650421,-3.0102586951
 H,O,-1.2925168236,3.3100814635,-1.6252335653
 H,O,-2.3004486912,1.0813051842,-1.3937099683
 H,O,3.7047294118,0.2136826521,3.4794643415
 H,O,-0.1254055977,1.7839855715,0.6205447123
 H,O,-0.1311195322,-0.3987515807,1.5560814209
 H,O,-3.1486901019,-1.2598626557,-0.6755824953
 H,O,-2.9803712057,1.5279444618,0.6869259514
 H,O,5.825709503,-0.0585601742,2.5075209933
 H,O,1.147216357,1.9040992631,-1.5938667448
 H,O,2.1514533692,-0.5624574916,-2.7074057551
 H,O,0.1437076106,-1.711340121,-0.8447047625
 H,O,-3.539216259,-0.9361028397,1.4656749569

Arsenolysis Transition Structure 1 B3LYP/6-31G*

E(RB+HF-LYP) = -3518.64714426

Zero-point correction= 0.258494
 (Hartree/Particle)
 Thermal correction to Energy= 0.281165
 Thermal correction to Enthalpy= 0.282109
 Thermal correction to Gibbs Free Energy= 0.203949
 Sum of electronic and zero-point Energies= -
 3518.388651
 Sum of electronic and thermal Energies= -
 3518.365980
 Sum of electronic and thermal Enthalpies= -
 3518.365036
 Sum of electronic and thermal Free Energies= -
 3518.443195

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.433	84.039	164.500

O,0,-0.7191321723,0.9060348611,-1.0258398911
 C,0,-0.558904575,-0.199925123,-0.3764345811
 C,0,-0.7061847525,-0.0419328326,1.130891572
 C,0,-1.3236686046,1.4301587511,1.2607930552
 C,0,-0.995385316,2.0467055442,-0.1202449961
 O,0,-1.3282717733,-1.0665433438,1.8050010222
 O,0,-2.6554859413,1.5192980268,1.6164571268
 C,0,0.2265679671,2.9533612144,-0.1553534676
 O,0,0.5955702095,3.3205688652,-1.4842068178
 O,0,-3.8084155091,0.8090822976,-0.5488851782
 As,0,-3.7023460854,-0.8905424133,-0.6907738998
 O,0,-3.6285639427,-1.6362333241,0.8244870886
 O,0,-2.5674113186,-1.4497138658,-1.7914693896
 O,0,-5.3618732911,-1.2237374341,-1.368849482
 N,0,1.6925002327,-0.5482327065,-0.6704074364
 C,0,2.8294487314,-0.1387000867,-0.0562300812
 C,0,3.9336960973,-0.7611891159,-0.6962133965
 N,0,3.4775931404,-1.561447113,-1.7121166605
 C,0,2.1535375013,-1.3883819108,-1.6365342998
 N,0,2.898812283,0.7381553995,1.0045123552
 C,0,4.1075313222,0.9692797127,1.4093642464
 N,0,5.234019414,0.4100691768,0.8544058469
 C,0,5.2715597359,-0.5026515072,-0.2482953585
 O,0,6.3691721114,-0.9124218752,-0.63493484
 H,0,-0.0160311454,3.8856248824,0.3692853863
 H,0,1.0669477193,2.474061268,0.3682187091
 H,0,-1.876172029,2.5111158784,-0.5643909658
 H,0,4.2827422691,1.6476090256,2.2436671466
 H,0,-0.7422658015,1.9526230227,2.0364899196
 H,0,0.3234109125,0.0345784245,1.5046616123
 H,0,-2.2805287724,-1.259737313,1.4181177847
 H,0,-3.2244588396,1.1784888883,0.8150103223
 H,0,6.1471756779,0.6396863938,1.2264510412
 H,0,0.6957743174,2.4772984019,-1.956890216
 H,0,1.4635334721,-1.890069593,-2.3078316361
 H,0,-0.7168366639,-1.1076128553,-0.9504657191
 H,0,-5.7158765809,-0.3193236216,-1.3177829218

Arsenolysis Transition Structure B3LYP/6-31G*

E(RB3LYP) = -3518.64802828

Zero-point correction= 0.259322
 (Hartree/Particle)
 Thermal correction to Energy= 0.281599
 Thermal correction to Enthalpy= 0.282543
 Thermal correction to Gibbs Free Energy= 0.205838
 Sum of electronic and zero-point Energies= -
 3518.388707

Sum of electronic and thermal Energies= -
 3518.366429
 Sum of electronic and thermal Enthalpies= -
 3518.365485
 Sum of electronic and thermal Free Energies= -
 3518.442190

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.706	83.225	161.440

C,0,-0.753758,0.584502,1.000961
 C,0,-0.535597,-0.121937,-0.341402
 O,0,-0.906544,0.590137,-1.366904
 C,0,-1.343726,1.940874,-0.968618
 C,0,-1.569521,1.887176,0.564182
 C,0,-0.304658,2.933822,-1.467113
 O,0,0.937901,2.875789,-0.784125
 O,0,-2.907449,1.925318,0.923904
 O,0,-1.280302,-0.197635,2.00449
 N,0,1.547258,-0.130722,-0.644423
 C,0,2.663053,-0.265537,0.128761
 C,0,3.710154,-0.729571,-0.701483
 N,0,3.247212,-0.89646,-1.984611
 C,0,1.970594,-0.536174,-1.880584
 N,0,2.75768,0.03058,1.466549
 C,0,3.938269,-0.171443,1.956814
 N,0,5.016139,-0.627808,1.234443
 C,0,5.023436,-0.944182,-0.158986
 O,0,6.073844,-1.329137,-0.675678
 O,0,-3.444239,-1.393197,1.344848
 As,0,-3.623005,-1.270579,-0.342905
 O,0,-5.201351,-2.17745,-0.524672
 O,0,-3.929704,0.333716,-0.814649
 O,0,-2.456764,-2.065695,-1.243036
 H,0,-0.168003,2.793551,-2.554424
 H,0,-0.695847,3.948155,-1.314197
 H,0,-2.299862,2.06337,-1.481768
 H,0,4.12983,0.024562,3.011018
 H,0,-1.076772,2.750697,1.03058
 H,0,0.232772,0.929163,1.331246
 H,0,-2.18972,-0.635069,1.727566
 H,0,-3.412534,1.239517,0.336221
 H,0,5.910447,-0.759644,1.690663
 H,0,1.241862,1.946242,-0.806987
 H,0,1.277268,-0.558648,-2.713777
 H,0,-0.62361,-1.195488,-0.495061
 H,0,-5.365815,-2.352416,0.417744

Arsenolysis Transition Structure B3LYP/6-31+G** (as shown in figure 3b)

E(RB3LYP) = -3518.84228642

Zero-point correction= 0.258548
 (Hartree/Particle)
 Thermal correction to Energy= 0.281303
 Thermal correction to Enthalpy= 0.282247
 Thermal correction to Gibbs Free Energy= 0.203476
 Sum of electronic and zero-point Energies= -
 3518.583738
 Sum of electronic and thermal Energies= -
 3518.560983
 Sum of electronic and thermal Enthalpies= -
 3518.560039
 Sum of electronic and thermal Free Energies= -
 3518.638810

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.520	83.942	165.788

C,0,-0.7070258485,0.3482160453,1.0268113268
 C,0,-0.437282305,-0.2873148516,-0.3320688396
 O,0,-0.841816566,0.4196292011,-1.3467179314
 C,0,-1.3113424373,1.7639701037,-0.9263377287
 C,0,-1.3832489553,1.7395711353,0.6233856534
 C,0,-0.3924598324,2.7938827825,-1.5581853371
 O,0,0.9335471384,2.8165596685,-1.032373708
 O,0,-2.670238201,1.9489247027,1.1028238259
 O,0,-1.4460574867,-0.4971784116,1.8442537959
 N,0,1.6301185423,-0.205324805,-0.5940369758
 C,0,2.7305832545,-0.2286151931,0.21147106
 C,0,3.8236575066,-0.6853389311,-0.5642386931
 N,0,3.4005625728,-0.9592185825,-1.8418273171
 C,0,2.1024083527,-0.6658131477,-1.793264753
 N,0,2.776072749,0.1516467502,1.5300060484
 C,0,3.9547461932,0.0500746564,2.05957569
 N,0,5.0739172203,-0.3870192807,1.3897037074
 C,0,5.1295177823,-0.7906224927,0.0240172689
 O,0,6.2138031104,-1.1536616308,-0.4465452413
 O,0,-2.7597876928,-1.6405112471,0.0399469359
 As,0,-4.1226358968,-0.9671039442,-0.7653803408
 O,0,-5.4590242532,-1.6843427712,0.2884927428
 O,0,-4.1871452653,0.7133890126,-0.5076911396
 O,0,-4.3952105329,-1.4757234801,-2.3253382389
 H,0,-0.3725906384,2.6377346374,-2.6483845677
 H,0,-0.8171813462,3.7862514304,-1.3679506042
 H,0,-2.322857274,1.830198119,-1.3394829389
 H,0,4.1065492143,0.3208924727,3.1023146308
 H,0,-0.745873559,2.53743045,1.0232986181
 H,0,0.2467266759,0.5548915029,1.5187516598
 H,0,-2.1350042455,-0.960554185,1.2241984233
 H,0,-3.3364345318,1.3822570144,0.5448931143
 H,0,5.9612167362,-0.4349188296,1.8744120594
 H,0,1.2697499518,1.9039450894,-0.9986177617
 H,0,1.4388803443,-0.7757140835,-2.6428750453
 H,0,-0.416212495,-1.35769937,-0.485281668
 H,0,-4.9436899821,-2.1044105368,0.992829269

4. Enzymatic Transition Structures

Arsenolysis Transition Structure B3LYP/6-31G* (as shown in figure 6a)

E(RB3LYP) = -4166.09200612

Zero-point correction=	0.467298
(Hartree/Particle)	
Thermal correction to Energy=	0.508248
Thermal correction to Enthalpy=	0.509192
Thermal correction to Gibbs Free Energy=	0.382135
Sum of electronic and zero-point Energies=	-
4165.624708	

Sum of electronic and thermal Energies= -
 4165.583758
 Sum of electronic and thermal Enthalpies= -
 4165.582814
 Sum of electronic and thermal Free Energies= -
 4165.709871

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	318.930	141.849	267.414

N,0,1.4850669813,-2.0904903984,0.087942836
 C,0,1.2062714978,-0.9096051055,-0.5598493008
 C,0,2.1736338609,-0.095804248,-1.2001179895
 C,0,3.5583822388,-0.4576488761,-1.1751332187
 N,0,3.7551056822,-1.6737384022,-0.5158770509
 C,0,2.753211399,-2.4087163483,0.0658225329
 N,0,1.5502225222,1.017056745,-1.7292936336
 C,0,0.2700180656,0.8042929405,-1.3798152562
 N,0,-0.0204490389,-0.3179802461,-0.6739664541
 O,0,4.5388059551,0.1731666702,-1.6480693842
 O,0,6.2210365248,-2.9685052171,-0.0996500309
 C,0,6.1261102797,-4.0506470444,0.5518446232
 C,0,7.4912396577,-4.7720949608,0.7823576612
 O,0,5.1072300729,-4.6040446103,1.0232243484
 O,0,4.5044037462,4.9467111525,-0.9991123559
 C,0,4.7931795178,3.774162116,-1.2749311491
 C,0,6.1646331659,3.1934620421,-0.9177094298
 N,0,3.9917943414,2.9118012123,-1.9315587412
 C,0,-2.9132479903,-0.2884176919,-0.4718773586
 O,0,-2.9284048293,0.6059280463,0.4369827862
 C,0,-3.5202503762,0.0798809636,1.7108418159
 C,0,-3.7532548728,-1.4358321011,1.484384371
 C,0,-3.15504329,-1.687830997,0.0287358349
 O,0,-5.0650992811,-1.8275975744,1.7010755388
 C,0,-2.5987382647,0.4179744216,2.8728726024
 O,0,-2.5275731434,1.7884756659,3.1987275486
 O,0,-3.7499313283,-2.612733942,-0.7917783166
 O,0,-6.1087945918,-1.9329259149,-1.5665526475
 As,0,-6.2130761917,-0.2785506351,-1.1844826395
 O,0,-7.8064754976,0.1303737351,-2.0079942764
 O,0,-6.4271080892,-0.0068747267,0.4801469861
 O,0,-5.0064303089,0.6698109428,-1.8826876453
 N,0,0.0000544586,2.7671818045,2.2203973399
 C,0,0.5677312248,4.0454779437,1.9412265328
 C,0,1.7751245506,3.959266356,1.3488695614
 C,0,2.0646183808,2.5005564042,1.1717509746
 C,0,0.855412872,1.88836438,1.8008744448
 H,0,-0.0019099642,4.9311602073,2.2022749314
 H,0,2.0918081844,2.2045207175,0.1060899276
 H,0,7.3656314632,-5.7004363229,1.3515612119
 H,0,7.9621718526,-4.9996051412,-0.1839008362
 H,0,6.4442641878,3.5447369142,0.0807772611
 H,0,6.1699590954,2.0998756425,-0.9458867798
 H,0,3.0150820817,3.1461391054,-2.065511053
 H,0,4.185063906,1.8931546259,-1.9305198418
 H,0,2.4141954693,4.7573546471,0.9905008012
 H,0,0.6570040403,0.822458226,1.8456357626
 H,0,3.1162479295,-3.3202679048,0.5393114214
 H,0,-0.5094975154,1.5163045384,-1.6413091148
 H,0,-3.0196150261,-0.1115802097,3.7411686773
 H,0,-1.6048343444,-0.0165426843,2.6815496266
 H,0,-1.7322722064,2.1761800978,2.7665810886
 H,0,-4.4757336658,0.6049214481,1.7714399357
 H,0,-2.102464706,-2.0003611644,0.1751507474
 H,0,-4.7154220268,-2.3377856398,-1.0627057936
 H,0,-3.1308937991,-2.0080874194,2.1878810188
 H,0,-5.686335993,-1.179935573,1.1944307005
 H,0,8.1806401156,-4.1066127905,1.3199044486
 H,0,6.9164083053,3.57268647,-1.6224203602

H,0,-2.6075807722,0.0094925208,-1.4632661216
 H,0,-7.9819007636,-0.7456143934,-2.3930253722
 H,0,4.7239570644,-2.064437527,-0.4229732053
 H,0,3.0133311854,2.1528821134,1.6029494574

Phosphorolysis Transition Structure B3LYP/6-31G* (as shown in figure 6b)

E(RB+HF-LYP) = -2274.16515016

Zero-point correction= 0.470170
 (Hartree/Particle)
 Thermal correction to Energy= 0.509533
 Thermal correction to Enthalpy= 0.510477
 Thermal correction to Gibbs Free Energy= 0.388876
 Sum of electronic and zero-point Energies= -
 2273.694980
 Sum of electronic and thermal Energies= -
 2273.655617
 Sum of electronic and thermal Enthalpies= -
 2273.654673
 Sum of electronic and thermal Free Energies= -
 2273.776275

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	319.737	137.858	255.932

N,0,9.0044799834,4.592710143,-4.8596023783
 C,0,7.653707748,4.351099501,-4.7643899358
 C,0,6.6622662916,5.3579192016,-4.6618740406
 C,0,7.0314822178,6.7405267865,-4.6180801134
 N,0,8.414666284,6.9004420657,-4.7329977755
 C,0,9.3072763414,5.8644870073,-4.8428702637
 N,0,5.4205707569,4.7599263693,-4.5647109031
 C,0,5.7401665617,3.4557320846,-4.6138374836
 N,0,7.0515072208,3.1246344748,-4.727831334
 O,0,6.2871278437,7.7459810108,-4.4891179291
 O,0,9.8481698245,9.3317745921,-4.7040417525
 C,0,11.1039158439,9.1939402876,-4.7912462502
 C,0,11.8903033377,10.5426462594,-4.7872451497
 O,0,11.7813601175,8.1454638742,-4.883026314
 O,0,2.4904075246,7.2335107391,-1.5237246738
 C,0,3.3508975471,7.6726543084,-2.3001584716
 C,0,3.9788227365,9.0516064467,-2.0753131627
 N,0,3.7891130727,7.048938015,-3.4090958036
 C,0,6.8326324182,0.3021671801,-5.3569354606
 O,0,6.5532040714,0.0138342275,-4.1474818344
 C,0,7.6655306774,-0.7517833535,-3.4973217799
 C,0,8.777744125,-0.8878430643,-4.5700715018
 C,0,8.2621410221,0.0505031402,-5.746815006
 O,0,9.0682037385,-2.2010466455,-4.9016666448
 C,0,8.0828287445,-0.0265034659,-2.2246956853
 O,0,7.1560268805,-0.1133074421,-1.1622242101
 O,0,8.5496426485,-0.2895150989,-7.0459364237
 O,0,7.3029236011,-2.4329908477,-7.7406010273
 P,0,6.1877791103,-2.6749594205,-6.685726551
 O,0,5.3230860451,-3.952903655,-7.3979374447
 O,0,6.7400694728,-3.2167963297,-5.343521546
 O,0,5.204209991,-1.5030512201,-6.531425792
 N,0,5.8313142459,2.4296609982,-0.8106567258
 C,0,4.545816327,2.9076190026,-0.4190646175
 C,0,4.3901999452,4.2263848641,-0.6466750168
 C,0,5.6567187974,4.7046114376,-1.2871391537
 C,0,6.4712006168,3.4522375873,-1.2836676926
 H,0,3.8348534245,2.1978943553,-0.009478515
 H,0,5.4843524676,4.9959555767,-2.3412658207
 H,0,12.973319967,10.3780659397,-4.8264048705
 H,0,11.5865527441,11.1533012442,-5.6487436012

H,0,4.1719730485,9.1779994122,-1.0051011982
 H,0,4.9064754644,9.1815065609,-2.6404131878
 H,0,3.5608470825,6.0729295667,-3.5642849625
 H,0,4.6608062786,7.3437210763,-3.8870075352
 H,0,3.5137920034,4.8446705738,-0.4923656548
 H,0,7.4707095323,3.3622740585,-1.6975103671
 H,0,10.3414969091,6.2004688593,-4.9093993835
 H,0,4.9743691814,2.6867879692,-4.5475951868
 H,0,9.0105609354,-0.5159206863,-1.8926001324
 H,0,8.3334110626,1.0151550633,-2.4771638427
 H,0,6.5920839196,0.6926771325,-1.1585545531
 H,0,7.2134124387,-1.7217220633,-3.2861474027
 H,0,8.6864091089,1.0545484937,-5.5547262962
 H,0,8.0713262747,-1.1703293297,-7.3132640763
 H,0,9.7071379722,-0.4433861087,-4.1859806256
 H,0,8.187630563,-2.672398024,-5.1545923863
 H,0,11.6408208022,11.1207198168,-3.8871563581
 H,0,3.2658456368,9.8307692798,-2.3753433484
 H,0,6.0678689757,0.7890624236,-5.9434383745
 H,0,5.7843505969,-4.0060210322,-8.2497212738
 H,0,8.8276097167,7.8632337745,-4.7131329489
 H,0,6.141897161,5.5626230059,-0.8029412485

5. Alternative Mechanisms

A. $D_N^*A_N^\ddagger$ Structures Arsenolysis

B3LYP/6-31G* $r_{C-O} = 2.7$

E(RB3LYP) = -3032.06636065

Zero-point correction= 0.167746
 (Hartree/Particle)
 Thermal correction to Energy= 0.182591
 Thermal correction to Enthalpy= 0.183535
 Thermal correction to Gibbs Free Energy= 0.125651
 Sum of electronic and zero-point Energies= -
 3031.898614
 Sum of electronic and thermal Energies= -
 3031.883770
 Sum of electronic and thermal Enthalpies= -
 3031.882826
 Sum of electronic and thermal Free Energies= -
 3031.940710

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	114.578	54.877	121.828

O,0,-0.9750173117,-0.4151954761,-0.5786602471
 C,0,-1.9335225026,-1.3618412245,-0.1245828252
 C,0,-2.7443081956,-1.9769553063,-1.2487200717
 O,0,-1.7241767663,-2.6088502192,-2.170015614
 C,0,-2.017895271,-3.8435084376,-2.3842281916
 C,0,-3.0752759543,-4.4212843574,-1.4830696396
 C,0,-3.7298441331,-3.0922272979,-0.8460055442
 O,0,-5.038328298,-2.840958994,-1.2285887386
 O,0,-3.8112290484,-5.4445232017,-1.7914406395
 O,0,-5.0754400711,-5.0583217053,-4.0670218294
 As,0,-4.220524371,-3.6461426913,-4.6784035463
 O,0,-2.6187292568,-3.9605801121,-5.0139226765
 O,0,-5.146916665,-3.5481638774,-6.2043607127
 O,0,-4.5420963884,-2.3006224623,-3.7351256551
 H,0,-2.6160643783,-0.8248104384,0.5425388045

H,0,-1.4549284683,-2.163696729,0.4644660143
 H,0,-0.5110147612,-0.8365828016,-1.3200638572
 H,0,-3.2234487086,-1.2276091648,-1.8795218434
 H,0,-2.2332674316,-4.6649753291,-0.7082458478
 H,0,-4.6515410765,-5.2829831726,-3.169260194
 H,0,-3.736469594,-3.2125014678,0.2452286836
 H,0,-5.0277223386,-2.7098921407,-2.2279491751
 H,0,-1.3696108637,-4.3861956801,-3.0621008221
 H,0,-5.7976851462,-4.2636407127,-6.1083958311

Zero-point correction= 0.168748
 (Hartree/Particle)
 Thermal correction to Energy= 0.183273
 Thermal correction to Enthalpy= 0.184217
 Thermal correction to Gibbs Free Energy= 0.127201
 Sum of electronic and zero-point Energies= -
 3031.907715
 Sum of electronic and thermal Energies= -
 3031.893190
 Sum of electronic and thermal Enthalpies= -
 3031.892246

Sum of electronic and thermal Free Energies= -
 3031.949262

B3LYP/6-31G* $r_{C-O} = 2.5$

E(RB3LYP) = -3032.07052699

Zero-point correction= 0.168256
 (Hartree/Particle)
 Thermal correction to Energy= 0.182916
 Thermal correction to Enthalpy= 0.183860
 Thermal correction to Gibbs Free Energy= 0.126463
 Sum of electronic and zero-point Energies= -
 3031.902271
 Sum of electronic and thermal Energies= -
 3031.887611
 Sum of electronic and thermal Enthalpies= -
 3031.886667
 Sum of electronic and thermal Free Energies= -
 3031.944064

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	114.782	54.445	120.803

O,0,-1.0118847657,-0.3806387122,-0.6695465311
 C,0,-1.9621883053,-1.3209246495,-0.1852686124
 C,0,-2.7187817787,-2.0293507575,-1.2898718236
 O,0,-1.6515478813,-2.690073384,-2.1364558486
 C,0,-1.9719476763,-3.9138397018,-2.3878983178
 C,0,-3.0588035261,-4.4843292603,-1.4995947115
 C,0,-3.687385096,-3.1434642006,-0.8495457375
 O,0,-5.0130753741,-2.8814923203,-1.1686124457
 O,0,-3.8278897746,-5.4743866129,-1.8526783072
 O,0,-5.142927412,-4.9841836978,-4.0394323122
 As,0,-4.3094890881,-3.5407460422,-4.5841170204
 O,0,-2.669485039,-3.8141518585,-4.7865446041
 O,0,-5.0878941913,-3.4760836499,-6.1900571625
 O,0,-4.7447520559,-2.1924543137,-3.6984836695
 H,0,-2.6806805166,-0.7618390321,0.4235001835
 H,0,-1.4832648776,-2.0709092424,0.4685797557
 H,0,-0.5198458774,-0.8353155541,-1.372214286
 H,0,-3.2004344681,-1.3386720018,-1.9841634032
 H,0,-2.2624152714,-4.7797930578,-0.7093543176
 H,0,-4.6798544203,-5.2509596061,-3.1613568364
 H,0,-3.6504936477,-3.2622017526,0.2415527107
 H,0,-5.0600722929,-2.6904403703,-2.1545086458
 H,0,-1.2673881019,-4.4816498621,-2.9829073372
 H,0,-5.6125555618,-4.2941633595,-6.2084707197

B3LYP/6-31G* $r_{C-O} = 2.3$

E(RB3LYP) = -3032.07646300

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	115.005	54.073	120.000

O,0,-1.0359562592,-0.3590130232,-0.7357966295
 C,0,-1.9738561787,-1.299442205,-0.22575892
 C,0,-2.7099824288,-2.0548896942,-1.3131472753
 O,0,-1.6321777027,-2.717624209,-2.1296511115
 C,0,-1.9756956803,-3.9318466199,-2.4302642502
 C,0,-3.0591505697,-4.5122411613,-1.5202113785
 C,0,-3.6615691942,-3.1725424099,-0.8460023644
 O,0,-5.0019823148,-2.9023854217,-1.1079484826
 O,0,-3.8603463462,-5.4739561958,-1.9017982514
 O,0,-5.1966229323,-4.9528273932,-4.0247891391
 As,0,-4.3498428464,-3.5057377756,-4.5103981187
 O,0,-2.6900581266,-3.7799071977,-4.6112274529
 O,0,-4.9809126513,-3.4366321266,-6.1764320465
 O,0,-4.8285541786,-2.1532539468,-3.6624092718
 H,0,-2.7047881334,-0.7342762904,0.3621154501
 H,0,-1.4843472281,-2.0208681007,0.4519162158
 H,0,-0.5418736228,-0.8268763032,-1.4284666255
 H,0,-3.2079101728,-1.3902594151,-2.0221618404
 H,0,-2.2893178416,-4.853800475,-0.7389527464
 H,0,-4.7170431248,-5.2428634221,-3.1490659563
 H,0,-3.5870888127,-3.296215348,0.2428211252
 H,0,-5.0923062121,-2.6882217141,-2.0801030847
 H,0,-1.2280854862,-4.5115839974,-2.9572940881
 H,0,-5.4655889558,-4.2747985542,-6.2624237572

B3LYP/6-31G* $r_{C-O} = 2.1$

E(RB3LYP) = -3032.09202993

Zero-point correction= 0.171651
 (Hartree/Particle)
 Thermal correction to Energy= 0.185726
 Thermal correction to Enthalpy= 0.186670
 Thermal correction to Gibbs Free Energy= 0.131015
 Sum of electronic and zero-point Energies= -
 3031.920379
 Sum of electronic and thermal Energies= -
 3031.906304
 Sum of electronic and thermal Enthalpies= -
 3031.905360
 Sum of electronic and thermal Free Energies= -
 3031.961015

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	116.545	52.930	117.136

O,0,-1.080127763,-0.3598097003,-0.7945144609
 C,0,-2.0088605743,-1.307107659,-0.2830967124
 C,0,-2.7161105249,-2.0863386946,-1.3729417237
 O,0,-1.6354834443,-2.750607429,-2.1521618044
 C,0,-2.0083964194,-3.9587689866,-2.5154244272
 C,0,-3.0272288422,-4.5221482217,-1.530104407
 C,0,-3.6673900161,-3.2090731894,-0.8893403789
 O,0,-5.0078198816,-2.9666760019,-1.1548175405
 O,0,-3.8428124219,-5.5593805542,-1.9017564762
 O,0,-5.2895183717,-4.8610752948,-3.9574297024
 As,0,-4.4467230218,-3.4882633862,-4.4294028223
 O,0,-2.7399563754,-3.7834750791,-4.4760600549
 O,0,-4.8475213247,-3.2953568715,-6.1644193344
 O,0,-4.8180994097,-2.0676233836,-3.6190173989
 H,0,-2.7549273468,-0.747601435,0.2913707846
 H,0,-1.513534968,-2.013145273,0.407632296
 H,0,-0.5900845616,-0.8213099857,-1.49438371
 H,0,-3.229107526,-1.4420892653,-2.0912748407
 H,0,-2.3477475114,-4.9211431736,-0.7489288924
 H,0,-4.4476675794,-5.2994293918,-2.6888070162
 H,0,-3.5862116817,-3.3170536043,0.2020491998
 H,0,-5.0944911629,-2.6472181886,-2.1110304911
 H,0,-1.2244472321,-4.5597607122,-2.9595278475
 H,0,-5.3507890391,-4.1076075187,-6.344062238

B3LYP/6-31G* $r_{C-O} = 1.9$

E(RB3LYP) = -3032.10945509

Zero-point correction=	0.172654
(Hartree/Particle)	
Thermal correction to Energy=	0.186663
Thermal correction to Enthalpy=	0.187607
Thermal correction to Gibbs Free Energy=	0.132093
Sum of electronic and zero-point Energies=	-
3031.936802	
Sum of electronic and thermal Energies=	-
3031.922792	
Sum of electronic and thermal Enthalpies=	-
3031.921848	
Sum of electronic and thermal Free Energies=	-
3031.977362	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	117.133	52.761	116.838

O,0,-1.0713713757,-0.3723969752,-0.8366157909
 C,0,-2.004995503,-1.3045739564,-0.3055293506
 C,0,-2.7188334578,-2.0927933657,-1.3869561801
 O,0,-1.6505686946,-2.7439047245,-2.1712242587
 C,0,-2.0519094995,-3.9505505218,-2.5843893206
 C,0,-3.0264170214,-4.5228049795,-1.5500361119
 C,0,-3.6535391492,-3.2212812375,-0.8843815483
 O,0,-5.007338076,-2.9839275703,-1.1111590563
 O,0,-3.8565463375,-5.5654604332,-1.8954062151
 O,0,-5.3392071794,-4.8583265383,-3.9748553605
 As,0,-4.4963401875,-3.4717625425,-4.3821634691
 O,0,-2.7712095189,-3.7703103388,-4.3337094774
 O,0,-4.7298924779,-3.2752581513,-6.1434223207
 O,0,-4.9011296192,-2.0491459201,-3.6035482472
 H,0,-2.7421759883,-0.7323305059,0.2680878439
 H,0,-1.5089914735,-2.0070055677,0.3884171451
 H,0,-0.6037784839,-0.849485649,-1.541874515
 H,0,-3.2561945871,-1.4463810107,-2.0857353534
 H,0,-2.325373262,-4.9250101219,-0.7944612583
 H,0,-4.4799832467,-5.303319801,-2.6507552854

H,0,-3.5483672986,-3.335708026,0.2038355914
 H,0,-5.1230962666,-2.6445867758,-2.0491897145
 H,0,-1.2381853842,-4.5588310702,-2.9639084967
 H,0,-5.1696129114,-4.1069072169,-6.3884692498

B. $D_N^*A_N^{\ddagger}$ Structures Phosphorolysis

B3LYP/6-31G* $r_{C-O} = 2.7$

E(RB3LYP) = -1139.73831950

Zero-point correction=	0.169737
(Hartree/Particle)	
Thermal correction to Energy=	0.183665
Thermal correction to Enthalpy=	0.184609
Thermal correction to Gibbs Free Energy=	0.128923
Sum of electronic and zero-point Energies=	-
1139.568583	
Sum of electronic and thermal Energies=	-
1139.554655	
Sum of electronic and thermal Enthalpies=	-
1139.553711	
Sum of electronic and thermal Free Energies=	-
1139.609396	

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	115.251	52.029	117.200

O,0,4.190586392,-1.6557143711,-0.0934018627
 C,0,3.7424338496,-0.3328531418,-0.3467721967
 C,0,2.2328041751,-0.2170612075,-0.435046459
 O,0,1.7186964156,-0.745769337,0.8922302765
 C,0,0.9342861828,0.1096433727,1.4408952229
 C,0,0.9327385798,1.4816542976,0.8184631173
 C,0,1.6643385915,1.2049925224,-0.5930274441
 O,0,0.8605680774,1.3587111001,-1.7121640528
 O,0,-0.0631428118,2.3105296723,0.8975839147
 O,0,-2.2939804664,1.2572408211,0.0440375508
 As,0,-1.8346289113,-0.4416674317,-0.0546126819
 O,0,-1.4783181401,-1.1024890402,1.4322096119
 O,0,-3.4407507572,-1.0088803187,-0.6034745469
 O,0,-0.710543666,-0.6763577261,-1.2731512474
 H,0,4.1634239708,-0.0343345455,-1.3132166506
 H,0,4.1222113944,0.3726651906,0.4131156117
 H,0,3.6337793282,-1.9957941728,0.6260941069
 H,0,1.7991882421,-0.9056105905,-1.1604606269
 H,0,1.8338977446,1.7627323838,1.5068394115
 H,0,-1.4544668698,1.7375082417,0.3693603622
 H,0,2.483728959,1.9294156541,-0.68945849
 H,0,0.1133145631,0.6868986493,-1.6292693714
 H,0,0.4797769937,-0.1785708513,2.3820768814
 H,0,-3.9366288756,-0.1763971753,-0.6808933259

B3LYP/6-31G* $r_{C-O} = 2.5$

E(RB3LYP) = -1139.74531580

Zero-point correction=	0.172166
(Hartree/Particle)	
Thermal correction to Energy=	0.185800
Thermal correction to Enthalpy=	0.186744

Thermal correction to Gibbs Free Energy= 0.132031
 Sum of electronic and zero-point Energies= -
 1139.573150
 Sum of electronic and thermal Energies= -
 1139.559516
 Sum of electronic and thermal Enthalpies= -
 1139.558571
 Sum of electronic and thermal Free Energies= -
 1139.613285

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	116.591	51.479	115.155

O,0,-1.0193459277,-0.4123939519,-0.6655224717
 C,0,-1.9685532183,-1.3624435036,-0.2026292178
 C,0,-2.7478716687,-2.0229175395,-1.3227913499
 O,0,-1.7133631348,-2.6704693539,-2.2022445244
 C,0,-2.019452565,-3.8985018093,-2.4478930922
 C,0,-3.0432314556,-4.4590277162,-1.4905525229
 C,0,-3.7323438481,-3.1425194888,-0.9010413936
 O,0,-5.0352143886,-2.9102477175,-1.2827383847
 O,0,-3.8202523376,-5.5100510831,-1.8711044742
 O,0,-5.0489434791,-4.8416784174,-3.9822281826
 P,0,-4.3379709447,-3.5887218681,-4.5461535805
 O,0,-2.8197325572,-3.8232276529,-4.8151459536
 O,0,-5.0250749072,-3.388573519,-6.0538675932
 O,0,-4.6039284063,-2.3058581792,-3.7331610297
 H,0,-2.6741413965,-0.8219049933,0.4373299489
 H,0,-1.4855268901,-2.13899106,0.4173424241
 H,0,-0.5524244889,-0.8318929707,-1.4062091843
 H,0,-3.2346273483,-1.3054427681,-1.9843851623
 H,0,-2.364707158,-4.8157028798,-0.6804783925
 H,0,-4.377216681,-5.2527802715,-2.7272698017
 H,0,-3.7275793361,-3.2392077903,0.1947480698
 H,0,-5.024044802,-2.7027873146,-2.2893765023
 H,0,-1.3350623277,-4.4577616679,-3.0709949858
 H,0,-5.5644477324,-4.1889594833,-6.1510826429

B3LYP/6-31G* $r_{C-O} = 2.3$

E(RB3LYP) = -1139.75570409

Zero-point correction= 0.173562
 (Hartree/Particle)
 Thermal correction to Energy= 0.187068
 Thermal correction to Enthalpy= 0.188012
 Thermal correction to Gibbs Free Energy= 0.133606
 Sum of electronic and zero-point Energies= -
 1139.582142
 Sum of electronic and thermal Energies= -
 1139.568636
 Sum of electronic and thermal Enthalpies= -
 1139.567692
 Sum of electronic and thermal Free Energies= -
 1139.622098

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.387	51.180	114.507

O,0,-1.0405935679,-0.3925110448,-0.7262514742
 C,0,-1.9810788635,-1.3398964152,-0.2390947919
 C,0,-2.7373287195,-2.0481036621,-1.345958561
 O,0,-1.6883897205,-2.6977605215,-2.1921614429
 C,0,-2.0247856711,-3.9183265763,-2.4904122409
 C,0,-3.0394192927,-4.483358716,-1.5142437657
 C,0,-3.7035580944,-3.1715870279,-0.8956835532
 O,0,-5.0260181241,-2.9321180715,-1.2207328936
 O,0,-3.8378440682,-5.5247151605,-1.8913775211

O,0,-5.1323070656,-4.8062845866,-3.9851145037
 P,0,-4.3954420129,-3.5500871955,-4.4854604928
 O,0,-2.8449784315,-3.7947939395,-4.6356450106
 O,0,-4.9142155567,-3.3507756391,-6.0552708524
 O,0,-4.7079994039,-2.2634244984,-3.7097419082
 H,0,-2.6992970388,-0.7893441374,0.3778423839
 H,0,-1.4910106392,-2.0897424007,0.4076800769
 H,0,-0.5684831638,-0.8320780588,-1.4519462313
 H,0,-3.2419261191,-1.3574238365,-2.0234958933
 H,0,-2.3567018246,-4.8640858908,-0.7222834532
 H,0,-4.4149218316,-5.2546812308,-2.7108591463
 H,0,-3.6630154731,-3.2751107424,0.198432615
 H,0,-5.0618109657,-2.6990211475,-2.2095455205
 H,0,-1.2859815853,-4.4950038306,-3.0299165193
 H,0,-5.4179497662,-4.1618286694,-6.2262092997

B3LYP/6-31G* $r_{C-O} = 2.1$

E(RB3LYP) = -1139.76940190

Zero-point correction= 0.174850
 (Hartree/Particle)
 Thermal correction to Energy= 0.188220
 Thermal correction to Enthalpy= 0.189164
 Thermal correction to Gibbs Free Energy= 0.135134
 Sum of electronic and zero-point Energies= -
 1139.594552
 Sum of electronic and thermal Energies= -
 1139.581182
 Sum of electronic and thermal Enthalpies= -
 1139.580238
 Sum of electronic and thermal Free Energies= -
 1139.634268

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	118.110	50.888	113.716

O,0,-1.0354958024,-0.4004809834,-0.7616987758
 C,0,-1.9748789737,-1.3410044896,-0.2583921909
 C,0,-2.7428440818,-2.0502529636,-1.3574631324
 O,0,-1.7053854921,-2.6857121753,-2.2143066105
 C,0,-2.0617231926,-3.9057758903,-2.5517853828
 C,0,-3.0368244936,-4.4820743334,-1.5336399947
 C,0,-3.6929493222,-3.1813193679,-0.8922389974
 O,0,-5.0282603524,-2.947029153,-1.1826787161
 O,0,-3.8463896588,-5.5313782965,-1.8871700491
 O,0,-5.206816851,-4.7935250417,-3.998855961
 P,0,-4.4444132445,-3.5390530417,-4.4396308995
 O,0,-2.8734400855,-3.8046682839,-4.4859241811
 O,0,-4.8100705594,-3.3301061085,-6.0471891929
 O,0,-4.7776335985,-2.245020117,-3.695572823
 H,0,-2.6820549881,-0.7855746896,0.3671624592
 H,0,-1.4786604388,-2.0917627413,0.3827395391
 H,0,-0.5845924661,-0.8473598516,-1.4967094238
 H,0,-3.2697541585,-1.3559517543,-2.0142169466
 H,0,-2.3356680123,-4.8658842046,-0.7643644078
 H,0,-4.4362473182,-5.2688155521,-2.6782253156
 H,0,-3.6300840109,-3.2923707687,0.1998532067
 H,0,-5.0922390224,-2.6928554839,-2.1594039175
 H,0,-1.2808828507,-4.4927025664,-3.0185772011
 H,0,-5.2477480254,-4.1613851417,-6.2891610853

B3LYP/6-31G* $r_{C-O} = 1.9$

E(RB3LYP) = -1139.78649814

Zero-point correction= 0.175917
 (Hartree/Particle)
 Thermal correction to Energy= 0.189167
 Thermal correction to Enthalpy= 0.190111
 Thermal correction to Gibbs Free Energy= 0.136386
 Sum of electronic and zero-point Energies= -
 1139.610581
 Sum of electronic and thermal Energies= -
 1139.597331
 Sum of electronic and thermal Enthalpies= -
 1139.596387
 Sum of electronic and thermal Free Energies= -
 1139.650112

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	118.704	50.617	113.075

O,0,-1.02091916,-0.4212074731,-0.794209866
 C,0,-1.9653931247,-1.3485212907,-0.274582291
 C,0,-2.7537610982,-2.0480190069,-1.3681220064
 O,0,-1.7385584323,-2.6628406621,-2.2462887743
 C,0,-2.1136582766,-3.8888688874,-2.6229837919
 C,0,-3.0424520748,-4.4730735881,-1.5560772875
 C,0,-3.6887222029,-3.1861389328,-0.889455588
 O,0,-5.0362779322,-2.9550067141,-1.1440358487
 O,0,-3.8607827746,-5.5329560528,-1.8771438124
 O,0,-5.239741325,-4.793567614,-4.0116136327
 P,0,-4.4730322746,-3.5326968906,-4.4021688425
 O,0,-2.8813220561,-3.8045858305,-4.3589529107
 O,0,-4.6996237789,-3.3260891682,-6.0299132426
 O,0,-4.8300904397,-2.2385287935,-3.6848294409
 H,0,-2.6544190176,-0.7844559976,0.3636758464
 H,0,-1.4673844001,-2.1068859918,0.3562667578
 H,0,-0.6018220987,-0.8760748919,-1.5436227692
 H,0,-3.3063930272,-1.3404082437,-1.9893582451
 H,0,-2.3154548096,-4.8525500822,-0.8131945399

Phosphorolysis

Distance	2.7	2.5	2.3	2.1	1.9
C	1.033	1.047	1.058	1.065	1.069
1'	1.541	1.349	1.248	1.149	1.054
2'	1.263	1.188	1.141	1.092	1.051
5'	1.057	1.060	1.061	1.065	1.072

Arsenolysis

Distance	2.7	2.5	2.3	2.1	1.9
C	1.039	1.052	1.065	1.066	1.071
1'	1.422	1.337	1.258	1.158	1.071
2'	1.936	1.748	1.562	1.090	1.046
5'	1.050	1.058	1.057	1.064	1.068

D. $D_N^{\ddagger} * A_N$ Structures

B3LYP/6-31G* $r_{C-N} = 2.3$

E(RB+HF-LYP) = -983.327394566

Zero-point correction= 0.237345
 (Hartree/Particle)
 Thermal correction to Energy= 0.253048
 Thermal correction to Enthalpy= 0.253993
 Thermal correction to Gibbs Free Energy= 0.193455

H,0,-4.4636866028,-5.2815089239,-2.6492255387
 H,0,-3.6051306992,-3.3066400262,0.1998920205
 H,0,-5.1249165214,-2.6905711355,-2.1083652259
 H,0,-1.2926402762,-4.4797015666,-3.0131505596
 H,0,-5.0988745966,-4.1611652359,-6.3199904108

C. $D_N^{\ddagger} * A_N^{\ddagger}$ Structure KIEs

*(before tunneling)

Sum of electronic and zero-point Energies= -
 983.090050
 Sum of electronic and thermal Energies= -
 983.074346
 Sum of electronic and thermal Enthalpies= -
 983.073402
 Sum of electronic and thermal Free Energies= -
 983.133939

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	158.790	60.885	127.411

N,0,0.1267647843,1.4261617053,0.2725665226
 C,0,-0.8585385596,1.3398436793,-0.6832554225

C,0,-1.3217014613,0.160463128,-1.2929774767
 C,0,-0.7441845448,-1.1126927718,-0.9441064666
 N,0,0.2804483106,-0.9092827483,0.0503370754
 C,0,0.6517977001,0.2780677988,0.5987264461
 N,0,-2.3242628645,0.4548299336,-2.1816370713
 C,0,-2.4314630077,1.7729403962,-2.0851594792
 N,0,-1.5902074874,2.3695412736,-1.1874877427
 O,0,-0.9749507594,-2.243646208,-1.3370215911
 C,0,-1.2525106328,4.6379260593,-1.3618285047
 O,0,0.0191275199,4.9065800427,-1.386909866
 C,0,0.4491070119,5.5710475236,-0.1196987967
 C,0,-0.8541640696,6.1800989703,0.4085119166
 C,0,-1.9624483154,5.2308162621,-0.1544114281
 O,0,-1.0766826001,7.5149937721,-0.0475625553
 C,0,1.1178345065,4.582749849,0.8350426336
 O,0,0.1794589675,3.8278730208,1.5462474251
 O,0,-3.1313334136,5.9094207965,-0.5287008686
 H,0,1.4325954332,0.2402997877,1.3535624514
 H,0,-3.1483629536,2.3502806391,-2.6589337902
 H,0,1.8157103586,3.9582365085,0.2593607877
 H,0,1.7150582806,5.1861171853,1.535747499
 H,0,0.1604522432,2.9108721772,1.1488170309
 H,0,1.1650262607,6.3281820611,-0.4535583151
 H,0,-1.7256168777,4.4776793277,-2.3219004797
 H,0,-2.1864417314,4.4386543953,0.560861937
 H,0,-2.8993140559,6.8589592909,-0.5164810165
 H,0,-0.8787812096,6.2166374916,1.4966716287
 H,0,-0.7275598556,7.6105441374,-0.9494703283
 H,0,0.7340130229,-1.7637284849,0.3536678453

B3LYP/6-31G* $r_{C-N} = 2.5$

Zero-point correction= 0.236716
 (Hartree/Particle)
 Thermal correction to Energy= 0.252560
 Thermal correction to Enthalpy= 0.253504
 Thermal correction to Gibbs Free Energy= 0.192526
 Sum of electronic and zero-point Energies= -
 983.081492
 Sum of electronic and thermal Energies= -
 983.065647
 Sum of electronic and thermal Enthalpies= -
 983.064703
 Sum of electronic and thermal Free Energies= -
 983.125681

		E (Thermal)	CV	S
		KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total		158.484	61.172	128.339
1	7	0	-1.418418	1.203057
2	6	0	-1.606587	-0.152591
3	6	0	-2.846628	-0.806543
4	6	0	-4.072764	-0.052710
5	7	0	-3.762254	1.348168
6	6	0	-2.523371	1.894957
7	7	0	-2.645881	-2.157883
8	6	0	-1.323086	-2.266172
9	7	0	-0.632291	-1.098138
10	8	0	-5.240739	-0.393042
11	6	0	1.762671	-0.981762
12	8	0	1.932387	0.018340
13	6	0	2.689624	1.118724
14	6	0	3.426221	0.379411
15	6	0	2.505073	-0.850043
16	8	0	4.727863	-0.067761
17	6	0	1.738479	2.214383
18	8	0	1.116967	1.861575

19	8	0	3.219995	-2.018335	-0.954558
20	1	0	-2.479860	2.973254	-0.382222
21	1	0	-0.811385	-3.221022	0.180032
22	1	0	1.020877	2.434617	1.089829
23	1	0	2.358289	3.113314	0.141766
24	1	0	0.155509	1.649899	-0.715163
25	1	0	3.358826	1.495107	1.548893
26	1	0	1.414714	-1.905960	1.100907
27	1	0	1.790504	-0.613616	-1.445213
28	1	0	4.149254	-1.825511	-0.720147
29	1	0	3.554805	1.003685	-1.235614
30	1	0	4.729505	-0.310539	0.965417
31	1	0	-4.578713	1.948201	-0.160364

B3LYP/6-31G* $r_{C-N} = 2.7$

E(RB+HF-LYP) = -983.310592173

Zero-point correction= 0.236096
 (Hartree/Particle)
 Thermal correction to Energy= 0.252091
 Thermal correction to Enthalpy= 0.253035
 Thermal correction to Gibbs Free Energy= 0.191500
 Sum of electronic and zero-point Energies= -
 983.074496
 Sum of electronic and thermal Energies= -
 983.058501
 Sum of electronic and thermal Enthalpies= -
 983.057557
 Sum of electronic and thermal Free Energies= -
 983.119092

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	158.190	61.433	129.512

N,0,0.0044976467,1.3857774841,0.2897444823
 C,0,-0.9372838555,1.2250547125,-0.7044062138
 C,0,-1.256144242,0.0142732038,-1.3497014807
 C,0,-0.5751835293,-1.2023779813,-0.9958085732
 N,0,0.3847562418,-0.920028023,0.0450965128
 C,0,0.6240698279,0.2878878563,0.6225564219
 N,0,-2.2456221592,0.2354389446,-2.2726600935
 C,0,-2.4764207618,1.5398536686,-2.1482796897
 N,0,-1.7368012851,2.1986108979,-1.2072449948
 O,0,-0.67456443,-2.3459352523,-1.4116835526
 C,0,-1.2153234534,4.8407080215,-1.4005937812
 O,0,0.0505875031,5.0215147269,-1.3494900081
 C,0,0.4491790172,5.6222586338,-0.0258661534
 C,0,-0.853145762,6.2688691731,0.4580613425
 C,0,-1.9705224448,5.4077885812,-0.2214737594
 O,0,-0.9881469599,7.6347243912,0.0703722648
 C,0,0.9941987407,4.5318765433,0.898560848
 O,0,-0.0405520597,3.8011222724,1.4782547806
 O,0,-3.0784329737,6.1572388316,-0.6397781842
 H,0,1.3780596781,0.3105036702,1.4049790344
 H,0,-3.2258421511,2.0557990188,-2.739822305
 H,0,1.6931292393,3.9044844674,0.3268617815
 H,0,1.5785470647,5.0561692413,1.6721289519
 H,0,-0.0364941908,2.8724059186,1.0855299567
 H,0,1.2249458247,6.3453413404,-0.2924171447
 H,0,-1.6347955377,4.5048319597,-2.3401284043
 H,0,-2.2732965435,4.5808525245,0.4249534299
 H,0,-2.8030844586,7.0930597327,-0.5737708359
 H,0,-0.9391531928,6.2409793276,1.5433477297
 H,0,-0.5656088403,7.7752992842,-0.7931812928
 H,0,0.9033180472,-1.7339161716,0.3548789302

B3LYP/6-31G* $r_{C-N} = 2.9$

E(RB+HF-LYP) = -983.303383398

Zero-point correction= 0.235572
 (Hartree/Particle)
 Thermal correction to Energy= 0.251716
 Thermal correction to Enthalpy= 0.252660
 Thermal correction to Gibbs Free Energy= 0.190557
 Sum of electronic and zero-point Energies= -
 983.067811
 Sum of electronic and thermal Energies= -
 983.051668
 Sum of electronic and thermal Enthalpies= -
 983.050723
 Sum of electronic and thermal Free Energies= -
 983.112827

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	157.954	61.639	130.708

N,0,-0.1324214755,1.4075690185,0.3586930792
 C,0,-1.1118636466,1.1964740014,-0.5906349397
 C,0,-1.2776675822,0.0239880626,-1.3549816599
 C,0,-0.3807229911,-1.0878693081,-1.1930110976
 N,0,0.5960059481,-0.7606251615,-0.1802869422
 C,0,0.6812043865,0.4014923276,0.5215793468
 N,0,-2.3575995501,0.1773966192,-2.1869037016
 C,0,-2.776151074,1.4080427013,-1.8950837358
 N,0,-2.0882328671,2.0780802579,-0.9212159386
 O,0,-0.3173432566,-2.1779373496,-1.7400228906
 C,0,-1.1503143391,4.7827626181,-1.3848929456
 O,0,0.1145652353,4.8418089727,-1.2455325563
 C,0,0.4755629094,5.5219513513,0.0589382359
 C,0,-0.7978776829,6.3049469371,0.3961154421
 C,0,-1.9330381726,5.4948297236,-0.3129023216
 O,0,-0.7838804933,7.6476125906,-0.0826792755
 C,0,0.8561980146,4.4514001256,1.0834580879
 O,0,-0.277423672,3.8080926677,1.5726730272
 O,0,-2.9464793041,6.2962099215,-0.8551769219
 H,0,1.4821373206,0.4670928129,1.2535264264
 H,0,-3.6422286118,1.8519750763,-2.3755097664
 H,0,1.5691310763,3.7584392048,0.614054341
 H,0,1.3877736755,4.9789876969,1.8919484621
 H,0,-0.2820555897,2.8685342687,1.2018896718
 H,0,1.327023515,6.1557647143,-0.2027812506
 H,0,-1.5416347585,4.3247993206,-2.2872118382
 H,0,-2.3432472276,4.7281577152,0.3516013605
 H,0,-2.5983453757,7.2094984407,-0.8373372574
 H,0,-0.9643321805,6.3571602769,1.4713003402
 H,0,-0.2909702779,7.6963058969,-0.918701871
 H,0,1.2630980477,-1.5024745018,-0.0018909107

B3LYP/6-31G* $r_{C-N} = 3.1$

E(RB+HF-LYP) = -983.297690255

Zero-point correction= 0.235039
 (Hartree/Particle)
 Thermal correction to Energy= 0.251257
 Thermal correction to Enthalpy= 0.252201

Thermal correction to Gibbs Free Energy= 0.189744
 Sum of electronic and zero-point Energies= -
 983.062652
 Sum of electronic and thermal Energies= -
 983.046434
 Sum of electronic and thermal Enthalpies= -
 983.045489
 Sum of electronic and thermal Free Energies= -
 983.107946

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	157.666	61.693	131.451

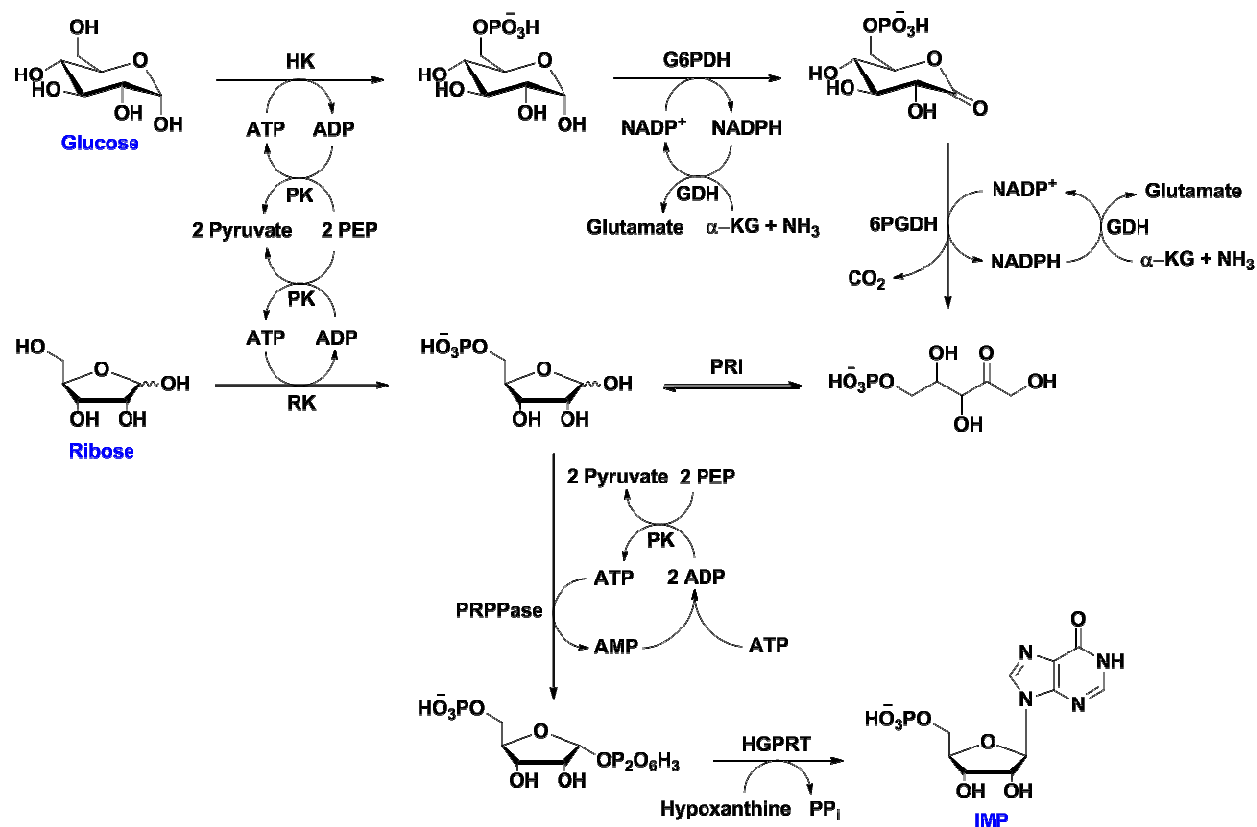
N,0,-0.1570836571,1.3768682873,0.313089445
 C,0,-1.1225943624,1.1253422398,-0.6423823684
 C,0,-1.2722133978,-0.0799596489,-1.3580068319
 C,0,-0.3746965912,-1.179567974,-1.1387297163
 N,0,0.5884649227,-0.8063318416,-0.126421619
 C,0,0.6580508954,0.3825267832,0.5293495125
 N,0,-2.3554592917,0.0262011463,-2.1927067468
 C,0,-2.7905508843,1.2615034866,-1.9455667276
 N,0,-2.1119291759,1.9801141668,-1.002584154
 O,0,-0.3002671182,-2.2921983236,-1.634812638
 C,0,-1.1586417674,4.9039537625,-2.3929613996
 O,0,0.1061754593,4.9707840555,-1.2767180719
 C,0,0.4883573001,5.5866523999,0.0488474061
 C,0,-0.7799483482,6.3536911226,0.4420982659
 C,0,-1.9291397684,5.5783907455,-0.2870827097
 O,0,-0.772156124,7.7180804579,0.0251855212
 C,0,0.8667155711,4.4553626759,1.0110526285
 O,0,-0.2736945823,3.7939939338,1.4568898568
 O,0,-2.9384327057,6.4057674184,-0.7920939675
 H,0,1.4454264041,0.4812289217,1.2724730424
 H,0,-3.6620295101,1.675660849,-2.4432462662
 H,0,1.5780216876,3.7871438364,0.5032445161
 H,0,1.4023092929,4.9357917988,1.8458263239
 H,0,-0.2739477391,2.8488022563,1.0779287752
 H,0,1.3402289612,6.2292299679,-0.1891968108
 H,0,-1.5604942324,4.4577516804,-2.2982289521
 H,0,-2.3465814622,4.7926140707,0.3512489295
 H,0,-2.5818312592,7.3154809183,-0.7539055379
 H,0,-0.9307091203,6.355225031,1.520623097
 H,0,-0.2744938903,7.8098631417,-0.8043716727
 H,0,1.2520144938,-1.5395003662,0.0951788701

E. $D_N^{\ddagger} * A_N$ KIEs

r(C-N) distance	2.3	2.5	2.7	2.9	3.1
C	1.052	1.042	1.032	1.025	1.023
N	1.029	1.031	1.032	1.036	1.037
1'	1.161	1.240	1.307	1.363	1.383
2'	0.969	0.983	1.002	1.024	1.024
5'	1.051	1.061	1.073	1.080	1.095

6. Synthetic Schemes for Specifically Labeled Inosine Substrates

Scheme S1: Synthesis of $[5'\text{-}^3\text{H}_2]\text{-}$, $[4'\text{-}^3\text{H}]\text{-}$, $[5'\text{-}^{14}\text{C}]\text{-}$, and $[5'\text{-}^{14}\text{C}, 2'\text{-}^2\text{H}]\text{IMP}$ from labeled glucose, and of $[1'\text{-}^3\text{H}]\text{-}$ and $[1'\text{-}^{14}\text{C}]\text{IMP}$ from labeled ribose.



Scheme S2: Synthesis of [5'-¹⁴C,9-¹⁵N]inosine from labeled ATP.