SUPPORTING INFORMATION

Allosteric activation shifts the rate-limiting step in a short-form ATP phosphoribosyltransferase

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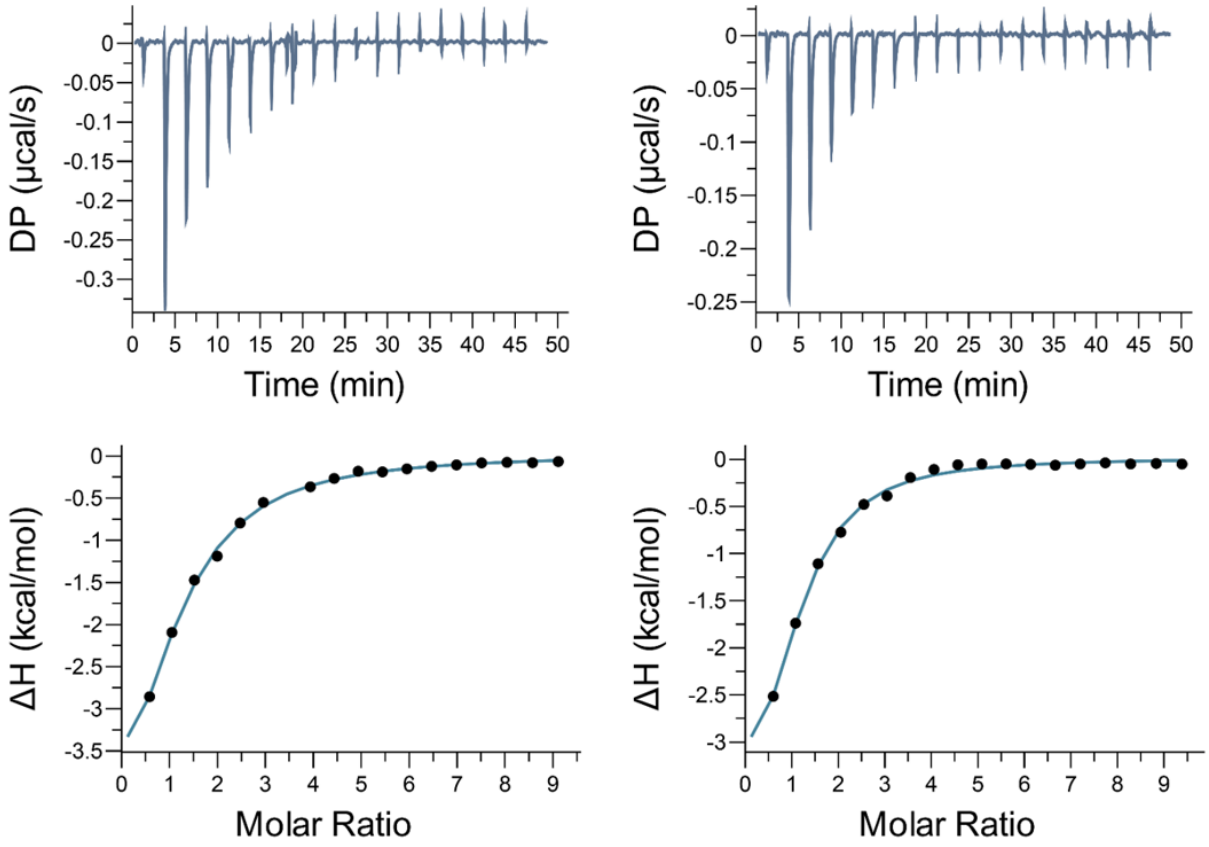

Figure S1. ITC curves for *Pa*HisG$_S$ titration with PRPP in two independent experiments. Controls lacking *Pa*HisG$_S$ have been subtracted from the data, and the solid lines represent data fitting to a single-site binding model.

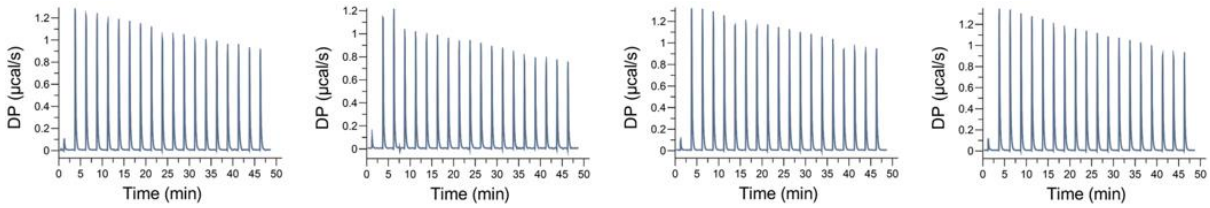

Figure S2. ITC curves for *Pa*HisG$_S$ (two graphs on the left) and buffer (two graphs on the right) titration with ATP in two independent experiments. No signal is detected beyond the heat of dilution when experimental and control sets are compared.

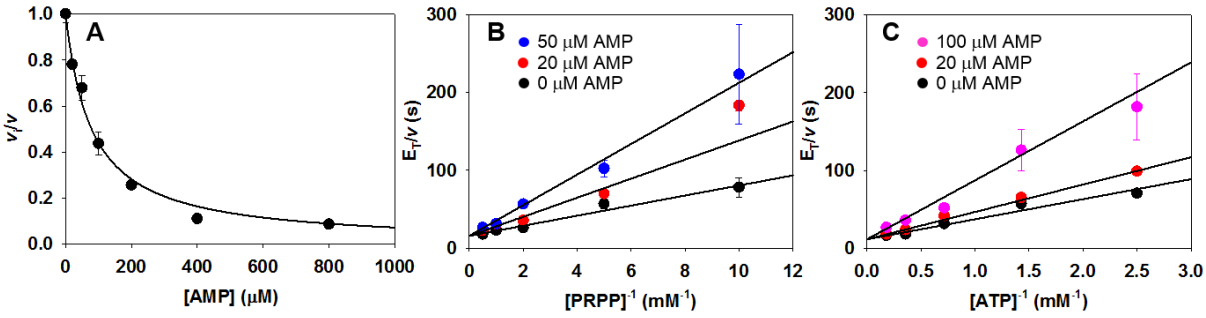

Figure S3. *Pa*HisG$_S$ inhibition by AMP. (A) Dose-response curve for AMP concentration. Line represents data fitting to eq 4. (B) and (C) Double-reciprocals of substrate saturation curves in the presence of AMP. Lines are the reciprocals of data fitting to eq 5.

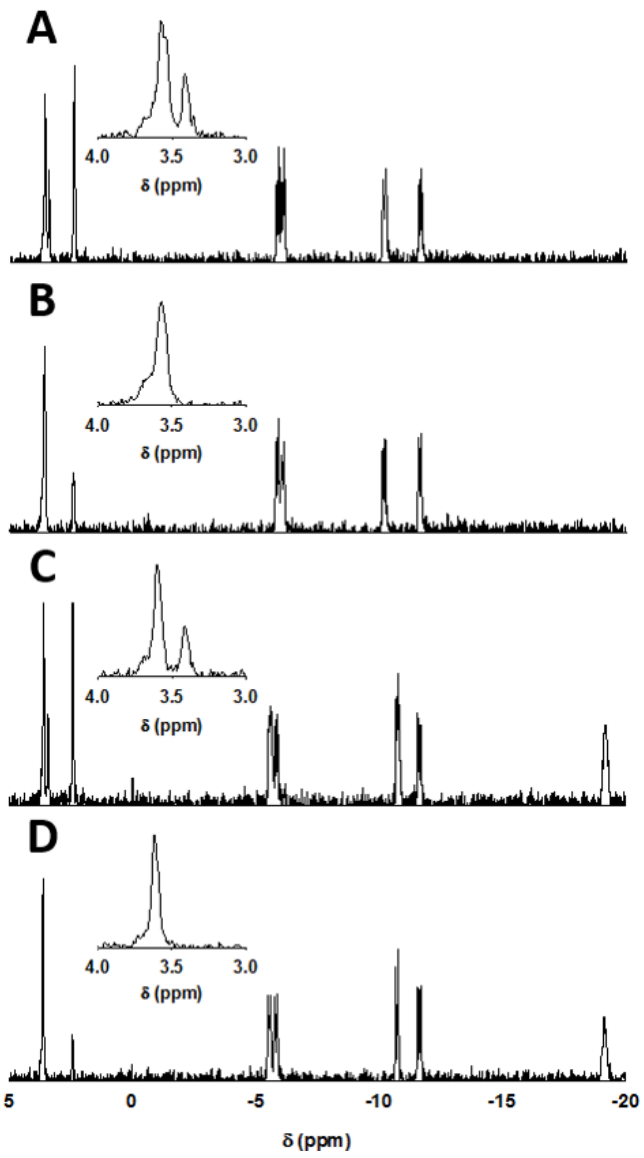

Figure S4. ^{31}P-NMR spectra of *Pa*HisG$_S$ reaction with either (A) ADP or (C) ATP as substrate. (B) and (D) are controls for (A) and (B), respectively, in the absence of *Pa*HisG$_S$. Insets in A – D are close-ups of the spectra between 4.0 and 3.0 ppm, showing the peak at *ca*. 3.3 ppm in A and C corresponding to the phosphorus in the N^1-5-phospho-β-D-ribose moiety of PRATP and PRADP, respectively, which is missing in insets in B and D.

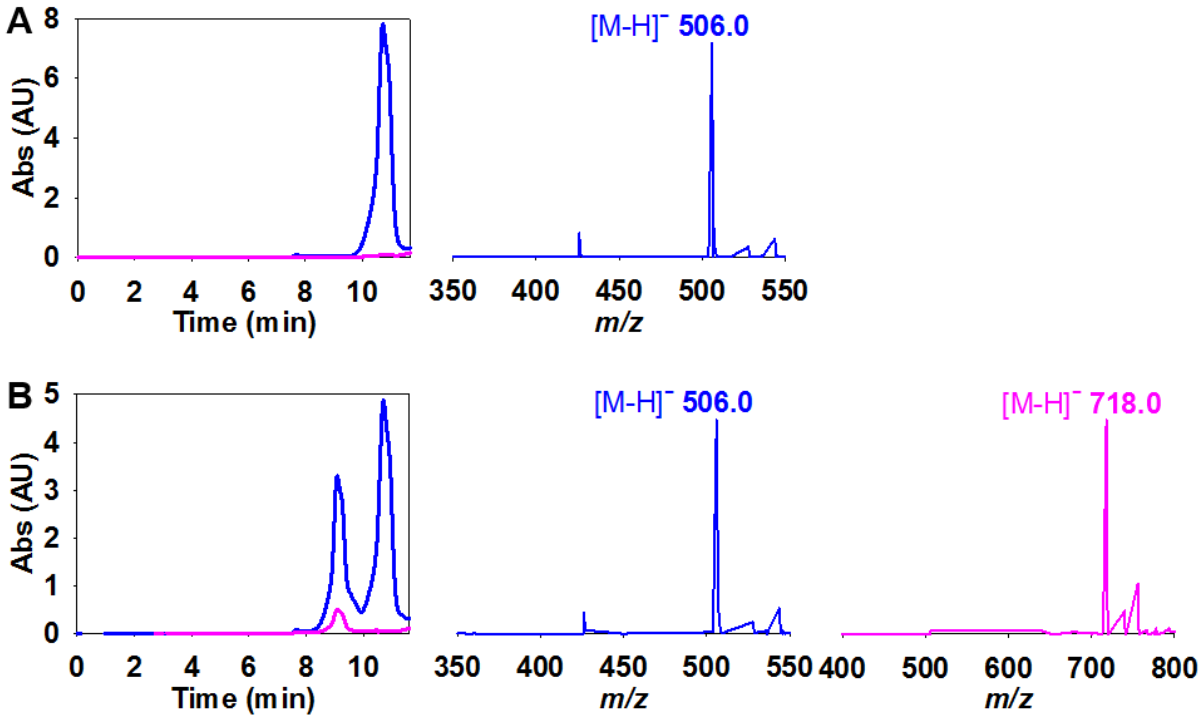

Figure S5. Analysis of *Pa*HisG$_S$-catalysed reaction with Mn^{2+} replacing Mg^{2+}. (A) Chromatogram of the control reaction lacking *Pa*HisG$_S$, showing a peak with absorbance at 260 nm (blue), corresponding to ATP, and mass spectra of the peak showing the expected *m/z* for ATP (blue). (B) Chromatogram of the reaction, showing peaks with absorbance at 260 nm (blue) and at both 260 nm and 290 nm (pink), corresponding to ATP and PRATP, respectively, and mass spectra of the peak absorbing at 260 nm showing the expected *m/z* for ATP (blue), and of the peak absorbing at both 260 nm and 290 nm showing the expected *m/z* for PRATP (pink).

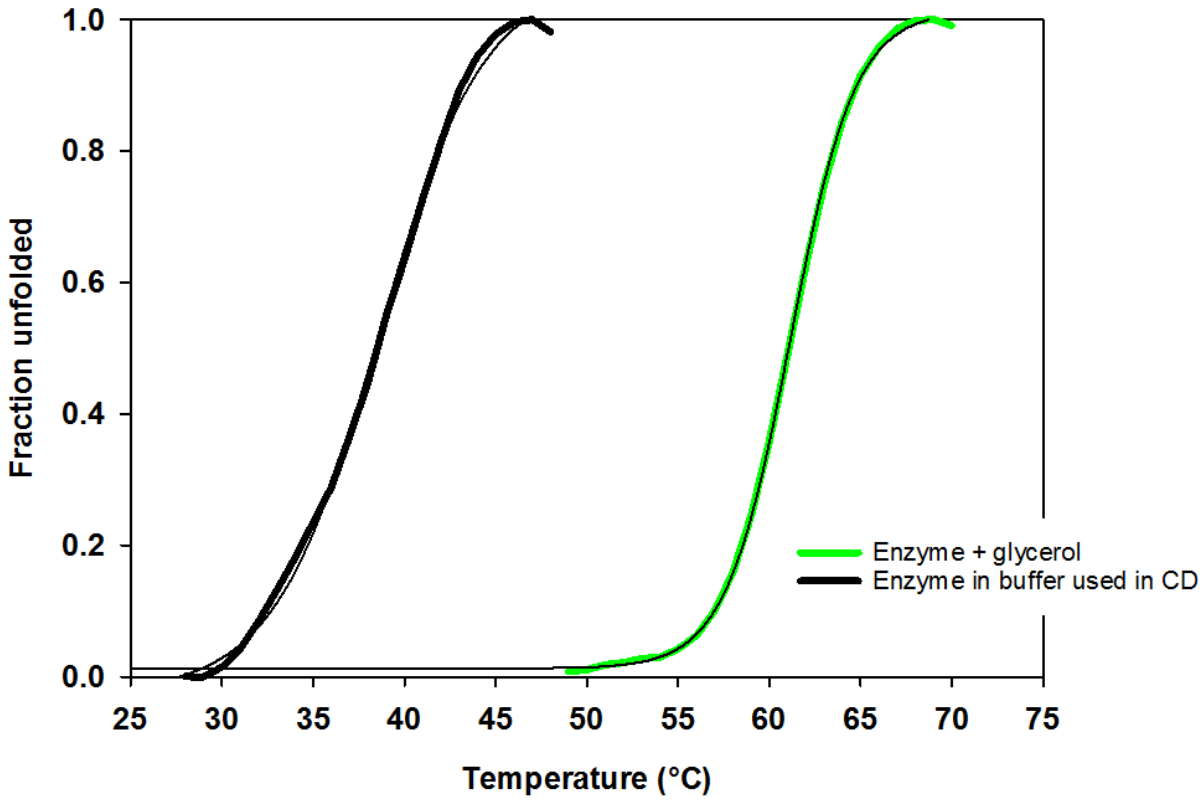

Figure S6. DSF-based thermal denaturation of *Pa*HisG$_S$ in the presence of 22% glycerol (*v/v*), and in 10 mM KH_2PO_4, 10 mM KF pH 8.0, which was the buffer used for circular dichroism (CD) thermal denaturation studies of *Pa*HisG$_S$,[1] indicating that the protein is more thermolabile in that buffer. Data were fitted to eq 8.

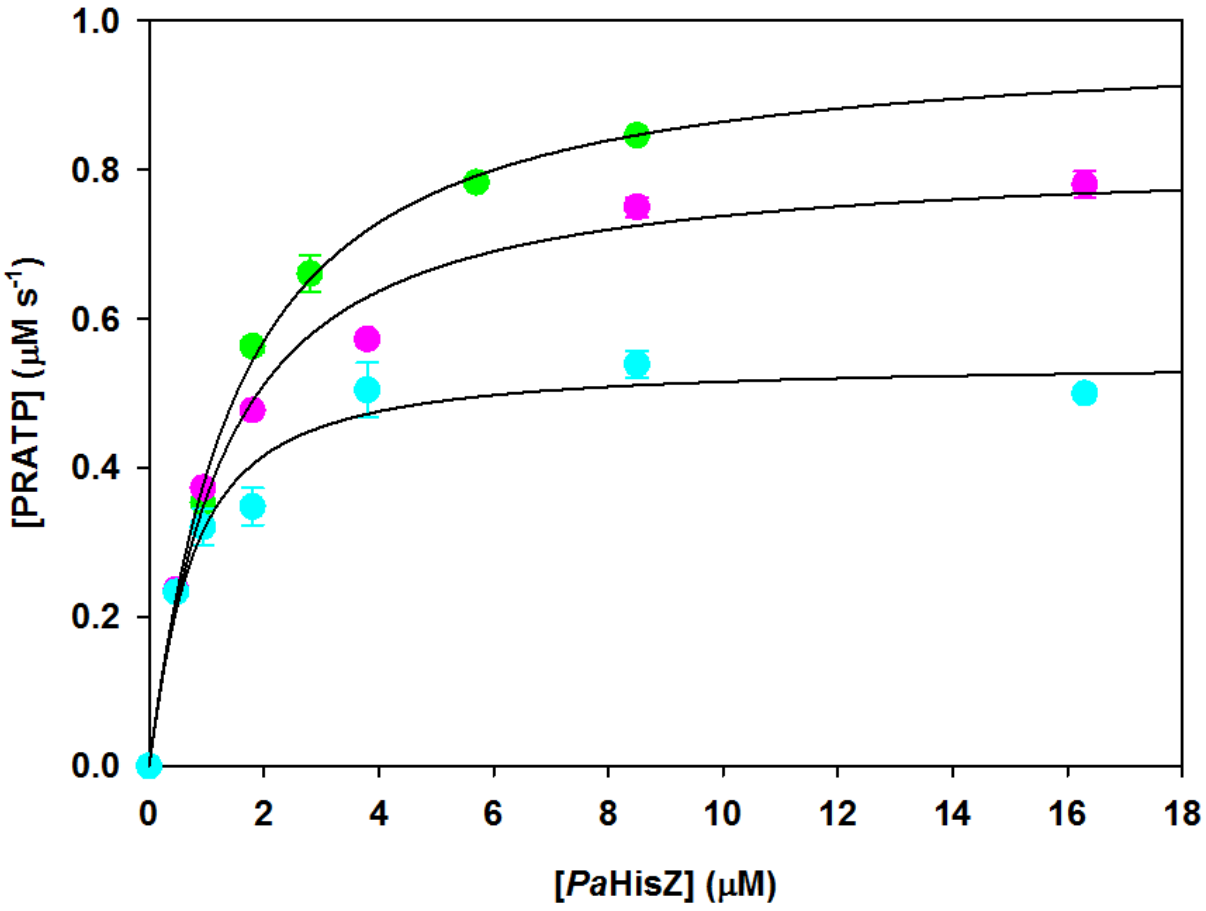

Figure S7. Determination of K_D for equilibrium dissociation of *Pa*HisZ from the *Pa*ATPPRT holoenzyme in 0% glycerol (green), 18% glycerol (pink), and 27% glycerol (cyan) (*v/v*). Lines are data fitting to eq 1.

Table S1. *Pa*ATPPRT and *Pa*HisG$_S$ steady-state parameters from initial velocity patterns.

Parameter	*Pa*ATPPRT[a]	*Pa*HisG$_S$[b]
k_{cat} (s^{-1})	1.5 ± 0.1	0.25 ± 0.02
K_{iPRPP} (mM)	0.4 ± 0.1	0.04 ± 0.03
K_{PRPP} (mM)	0.7 ± 0.1	0.6 ± 0.1
K_{ATP} (mM)	1.4 ± 0.2	2.3 ± 0.3
k_{cat}/K_{PRPP} (M^{-1} s^{-1})	2142 ± 337	416 ± 77
k_{cat}/K_{ATP} (M^{-1} s^{-1})	1071 ± 168	108 ± 16

[a]Values represent mean ± fitting error of duplicate measurements. [b]Values represent mean ± fitting error of quadruplicate measurements.

Table S2. *Pa*HisG$_S$ T_m's by DSF in the presence and absence of ligands.[a]

Ligand	T_m (°C)
Enzyme (no ligand)	60.0 ± 0.1
PRPP	66.0 ± 0.1
ATP	59.0 ± 0.1
PRATP	65.0 ± 0.1
PP_i	59.0 ± 0.1
Enzyme (no ligand) in 22% glycerol (*v*/*v*)	61.0 ± 0.1
Enzyme (no ligand) in 10 mM K_2HPO_4, 10 mM KF, pH 8.0[b]	39.0 ± 0.2

[a]Values represent mean ± fitting error of triplicate measurements. [b]Buffer used in a previous circular dichroism-based thermal denaturation.[1]

Table S3. Steady-state kinetic constants for *Pa*HisG$_S$[a] with either ATP or ADP.

Parameter	ATP	ADP
k_{cat} (s^{-1})	0.15 ± 0.01	0.14 ± 0.01
$K_M^{A(X)P}$ (mM), X = T or D	0.96 ± 0.09	3.2 ± 0.3
K_M^{PRPP} (mM)	0.39 ± 0.07	0.91 ± 0.08
$k_{cat}/K_M^{A(X)P}$ (M^{-1} s^{-1}), X = T or D	156 ± 20	43 ± 5
k_{cat}/K_M^{PRPP} (M^{-1} s^{-1})	384 ± 70	153 ± 6

[a]Values represent mean ± fitting error of duplicate measurements.

Table S4. Effect of Mn^{2+} on *Pa*ATPPRT and *Pa*HisG$_S$ steady-state kinetic parameters.[a]

Parameter	*Pa*HisG$_S$ Mg^{2+}	*Pa*HisG$_S$ Mn^{2+}	*Pa*ATPPRT Mg^{2+}	*Pa*ATPPRT Mn^{2+}
k_{cat} (s^{-1})	0.15 ± 0.01	0.39 ± 0.05	2.7 ± 0.1	2.1 ± 0.1
K_M^{PRPP} (mM)	0.33 ± 0.03	0.6 ± 0.2	0.43 ± 0.06	0.28 ± 0.06
K_M^{ATP} (mM)	1.4 ± 0.2	0.30 ± 0.05	0.72 ± 0.09	0.19 ± 0.03
k_{cat}/K_M^{PRPP} (M^{-1} s^{-1})	450 ± 50	700 ± 200	6000 ± 900	7500 ± 2000
k_{cat}/K_M^{ATP} (M^{-1} s^{-1})	110 ± 20	1300 ± 300	3800 ± 500	11100± 2000

[a]Values represent mean ± fitting error of duplicate measurements.

Table S5. NBO charge distribution of key atoms at the transition state of *Pa*HisG$_S$.

Atom	Transition state with Mg^{2+} NBO charge	Transition state with Mn^{2+} NBO charge
ADP N1	–0.563	–0.562
ADP N6	–0.783	–0.783
ADP C6	0.455	0.453
5-phosphoribosyl C1	0.410	0.399
5-phosphoribosyl O4	–0.459	–0.459
PP_i Os bonded to metal ion 1	–1.208 (average of 2 O atoms)	–1.053 (average of 2 O atoms)
PP_i Os bonded to metal ion 2	–1.162 (average of 2 charges)	–1.026 (average of 2 charges)
Metal ion 1 (bonded to PP_i)	1.437	0.610
Metal ion 2 (bonded to PP_i and ADP)	1.439	0.688

Table S6. Solvent viscosity effects on *Pa*HisG$_S$ steady-state kinetic parameters.[a]

Parameter	0% glycerol (*v/v*)	18% glycerol (*v/v*)	27% glycerol (*v/v*)
k_{cat} (s^{-1})	0.15 ± 0.02	0.28 ± 0.05	0.40 ± 0.02
K_M^{PRPP} (mM)	0.36 ± 0.04	0.35 ± 0.02	0.41 ± 0.08
K_M^{ATP} (mM)	1.2 ± 0.1	1.9 ± 0.2	1.9 ± 0.2
k_{cat}/K_M^{PRPP} (M^{-1} s^{-1})	416 ± 70	800 ± 150	976 ± 197
k_{cat}/K_M^{ATP} (M^{-1} s^{-1})	125 ± 19	147 ± 30	210 ± 24

[a]Values represent mean ± fitting error of duplicate measurements.

Table S7. Solvent viscosity effects on *Pa*ATPPRT steady-state kinetic parameters.[a]

Parameter	0% glycerol (*v/v*)	18% glycerol (*v/v*)	27% glycerol (*v/v*)
k_{cat} (s^{-1})	2.6 ± 0.1	1.8 ± 0.1	1.03 ± 0.03
K_M^{PRPP} (mM)	0.29 ± 0.04	0.18 ± 0.03	0.10 ± 0.01
K_M^{ATP} (mM)	0.62 ± 0.05	0.8 ± 0.1	0.35 ± 0.03
k_{cat}/K_M^{PRPP} (M^{-1} s^{-1})	9000 ± 1000	10000 ± 2000	10300 ± 1000
k_{cat}/K_M^{ATP} (M^{-1} s^{-1})	4200 ± 400	2300 ± 300	2900 ± 300

[a]Values represent mean ± fitting error of duplicate measurements.

Coordinates of DFT-calculated structures

freeTS.log – Transition structure with Mg. No bonds fixed

C-N = 2.27 Å

C-O = 2.36 Å

Free Energy = -6563.285823

Zero-point Energy = -6563.129757

Potential Energy = -6564.43503489

Nimag = 1 (-213.6872 cm-1)

B3LYP/6-31G* Lanl2DZ Mg

Charge = 0 Multiplicity = 1

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H 1.59715 7.36192 -4.48860

freeTSMn.log - Transition structure with Mn. No bonds fixed

C-N = 2.27 Å

C-O = 2.38 Å

B3LYP/6-31G* Lanl2DZ Mn

Free Energy = -6769.088921

Zero-point Energy = -6768.934608

Potential Energy = -6770.24007644

Nimag = 1 (-198.4577 cm-1)

Charge = 0 Multiplicity = 1

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H -3.98173 5.23200 -1.90836
H -3.27601 6.78155 -2.39493
H -1.22707 5.96776 -1.93786
H -0.16250 3.59942 0.46239
H 0.23593 4.50242 -1.00314
H -3.58990 4.39252 0.22482
H -2.43303 3.41586 1.02811
H -8.40598 -6.23721 -3.45535
H -8.40770 -6.60731 -1.73440
H -2.58122 -4.78714 -2.77448
H -1.74779 -4.52716 -1.20582
H -3.84998 -3.81304 -0.23750
H -4.67640 -4.17386 -1.72539
H -3.55309 -2.88176 -1.62948
H 1.97617 5.50071 -5.03498
H 2.84882 6.31935 -3.73720
H 9.21423 -2.07650 -1.78296
H 6.75672 -0.73160 -0.01144
H -9.04883 0.39344 -4.01015
H -8.05148 -0.73197 -3.73845
H 5.66890 -4.17256 3.71016
H 5.51518 -3.81519 2.16952
H -8.45816 -3.75650 1.01872
H -8.43372 -3.53546 -0.51408
H 7.15637 -4.56076 -1.76341
H 7.65756 -4.45678 -0.34292
H 5.84924 -3.38410 -0.16815
H 6.53312 -2.52314 0.90143
H 2.53034 2.77449 -1.30988
H 2.18001 3.65186 -2.55677
H -3.68515 4.30438 5.25880
H -3.79248 3.18616 4.14070
H -2.36247 2.32070 5.06633
H -2.14758 0.75570 5.10039
H -4.81937 -3.16781 1.37362
H -3.42294 -3.49742 2.02153
H -0.54250 -3.38454 3.54752
H 0.53327 -2.80362 4.49361
H 3.27384 -3.74123 2.89452
H 1.65934 -3.60159 2.90293
H -6.09854 0.35507 2.03578
H -6.39661 1.94688 1.30599
H -7.46052 0.03687 0.10901
H -4.57961 -0.84339 -0.31125
H -6.96134 -2.35046 0.26470
H -5.24282 -1.69903 -2.52249
H -7.32951 -2.50064 -2.17087
H -6.52358 0.62785 -3.20029
H -5.10720 2.90883 -2.98539
H -1.25758 -2.20965 -2.43735
H -0.27898 2.96684 -3.06220
H 3.40595 -0.65666 -4.01856
H 3.77254 -2.34927 -3.60675
H 3.95061 -0.60198 -1.24721
H 2.63612 -3.18663 -1.78504
H 3.10372 -3.39228 0.38189
H 0.43849 -2.39171 -1.46906
H -0.08996 -1.70356 0.70339
H 0.51829 0.39676 -0.88065
H 7.00796 2.77029 -3.62256
H -3.78291 6.54903 -0.71126
H -7.07786 -7.21368 -2.76833

H -2.99640 -5.79013 -1.36878

Mn 2.50790 -1.49507 1.67823

O 4.38417 -1.11935 2.71543

H 4.72597 -2.00794 2.99279

H 5.05939 -0.78146 2.08310

H 0.96204 1.80148 -2.93983

H 4.02973 -0.08566 4.43750

O -0.56395 3.71850 3.50270

H 0.08762 3.88559 4.20560

H -1.44480 3.99934 3.84428

H 0.12181 -0.69305 3.29779

H 7.50135 -0.51061 1.36793

H 9.09300 -3.61323 -1.90576

H 8.22226 -2.52032 -3.41609

H 1.66443 7.23194 -4.71264

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fixed bonds at

C-N = 2.9

C-O = 1.4

B3LYP/6-31G* Lanl2DZ Mg

Zero-point correction= 1.305334 (Hartree/Particle)

Thermal correction to Energy= 1.417149

Thermal correction to Enthalpy= 1.418094

Thermal correction to Gibbs Free Energy= 1.149400

Sum of electronic and zero-point Energies= -6563.173805

Sum of electronic and thermal Energies= -6563.061989

Sum of electronic and thermal Enthalpies= -6563.061045

Sum of electronic and thermal Free Energies= -6563.329739

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	889.275	406.194	565.513

C,0,-6.0980201217,5.1078923051,-1.6956588565

N,0,-5.4904213768,3.8149741672,-1.9568600753

C,0,-6.0434830118,2.6555622119,-1.6054424761

N,0,-7.2627432202,2.6080797228,-1.012364787

N,0,-5.4157768765,1.5053703652,-1.8787131615

C,0,3.9262370916,4.2366170308,-3.7770063974

N,0,2.5418712012,3.9203098956,-3.4898191004

C,0,2.0909508088,2.6794302063,-3.3128875372

N,0,0.7936694952,2.480906713,-3.0502903007

N,0,2.9194017828,1.6213931674,-3.4556069857

C,0,7.5772068091,-1.0565153302,6.8900674852

C,0,6.8632403843,-0.6136002522,5.6136576744

O,0,7.6140782556,-0.3600174184,4.6148385684

O,0,5.6113786555,-0.5132606515,5.6424133604

C,0,2.5648360782,-1.0253843118,5.0166423266

N,0,3.6047127313,-0.923670143,3.9637904029

C,0,-1.3805134623,6.9529756033,-3.0668490735

C,0,-0.330977395,5.8518289908,-2.9340983323

O,0,0.814021306,6.0493347745,-3.3816820434

O,0,-0.7241619663,4.7625272219,-2.3565843274

O,0,-7.3498676839,1.3730777929,5.6479954578

O,0,-6.4308071901,-1.1969001815,-0.9982514579

O,0,8.2080144211,3.7027768621,2.2923021782

O,0,-5.5623135195,-4.6635791122,1.6579732987

O,0,8.4237630506,-1.9142082015,2.5794129476

O,0,-6.1975356483,-1.0720239921,5.511705245

O,0,-7.1248419845,-2.9309833653,3.0490567547
O,0,-3.1143159796,3.8874154673,-3.2681735391
O,0,3.446044046,-3.2557886177,-5.4538893422
O,0,5.614484081,-1.5694040971,-5.1242587338
O,0,3.9510256477,-3.2854912282,2.5853046517
O,0,-0.3853847145,-5.4878531083,1.7266319236
O,0,-2.7452052778,-4.3344619789,1.5793418407
O,0,2.3291276504,-1.1536394449,-2.7101056211
P,0,3.5801203079,-1.7668885419,-2.0760044139
O,0,4.429763735,-2.7134248171,-2.8819020548
O,0,3.1132170887,-2.545988767,-0.7025927713
P,0,1.6360359835,-2.773437769,-0.0634542827
O,0,1.0445273244,-1.480330481,0.453004996
O,0,0.8091054542,-3.1983484626,-1.4595852136
O,0,1.7159049451,-3.9647638736,0.8581883072
O,0,4.4345755425,-0.5159718519,-1.5371071037
C,0,5.8597031768,-0.6436840733,-1.3201601083
C,0,6.2726037349,0.1539856117,-0.1045536611
C,0,5.5364890396,-0.2000116964,1.1935911504
O,0,5.885435382,-1.4380793045,1.7596060487
C,0,5.8147704126,1.0723073314,2.0314283365
O,0,7.1490951586,1.1026558701,2.4918806654
C,0,5.6740827667,2.1630965486,0.9549106079
O,0,6.0040605463,1.5499405902,-0.2978565852
N,0,4.338992357,2.7678251784,0.8540634236
C,0,3.0814904073,2.3322788668,1.232169261
C,0,2.1836178712,3.2221850454,0.6208263623
N,0,2.853999796,4.1856847218,-0.1089668641
C,0,4.1143365604,3.8783115538,0.0563621332
N,0,2.7331920216,1.3127237196,2.0448834875
C,0,1.4102134652,1.2176501094,2.1817061936
N,0,0.4447607096,1.9633907102,1.6384367933
C,0,0.8022626519,2.9971642671,0.8343061113
N,0,-0.1819898898,3.7415657964,0.2926746172
O,0,-8.0662454466,1.1036129072,3.1278158951
P,0,-6.8814849079,0.6884440445,2.1627186469
O,0,-7.4653405641,0.3825817042,0.7919186925
O,0,-6.0437748485,-0.4612185476,2.7841289699
O,0,-5.9570797849,2.0234385919,2.0565404533
C,0,-4.5261763453,2.1111870166,2.163518174
C,0,-3.7880274688,1.0661902762,1.3182296531
O,0,-2.6731225813,1.6676983171,0.6264364657
C,0,-3.1885445774,-0.1429809948,2.082057248
O,0,-3.8594435276,-1.3535071464,1.7123688597
C,0,-1.7327619603,-0.2090542757,1.5924987309
O,0,-1.3343439633,-1.5542337475,1.4089690009
C,0,-1.7879970364,0.6168669156,0.295230448
O,0,-2.3363703861,-0.2305619728,-0.674899324
P,0,-2.075596858,-0.0994387403,-2.3014659604
O,0,-2.7534920758,1.1014126612,-2.8728653317
O,0,-0.5976452827,-0.341624107,-2.5968434484
O,0,-2.925534097,-1.4516415599,-2.6968970536
P,0,-2.2761296307,-2.9584862707,-2.5992841877
O,0,-1.8613562887,-3.190630231,-1.1322750753
O,0,-1.1320690516,-3.0803208759,-3.5733293991
O,0,-3.5295350877,-3.8738330371,-2.960474078
Mg,0,0.5500105362,-1.9082989677,-3.1559438116
H,0,-5.4319244143,5.8720989037,-2.0995775759
H,0,-6.2218443189,5.2983715276,-0.620646525
H,0,-4.560249139,3.811556915,-2.4456109441
H,0,-7.4557000776,1.7997756796,-0.4066617822
H,0,-7.6315694922,3.4795265038,-0.659433776
H,0,-4.4747647641,1.4849699553,-2.2836290162
H,0,-5.8385206889,0.6074838438,-1.6511495659
H,0,4.5960113773,3.9487356215,-2.9546434337
H,0,3.9974204442,5.3177896295,-3.9069696009
H,0,1.8696535046,4.7137152952,-3.3816090228
H,0,0.4358031243,1.5441120577,-2.8981570405
H,0,0.1882496581,3.2964832103,-2.8496284181
H,0,3.9137231012,1.7796079791,-3.3892598943

H,0,2.6206109377,0.6965836228,-3.1456383079
H,0,6.8627939265,-1.3003726801,7.6790357891
H,0,8.2422313057,-0.2553729899,7.2316833693
H,0,2.4491913391,-0.0573657466,5.5070023071
H,0,1.6164415689,-1.3414897654,4.5765763829
H,0,3.6938666742,-1.833637122,3.4370825525
H,0,4.5338668387,-0.7084629937,4.4440624401
H,0,3.3943266488,-0.1712632587,3.2835766395
H,0,-1.7558905282,7.2297300124,-2.0744560073
H,0,-2.2316157404,6.5756050352,-3.6459612181
H,0,-8.1246566201,1.4474423428,6.2254856432
H,0,-6.86980754,-0.6935355469,-0.2430400631
H,0,8.9424345064,3.5274620682,1.6847241513
H,0,7.9230388272,2.8024331817,2.5591032021
H,0,-6.0515503186,-5.4922452789,1.5402631787
H,0,-6.1395298361,-4.078953305,2.2264962201
H,0,8.3303791203,-2.8338578269,2.8734427878
H,0,8.3305195222,-1.3823726577,3.4104140532
H,0,-5.8946858945,-0.8225851527,4.6120623253
H,0,-6.7716180548,-1.8368833604,5.3416566674
H,0,-6.7283980334,-2.0252431814,2.9519942484
H,0,-8.0184540975,-2.8444787036,2.6826244018
H,0,-2.8599571476,2.9622063005,-3.4433165675
H,0,-2.3103450006,4.2686876005,-2.8198374967
H,0,4.121866338,-2.5747703652,-5.68342255
H,0,3.6881272903,-3.4302422485,-4.5186221471
H,0,6.4220932333,-2.0422856307,-5.3786635862
H,0,5.3951932423,-1.9098521615,-4.2272926351
H,0,4.6477371127,-2.8938794457,2.0187884473
H,0,3.2452522209,-3.6147778827,1.9894443201
H,0,0.3723314735,-4.874897727,1.5321258012
H,0,-0.2710296005,-6.2034241365,1.0828289218
H,0,-3.5311823054,-4.7809736372,1.9387804815
H,0,-1.8880366817,-4.8468071109,1.7197218588
H,0,6.134505727,-1.6901102234,-1.1597457203
H,0,6.3671618647,-0.2810008265,-2.2202350267
H,0,7.3526457476,0.000130303,0.0414542214
H,0,4.4656632505,-0.2509358575,0.9781754025
H,0,6.853113836,-1.4924315167,1.9928962368
H,0,5.1097009871,1.2153346482,2.8537451656
H,0,7.2216183104,0.5667924087,3.341600915
H,0,6.3775297628,2.9786030466,1.1425231253
H,0,4.9502135424,4.4222026428,-0.364001218
H,0,1.0648672641,0.4039459365,2.8169092241
H,0,-0.041051236,4.3027618809,-0.5492567
H,0,-4.2733321686,3.1070488638,1.7925521878
H,0,-4.2386762669,2.0524949788,3.2190107418
H,0,-4.4838186387,0.6873008635,0.5624924556
H,0,-3.2528971974,-0.0280923503,3.1671621268
H,0,-4.8012588502,-1.2050741257,2.0087369883
H,0,-1.0802184792,0.3147130118,2.2886109634
H,0,-0.3685092969,-1.560717581,1.0642128624
H,0,-0.8413471224,1.0421010626,-0.0203912815
H,0,-7.072163369,5.2106165818,-2.1910654732
H,0,4.2705540418,3.7541655048,-4.7010957385
H,0,8.209613962,-1.9269235281,6.6815630052
H,0,2.8936799874,-1.7599203947,5.7526288002
Mg,0,-2.8349384747,-2.6506623147,0.506072891
O,0,-4.6831017771,-3.1764832997,-0.4388181413
H,0,-5.1269321101,-3.789473452,0.207414137
H,0,-5.3269150455,-2.435981259,-0.6329003176
H,0,-1.1282570899,3.4178088012,0.4557949894
H,0,-4.1304730546,-3.8715768738,-2.1768904158
O,0,1.0624888235,-2.3289919199,-5.0545166764
H,0,0.4362837473,-2.9210538199,-5.4989720975
H,0,2.0082399852,-2.633316326,-5.2909542393
H,0,-0.124573806,-3.4515274151,-1.230922372
H,0,-7.145993498,-1.4782036755,-1.5903531652
H,0,-6.9810569822,0.4620018795,5.7951420347
H,0,-7.7935870998,1.2928724835,4.0837161254

H,0,-0.9616687006,7.8331811846,-3.5581400043

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fixed bonds at

C-N = 2.65

C-O = 1.70

B3LYP/6-31G* Lanl2DZ Mg

Zero-point correction= 1.306527 (Hartree/Particle)

Thermal correction to Energy=1.418292

Thermal correction to Enthalpy=1.419236

Thermal correction to Gibbs Free Energy= 1.152773

Sum of electronic and zero-point Energies= -6563.141265

Sum of electronic and thermal Energies= -6563.029500

Sum of electronic and thermal Enthalpies=-6563.028556

Sum of electronic and thermal Free Energies= -6563.295019

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	889.992	407.893	560.820

C,0,-6.0534120239,4.3388881671,-1.4237117835

N,0,-5.2651018425,3.4460750444,-2.267387414

C,0,-5.6100189184,2.2104479585,-2.6127000589

N,0,-6.654587393,1.5880657084,-2.0304986226

N,0,-4.9527263742,1.5995360687,-3.6325167849

C,0,3.056080565,3.0695001063,-4.9204207208

N,0,1.8050328777,2.5924279322,-4.3592329119

C,0,1.6139740455,1.3852937801,-3.8463462141

N,0,0.3714487258,1.0132459512,-3.4898050434

N,0,2.6272920074,0.5025405859,-3.7155688463

C,0,8.420420419,0.7476702584,6.0938427344

C,0,7.583464168,0.8016335018,4.817166829

O,0,8.2256393803,0.6834101898,3.7227305279

O,0,6.344128513,0.9794139025,4.9315814214

C,0,3.2388301307,0.3903622094,4.8354506604

N,0,4.1621104147,0.1258018302,3.7053223564

C,0,-1.2365375193,6.3515654785,-4.1788404966

C,0,-0.1586691154,5.2805885635,-4.3415462882

O,0,0.7838147073,5.4442580162,-5.116584616

O,0,-0.3192104574,4.2075228365,-3.6044838928

O,0,-9.733370943,1.9928908353,3.0792943959

O,0,-6.7210865836,-1.3594109708,0.7537397582

O,0,8.5707614972,3.8364672504,0.2348052159

O,0,-5.1740601583,-3.5822300745,3.5252959278

O,0,8.8055460128,-1.4353484652,2.1768116833

O,0,-8.2237247636,0.6574701315,4.8676807307

O,0,-6.6112176951,-1.3457952961,3.5074626726

O,0,-2.6483982345,3.1105204249,-3.117971978

O,0,2.9086191749,-4.3134508623,-4.6778919341

O,0,1.2850350522,-5.0197950505,-2.6389916447

O,0,4.3824840006,-2.5458987554,3.105936698

O,0,-0.1841899363,-4.4924302884,3.3692000624

O,0,-2.4779780161,-3.1586383273,3.2040789491

O,0,2.085010092,-2.061300738,-2.3961660718

P,0,3.4099424632,-2.5119898562,-1.7796821893

O,0,4.1449701766,-3.6529378645,-2.4311713761

O,0,3.1337170254,-2.9107797106,-0.2026509129

P,0,1.782000727,-2.8381847365,0.7063343456

O,0,1.3071180418,-1.4125504883,0.9048381967

O,0,0.7442043829,-3.6198342634,-0.3285360718

O,0,2.0136548455,-3.6937979078,1.9299309477

O,0,4.3134549558,-1.1830418003,-1.6831740873

C,0,5.7553313619,-1.2839743041,-1.6286468659
C,0,6.3161210422,-0.1723424349,-0.7719410402
C,0,5.773690308,-0.1046378062,0.6606324155
O,0,6.2004461081,-1.1363825033,1.5126960258
C,0,6.1656765724,1.3438526107,1.0429887837
O,0,7.5475678445,1.4466204241,1.3127624018
C,0,5.8954638766,2.0842332221,-0.2812526992
O,0,5.989586961,1.1091789045,-1.3304364503
N,0,4.5891077491,2.7469798049,-0.3723653778
C,0,3.3649271021,2.4569680704,0.2019452576
C,0,2.4249738046,3.1975320032,-0.5284791111
N,0,3.0383456101,3.9410059296,-1.5183966942
C,0,4.3061940536,3.6443565498,-1.3906711898
N,0,3.080000498,1.6772181626,1.265766392
C,0,1.7733735028,1.6415755454,1.5180441442
N,0,0.7599258758,2.2411814366,0.8789135189
C,0,1.0616796591,3.0528216296,-0.171164902
N,0,0.0569927898,3.6680581292,-0.8201972061
O,0,-7.5543663047,3.2073380037,2.2038004213
P,0,-6.4532982081,2.0846043724,1.9659876043
O,0,-6.8194301933,1.2147214751,0.7472017653
O,0,-6.0572930337,1.3142037834,3.2191318091
O,0,-5.2014738956,3.055449299,1.5182717663
C,0,-3.915596834,2.8103709174,2.0763518733
C,0,-3.3081003948,1.497100744,1.5645718607
O,0,-2.2843934597,1.7654233381,0.551361042
C,0,-2.6185789354,0.5911730591,2.6049525793
O,0,-3.3665269033,-0.6345210219,2.7135637005
C,0,-1.2196024743,0.3056570926,2.0054612963
O,0,-0.8765716719,-1.050502132,2.1704184723
C,0,-1.4073867151,0.7459845559,0.5590372887
O,0,-2.2237785355,-0.6165305888,-0.046814852
P,0,-2.1179680207,-0.8785620136,-1.6658447061
O,0,-2.7337931624,0.2480118297,-2.4323871663
O,0,-0.7095207205,-1.3431569699,-2.0290700906
O,0,-3.0964010769,-2.213131736,-1.6969094692
P,0,-2.4577396428,-3.6762743568,-1.2879744063
O,0,-1.8616999051,-3.5135722493,0.1343377121
O,0,-1.4717977548,-4.131086124,-2.3288810586
O,0,-3.77244076,-4.5772044364,-1.2174282618
Mg,0,0.3459649932,-3.0983404747,-2.4381713608
H,0,-5.8778945153,5.3663478441,-1.7531436965
H,0,-5.784776257,4.2427930965,-0.3683007072
H,0,-4.2994125272,3.6936608854,-2.5251524621
H,0,-6.8994008241,0.6902648631,-2.42595013
H,0,-6.7954384228,1.6725450203,-1.0100792432
H,0,-4.1447159463,2.1350597445,-3.9614247769
H,0,-4.665895471,0.6435988068,-3.4337617273
H,0,3.8323966328,3.1894025361,-4.15502571
H,0,2.838288573,4.047937303,-5.350785768
H,0,1.046224466,3.2867969311,-4.2024393631
H,0,0.176238771,0.1269534723,-3.0279190202
H,0,-0.4114739717,1.5954361147,-3.7508948485
H,0,3.5527458548,0.8729122139,-3.5429927286
H,0,2.4315357259,-0.3861939622,-3.2503690075
H,0,7.7877653718,0.7734499862,6.9835266371
H,0,9.1096342721,1.5996418689,6.1115925368
H,0,3.162658236,1.4670484159,4.997627249
H,0,2.2538376151,-0.0304629098,4.6203123917
H,0,4.2002966053,-0.9072273328,3.48406235
H,0,5.136489882,0.454469047,3.9970920349
H,0,3.8770606776,0.6323462378,2.8485875195
H,0,-1.264881813,6.6986949734,-3.1391584094
H,0,-2.2241424142,5.9330221917,-4.4077294325
H,0,-10.0354079776,1.3482892622,2.4218148741
H,0,-6.7106738001,-0.3353346344,0.7396396951
H,0,9.2562521667,3.4876142876,-0.3548036226
H,0,8.3344552276,3.0600649052,0.7866323858
H,0,-5.7626339744,-4.2869133619,3.8365640779
H,0,-5.6642259696,-2.7160575056,3.6861145906

H,0,8.7436271593,-2.2275716534,2.7330237806

H,0,8.8055666106,-0.6835410931,2.8216631084

H,0,-7.4228091593,1.1394008169,4.5654148424

H,0,-8.016788263,-0.2485586703,4.5678304913

H,0,-6.1832080033,-0.4480094399,3.4711871449

H,0,-6.8922852649,-1.4582811337,2.5695634289

H,0,-2.4332454843,2.2754932833,-2.6604280546

H,0,-1.7836072126,3.5938253471,-3.3124805865

H,0,3.4582188769,-4.7828052924,-5.3228078769

H,0,3.519227078,-3.9845125015,-3.9519932746

H,0,1.9578864075,-5.0540909989,-3.3583041857

H,0,1.7416478466,-5.2624915002,-1.8177159617

H,0,5.0153791888,-2.3714094434,2.3782038583

H,0,3.6212741269,-3.0308084781,2.7199301574

H,0,0.6334254021,-4.1074783576,2.9547807872

H,0,-0.223543459,-5.3903001216,3.0067360568

H,0,-3.267861911,-3.6299592316,3.5385891614

H,0,-1.6354694453,-3.6899196911,3.3537723362

H,0,6.0610236843,-2.2436465239,-1.2025154074

H,0,6.1377384019,-1.2183143348,-2.6522899802

H,0,7.4091252793,-0.2987545264,-0.7379589056

H,0,4.6832908027,-0.1730529795,0.6135840271

H,0,7.1891805621,-1.14679671,1.6437005146

H,0,5.5735842806,1.751306185,1.8668179381

H,0,7.7157695339,1.1925076744,2.2733227983

H,0,6.6499507893,2.8592844445,-0.4421844898

H,0,5.1067253942,4.0476669361,-1.9978667

H,0,1.4911612923,1.0122547648,2.3586361703

H,0,0.1709574651,4.0528223399,-1.7647960651

H,0,-3.2810263175,3.6478683152,1.774751689

H,0,-3.9870143005,2.789952955,3.1675497743

H,0,-4.0874428497,0.9129913878,1.0714837511

H,0,-2.5639120812,1.0541311255,3.5921385027

H,0,-3.0858249493,-1.0977464516,3.5269864973

H,0,-0.48702332,0.9718123055,2.4581493607

H,0,0.0368494851,-1.2127958223,1.7176965893

H,0,-0.5721178179,0.854834924,-0.1114178069

H,0,-7.1148015533,4.1082581321,-1.5441073258

H,0,3.4168892792,2.3889679683,-5.7000238161

H,0,9.035592414,-0.1589457246,6.1013608698

H,0,3.6513412314,-0.075633913,5.7310923155

Mg,0,-2.5579863807,-2.1457537383,1.4063370025

O,0,-4.5279105805,-2.8977282839,0.9890955206

H,0,-4.8482929184,-3.3154264151,1.8329565572

H,0,-5.2579888856,-2.2618886114,0.7466095102

H,0,-0.8870982365,3.448992613,-0.5298483005

H,0,-4.3023194824,-4.2375103844,-0.4583741359

O,0,0.3984570706,-3.1187010531,-4.5361024287

H,0,-0.2261543217,-3.7694741408,-4.8950362996

H,0,1.2999229896,-3.4121831824,-4.8137866145

H,0,-0.1818369604,-3.6890276992,0.0398155421

H,0,-7.444665771,-1.6311562642,0.1688896818

H,0,-9.3172793985,1.452526814,3.8095628536

H,0,-8.4394096409,2.815104294,2.4922802448

H,0,-1.0393873758,7.1986481165,-4.8387041889

twofixCO19.log

fixed bonds at

C-N = 2.48

C-O = 1.90

B3LYP/6-31G* Lanl2DZ Mg

Free Energy = -6563.284078

Zero-point Energy = -6563.127692

Potential Energy = -6564.43315859

Nimag = 1 (-314.5498 cm-1)

Charge = 0 Multiplicity = 1

C 6.16481 2.89172 -3.22129
N 5.49938 2.77765 -1.92809
C 6.10020 2.32089 -0.84159
N 7.39449 1.87714 -0.92324
N 5.50542 2.35943 0.36296
C -3.44630 5.91450 -1.08506
N -2.08166 5.49236 -0.84456
C -1.74582 4.54431 0.03042
N -0.45556 4.21739 0.18597
N -2.68745 3.95771 0.80027
C -7.74214 -5.99506 -3.19131
C -6.97425 -4.73641 -2.79356
O -7.67965 -3.75059 -2.40155
O -5.72079 -4.75290 -2.89524
C -2.69427 -4.57796 -1.97844
N -3.76019 -3.65636 -1.51643
C 1.81290 6.69264 -3.57601
C 0.72830 6.13265 -2.65981
O -0.27512 6.83152 -2.40980
O 0.92244 4.94850 -2.19174
O 9.46596 -2.77915 -2.78724
O 6.77718 -0.78170 1.05183
O -8.18316 0.49438 -4.40955
O 5.16861 -4.13024 2.71799
O -8.56064 -2.94853 0.00494
O 7.81168 -4.74380 -1.82742
O 6.35911 -3.57819 0.40417
O 2.78351 3.12024 -1.90313
O -3.39168 3.10907 5.28560
O -1.69958 1.00173 5.39239
O -4.20294 -3.91341 1.17455
O 0.23142 -4.38829 3.26959
O 2.54652 -3.70245 2.13557
O -2.29272 1.65813 2.46335
P -3.60337 0.89183 2.62805
O -4.44243 1.14969 3.85100
O -3.25671 -0.72148 2.57882
P -1.85723 -1.50768 2.29870
O -1.36022 -1.27115 0.88290
O -0.88921 -0.70392 3.37285
O -2.03977 -2.93681 2.75516
O -4.44285 1.14128 1.27163
C -5.87459 0.92480 1.28175
C -6.33578 0.38072 -0.05243
C -5.62038 -0.89011 -0.53046
O -6.00637 -2.06741 0.13063
C -5.88781 -0.82254 -2.05521
O -7.22000 -1.17485 -2.35780
C -5.74749 0.68710 -2.30813
O -6.11509 1.34368 -1.09680
N -4.38829 1.13185 -2.68257
C -3.14533 0.54527 -2.57421
C -2.22676 1.57621 -2.80580
N -2.86759 2.77014 -3.05996
C -4.13759 2.46042 -2.97648
N -2.81606 -0.74426 -2.32651
C -1.50743 -0.92156 -2.26385
N -0.51823 -0.01908 -2.40955
C -0.84548 1.28188 -2.68188
N 0.10142 2.21738 -2.79438
O 7.27291 -1.80509 -3.89576
P 6.44944 -1.58544 -2.54728
O 7.36224 -0.94867 -1.48448
O 5.66075 -2.81780 -2.11676
O 5.40239 -0.40953 -3.01629
C 4.00706 -0.65330 -3.15740
C 3.31452 -0.66582 -1.78760
O 2.15791 0.24418 -1.81748
C 2.77049 -1.99770 -1.23840
O 3.49389 -2.35703 -0.05785

C 1.27966 -1.71051 -0.89132
O 0.94724 -2.19869 0.37823
C 1.18864 -0.20135 -1.06576
O 2.29214 0.10460 0.80065
P 2.07518 1.48965 1.51843
O 2.76375 2.64002 0.81408
O 0.60907 1.71767 1.91831
O 2.91684 1.22251 2.94915
P 2.20029 0.32621 4.10416
O 1.74716 -1.01147 3.45322
O 1.08376 1.09380 4.76154
O 3.42471 0.04055 5.09913
Mg -0.60094 1.48014 3.58624
H 5.58671 3.58535 -3.83513
H 6.21390 1.92252 -3.72975
H 4.47562 2.98514 -1.90087
H 7.77027 1.58631 -0.02915
H 7.54801 1.13760 -1.61283
H 4.51149 2.62468 0.48023
H 5.83329 1.68639 1.04469
H -4.06251 5.10147 -1.49167
H -3.41495 6.71488 -1.82642
H -1.33463 5.95939 -1.41076
H -0.18186 3.45348 0.79949
H 0.19691 4.53093 -0.54636
H -3.65131 4.02225 0.50991
H -2.45353 3.11862 1.33662
H -7.06208 -6.80484 -3.46345
H -8.39967 -5.76785 -4.03790
H -2.52617 -4.43579 -3.04769
H -1.77361 -4.39463 -1.41892
H -3.89967 -3.74900 -0.47087
H -4.66992 -3.92597 -2.01897
H -3.53724 -2.67279 -1.73256
H 1.98402 6.00767 -4.41430
H 2.75721 6.77321 -3.02447
H 9.33582 -2.12736 -2.07583
H 6.94913 -0.80635 0.04440
H -8.94624 0.90302 -3.97365
H -7.95221 -0.24595 -3.80839
H 5.74268 -4.66908 3.28285
H 5.58386 -4.11315 1.80584
H -8.51477 -3.70945 0.60477
H -8.45474 -3.34114 -0.89799
H 7.01632 -4.35176 -2.24246
H 7.64734 -4.55295 -0.88440
H 5.92076 -3.35471 -0.46519
H 6.65067 -2.69274 0.70789
H 2.62730 2.96694 -0.94149
H 2.26433 3.95045 -2.10559
H -4.00400 3.53285 5.90475
H -3.93438 2.50317 4.69841
H -2.41406 1.64135 5.61391
H -2.11341 0.12608 5.34014
H -4.87063 -3.19657 1.17605
H -3.49250 -3.64223 1.79738
H -0.60761 -3.94982 2.96931
H 0.25051 -4.21373 4.22297
H 3.31061 -4.12099 2.58362
H 1.68548 -4.03231 2.53782
H -6.15336 0.21307 2.06383
H -6.36045 1.88199 1.49596
H -7.41360 0.17574 0.02755
H -4.54735 -0.77293 -0.35116
H -6.97884 -2.26360 0.02485
H -5.17942 -1.40875 -2.64602
H -7.29129 -2.17759 -2.41738
H -6.41903 1.01183 -3.10737
H -4.95904 3.15014 -3.11847
H -1.18401 -1.93612 -2.05303

H -0.14556 3.20558 -2.81765
H 3.61156 0.18653 -3.73358
H 3.82612 -1.58025 -3.71019
H 3.98273 -0.22772 -1.04615
H 2.87721 -2.80071 -1.96839
H 3.37356 -3.31239 0.09711
H 0.65551 -2.17394 -1.65926
H -0.01259 -1.88360 0.59983
H 0.53107 0.47334 -0.54938
H 7.17698 3.28503 -3.09219
H -3.92145 6.30481 -0.17512
H -8.38671 -6.31517 -2.36500
H -3.02944 -5.60130 -1.80539
Mg 2.55877 -1.66385 1.74486
O 4.52552 -1.48208 2.64596
H 4.85387 -2.39274 2.85639
H 5.22974 -1.08945 2.07902
H 1.08955 2.04419 -2.61608
H 4.09039 -0.47552 4.59950
O -0.81549 3.44693 4.27630
H -0.22553 3.60397 5.03125
H -1.73720 3.57762 4.60391
H 0.05128 -1.04404 3.42444
H 7.65401 -0.74396 1.46596
H 9.03147 -3.59943 -2.43362
H 8.18054 -2.18757 -3.67491
H 1.53127 7.67612 -3.95689

218COCNfixed.log

Fixed bonds at
C-N = 2.18
C-O = 2.18

B3LYP/6-31G* Lanl2DZ Mg

Free Energy = -6563.284078
Zero-point Energy = -6563.127692
Potential Energy = -6564.43315859
Nimag = 1 (-314.5498 cm-1)

Charge = 0 Multiplicity = 1
C 6.16481 2.89172 -3.22129
N 5.49938 2.77765 -1.92809
C 6.10020 2.32089 -0.84159
N 7.39449 1.87714 -0.92324
N 5.50542 2.35943 0.36296
C -3.44630 5.91450 -1.08506
N -2.08166 5.49236 -0.84456
C -1.74582 4.54431 0.03042
N -0.45556 4.21739 0.18597
N -2.68745 3.95771 0.80027
C -7.74214 -5.99506 -3.19131
C -6.97425 -4.73641 -2.79356
O -7.67965 -3.75059 -2.40155
O -5.72079 -4.75290 -2.89524
C -2.69427 -4.57796 -1.97844
N -3.76019 -3.65636 -1.51643
C 1.81290 6.69264 -3.57601
C 0.72830 6.13265 -2.65981
O -0.27512 6.83152 -2.40980
O 0.92244 4.94850 -2.19174
O 9.46596 -2.77915 -2.78724
O 6.77718 -0.78170 1.05183
O -8.18316 0.49438 -4.40955
O 5.16861 -4.13024 2.71799
O -8.56064 -2.94853 0.00494
O 7.81168 -4.74380 -1.82742
O 6.35911 -3.57819 0.40417
O 2.78351 3.12024 -1.90313

O -3.39168 3.10907 5.28560
O -1.69958 1.00173 5.39239
O -4.20294 -3.91341 1.17455
O 0.23142 -4.38829 3.26959
O 2.54652 -3.70245 2.13557
O -2.29272 1.65813 2.46335
P -3.60337 0.89183 2.62805
O -4.44243 1.14969 3.85100
O -3.25671 -0.72148 2.57882
P -1.85723 -1.50768 2.29870
O -1.36022 -1.27115 0.88290
O -0.88921 -0.70392 3.37285
O -2.03977 -2.93681 2.75516
O -4.44285 1.14128 1.27163
C -5.87459 0.92480 1.28175
C -6.33578 0.38072 -0.05243
C -5.62038 -0.89011 -0.53046
O -6.00637 -2.06741 0.13063
C -5.88781 -0.82254 -2.05521
O -7.22000 -1.17485 -2.35780
C -5.74749 0.68710 -2.30813
O -6.11509 1.34368 -1.09680
N -4.38829 1.13185 -2.68257
C -3.14533 0.54527 -2.57421
C -2.22676 1.57621 -2.80580
N -2.86759 2.77014 -3.05996
C -4.13759 2.46042 -2.97648
N -2.81606 -0.74426 -2.32651
C -1.50743 -0.92156 -2.26385
N -0.51823 -0.01908 -2.40955
C -0.84548 1.28188 -2.68188
N 0.10142 2.21738 -2.79438
O 7.27291 -1.80509 -3.89576
P 6.44944 -1.58544 -2.54728
O 7.36224 -0.94867 -1.48448
O 5.66075 -2.81780 -2.11676
O 5.40239 -0.40953 -3.01629
C 4.00706 -0.65330 -3.15740
C 3.31452 -0.66582 -1.78760
O 2.15791 0.24418 -1.81748
C 2.77049 -1.99770 -1.23840
O 3.49389 -2.35703 -0.05785
C 1.27966 -1.71051 -0.89132
O 0.94724 -2.19869 0.37823
C 1.18864 -0.20135 -1.06576
O 2.29214 0.10460 0.80065
P 2.07518 1.48965 1.51843
O 2.76375 2.64002 0.81408
O 0.60907 1.71767 1.91831
O 2.91684 1.22251 2.94915
P 2.20029 0.32621 4.10416
O 1.74716 -1.01147 3.45322
O 1.08376 1.09380 4.76154
O 3.42471 0.04055 5.09913
Mg -0.60094 1.48014 3.58624
H 5.58671 3.58535 -3.83513
H 6.21390 1.92252 -3.72975
H 4.47562 2.98514 -1.90087
H 7.77027 1.58631 -0.02915
H 7.54801 1.13760 -1.61283
H 4.51149 2.62468 0.48023
H 5.83329 1.68639 1.04469
H -4.06251 5.10147 -1.49167
H -3.41495 6.71488 -1.82642
H -1.33463 5.95939 -1.41076
H -0.18186 3.45348 0.79949
H 0.19691 4.53093 -0.54636
H -3.65131 4.02225 0.50991
H -2.45353 3.11862 1.33662
H -7.06208 -6.80484 -3.46345

H -8.39967 -5.76785 -4.03790
H -2.52617 -4.43579 -3.04769
H -1.77361 -4.39463 -1.41892
H -3.89967 -3.74900 -0.47087
H -4.66992 -3.92597 -2.01897
H -3.53724 -2.67279 -1.73256
H 1.98402 6.00767 -4.41430
H 2.75721 6.77321 -3.02447
H 9.33582 -2.12736 -2.07583
H 6.94913 -0.80635 0.04440
H -8.94624 0.90302 -3.97365
H -7.95221 -0.24595 -3.80839
H 5.74268 -4.66908 3.28285
H 5.58386 -4.11315 1.80584
H -8.51477 -3.70945 0.60477
H -8.45474 -3.34114 -0.89799
H 7.01632 -4.35176 -2.24246
H 7.64734 -4.55295 -0.88440
H 5.92076 -3.35471 -0.46519
H 6.65067 -2.69274 0.70789
H 2.62730 2.96694 -0.94149
H 2.26433 3.95045 -2.10559
H -4.00400 3.53285 5.90475
H -3.93438 2.50317 4.69841
H -2.41406 1.64135 5.61391
H -2.11341 0.12608 5.34014
H -4.87063 -3.19657 1.17605
H -3.49250 -3.64223 1.79738
H -0.60761 -3.94982 2.96931
H 0.25051 -4.21373 4.22297
H 3.31061 -4.12099 2.58362
H 1.68548 -4.03231 2.53782
H -6.15336 0.21307 2.06383
H -6.36045 1.88199 1.49596
H -7.41360 0.17574 0.02755
H -4.54735 -0.77293 -0.35116
H -6.97884 -2.26360 0.02485
H -5.17942 -1.40875 -2.64602
H -7.29129 -2.17759 -2.41738
H -6.41903 1.01183 -3.10737
H -4.95904 3.15014 -3.11847
H -1.18401 -1.93612 -2.05303
H -0.14556 3.20558 -2.81765
H 3.61156 0.18653 -3.73358
H 3.82612 -1.58025 -3.71019
H 3.98273 -0.22772 -1.04615
H 2.87721 -2.80071 -1.96839
H 3.37356 -3.31239 0.09711
H 0.65551 -2.17394 -1.65926
H -0.01259 -1.88360 0.59983
H 0.53107 0.47334 -0.54938
H 7.17698 3.28503 -3.09219
H -3.92145 6.30481 -0.17512
H -8.38671 -6.31517 -2.36500
H -3.02944 -5.60130 -1.80539
Mg 2.55877 -1.66385 1.74486
O 4.52552 -1.48208 2.64596
H 4.85387 -2.39274 2.85639
H 5.22974 -1.08945 2.07902
H 1.08955 2.04419 -2.61608
H 4.09039 -0.47552 4.59950
O -0.81549 3.44693 4.27630
H -0.22553 3.60397 5.03125
H -1.73720 3.57762 4.60391
H 0.05128 -1.04404 3.42444
H 7.65401 -0.74396 1.46596
H 9.03147 -3.59943 -2.43362
H 8.18054 -2.18757 -3.67491
H 1.53127 7.67612 -3.95689

twofixCO24.log

fixed bonds at

C-N = 2.00

C-O = 2.40

B3LYP/6-31G* Lanl2DZ Mg

Zero-point correction= 1.305798 (Hartree/Particle)

Thermal correction to Energy= 1.418694

Thermal correction to Enthalpy= 1.419638

Thermal correction to Gibbs Free Energy=1.150443

Sum of electronic and zero-point Energies=-6563.133223

Sum of electronic and thermal Energies= -6563.020328

Sum of electronic and thermal Enthalpies= -6563.019383

Sum of electronic and thermal Free Energies= -6563.288578

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	890.244	410.368	566.569

C,0,6.1442185595,2.9043828187,-3.1743615118

N,0,5.4954688199,2.7886345749,-1.8729297386

C,0,6.1113921351,2.3344467173,-0.7925908652

N,0,7.4036361167,1.8887395254,-0.8934973178

N,0,5.5344414251,2.3802895754,0.419283942

C,0,-3.4683565739,5.8480008608,-1.0477911975

N,0,-2.0979554097,5.429580428,-0.8342057808

C,0,-1.7396129897,4.5062491298,0.0591880495

N,0,-0.4466871358,4.1835627235,0.1944918962

N,0,-2.6640539611,3.9380925468,0.8623537807

C,0,-7.8580367574,-5.9386967007,-3.0973283452

C,0,-7.0688743041,-4.6883848509,-2.7159380688

O,0,-7.758178602,-3.6820934859,-2.3474312781

O,0,-5.8151380182,-4.7307642433,-2.8074055707

C,0,-2.7834573325,-4.6260874354,-1.9179023552

N,0,-3.8235825471,-3.6812983372,-1.4436449267

C,0,1.7667698589,6.6580986692,-3.5936986983

C,0,0.6804933255,6.0857289798,-2.6873428441

O,0,-0.3344805402,6.7699783805,-2.4476216773

O,0,0.8878275907,4.9048475189,-2.213736835

O,0,9.4842225935,-2.7145327589,-2.8263760752

O,0,6.8350157289,-0.7877841045,1.0453372581

O,0,-8.1113008343,0.5315870523,-4.4370903811

O,0,5.2225501368,-4.1298179192,2.6838279422

O,0,-8.5980511152,-2.8217485758,0.0553588379

O,0,7.8599988413,-4.7093565939,-1.8699323636

O,0,6.4003644558,-3.5725929162,0.3650268528

O,0,2.7701176711,3.1118970652,-1.8022251267

O,0,-3.354719044,3.074780717,5.3287595844

O,0,-1.6614035581,0.96494705,5.4119279251

O,0,-4.2353710468,-3.8868352187,1.2510084707

O,0,0.3006193954,-4.3543918217,3.2695522098

O,0,2.6071522794,-3.6710703705,2.1019509661

O,0,-2.2473218632,1.6412562112,2.5013479066

P,0,-3.5605200269,0.8774817493,2.6549969553

O,0,-4.4155507976,1.1394009944,3.8654901596

O,0,-3.2153405322,-0.735149284,2.6114133921

P,0,-1.8179598245,-1.5238560712,2.3181277934

O,0,-1.332720876,-1.2811894718,0.8987936666

O,0,-0.8392538315,-0.7311374769,3.3859115159

O,0,-2.0096987655,-2.9550948904,2.7646718898

O,0,-4.3857076098,1.1289129056,1.2875926631

C,0,-5.8223713919,0.9566282206,1.289532262

C,0,-6.2918537953,0.4247926525,-0.0466828379

C,0,-5.6088370979,-0.8646939626,-0.5199470347

O,0,-6.014213914,-2.0310748194,0.1482090178
C,0,-5.8793449107,-0.79850772,-2.0448009079
O,0,-7.2180891792,-1.1243506645,-2.345064911
C,0,-5.7106431252,0.7079089931,-2.3067994848
O,0,-6.0345799841,1.3790445865,-1.0921522818
N,0,-4.3494591641,1.1217364206,-2.7150266592
C,0,-3.1149331375,0.5345582764,-2.5555906043
C,0,-2.1837505329,1.5459098948,-2.8161102151
N,0,-2.8082805853,2.7292442101,-3.1407748557
C,0,-4.0827052827,2.4338980067,-3.0668465576
N,0,-2.8060309065,-0.7450514332,-2.2302411232
C,0,-1.5106319177,-0.9344453665,-2.1050896362
N,0,-0.5157182159,-0.036534644,-2.2865171655
C,0,-0.8069438277,1.2628713433,-2.6235370079
N,0,0.1444919328,2.1855967809,-2.7295077356
O,0,7.274349218,-1.7521138893,-3.9204335284
P,0,6.4606113648,-1.5572251162,-2.5605431672
O,0,7.3813222098,-0.9295697547,-1.4986300086
O,0,5.6874357512,-2.8037567838,-2.1453844415
O,0,5.4047080467,-0.378583333,-2.9976626586
C,0,4.0130426896,-0.6254354585,-3.1709962506
C,0,3.2879992525,-0.6400840142,-1.8180524356
O,0,2.099436964,0.2118529516,-1.9002716571
C,0,2.7868400377,-1.9877745488,-1.2672957065
O,0,3.5228282946,-2.3284172289,-0.0911801489
C,0,1.283497334,-1.7525059659,-0.9229936565
O,0,0.990325639,-2.1806850483,0.3798485126
C,0,1.1087674557,-0.2550466472,-1.1564261348
O,0,2.401444468,0.1625400962,0.822110562
P,0,2.1427093201,1.5104905651,1.5659349154
O,0,2.8116728553,2.7055588082,0.910791457
O,0,0.6643303818,1.7068993268,1.9558215096
O,0,2.9624371009,1.2455431306,3.0198759603
P,0,2.2416035872,0.3118175671,4.134107994
O,0,1.7954110747,-1.0100872878,3.4435039256
O,0,1.1134052175,1.0508571006,4.8068626146
O,0,3.4535936749,-0.0036159849,5.1374977848
Mg,0,-0.5475558134,1.4585477161,3.6148559983
H,0,5.5563641749,3.5962424062,-3.7811486163
H,0,6.1911962236,1.9353099082,-3.6833217527
H,0,4.47127136,2.9851756155,-1.8330628531
H,0,7.7923312476,1.597938572,-0.00495365
H,0,7.5461844315,1.1492370979,-1.5862566711
H,0,4.5407072834,2.6478517194,0.5508464271
H,0,5.8708311957,1.7096731132,1.0990335158
H,0,-4.0982580563,5.0254106956,-1.4132380909
H,0,-3.4565819627,6.6268992669,-1.8121785228
H,0,-1.3659838235,5.8926104843,-1.4224177776
H,0,-0.153802644,3.439485922,0.8243498551
H,0,0.1937304605,4.496315507,-0.5477232083
H,0,-3.6336279615,3.9964277052,0.5901743426
H,0,-2.419025675,3.1067242593,1.4066608967
H,0,-7.1918629531,-6.7652855332,-3.3525111669
H,0,-8.5074041895,-5.7132349975,-3.9506224141
H,0,-2.623887827,-4.4875953335,-2.9888978407
H,0,-1.8525495678,-4.4649937153,-1.3686090598
H,0,-3.9536324,-3.7656161398,-0.3949683893
H,0,-4.7453881678,-3.9293215445,-1.9362516635
H,0,-3.5824154265,-2.7041973927,-1.6621285541
H,0,1.9683074002,5.9660454065,-4.4191888336
H,0,2.6991954409,6.767773026,-3.0270057548
H,0,9.3364041616,-2.0669238701,-2.1143270566
H,0,6.9871704576,-0.7996812149,0.035296345
H,0,-8.894834079,0.9442376929,-4.04326167
H,0,-7.9118406804,-0.2060674146,-3.8213721789
H,0,5.7956710531,-4.6771697321,3.2412723841
H,0,5.6315764735,-4.1105838029,1.7689697852
H,0,-8.5852317226,-3.5748096792,0.6666309411
H,0,-8.5100599152,-3.2310115279,-0.8420210204
H,0,7.0627612776,-4.3320986252,-2.294313262

H,0,7.6835188788,-4.5131908436,-0.9298155951
H,0,5.9555934968,-3.3435780511,-0.5002339161
H,0,6.6928257163,-2.6892510386,0.6745479955
H,0,2.6415652975,2.998811733,-0.8286985554
H,0,2.2544368331,3.9341004503,-2.0346069843
H,0,-3.9619584434,3.4840062224,5.962517931
H,0,-3.9017037831,2.4822546231,4.7332543779
H,0,-2.3861551233,1.592632166,5.6325747915
H,0,-2.0562057072,0.0806200927,5.3619651036
H,0,-4.8843397194,-3.1538823961,1.2528674929
H,0,-3.5052566201,-3.6243996188,1.8557091442
H,0,-0.5528655219,-3.943389556,2.9726691775
H,0,0.3390847422,-4.1389847525,4.2140327088
H,0,3.3682774785,-4.0945760959,2.5504195079
H,0,1.7467838555,-3.9960093888,2.5064868411
H,0,-6.1277354973,0.2546031442,2.0704242406
H,0,-6.2821564159,1.9276769279,1.4996018776
H,0,-7.3757354908,0.2517456602,0.0260431539
H,0,-4.5333253937,-0.7673746736,-0.3450428669
H,0,-6.9938110091,-2.1991627687,0.0604265279
H,0,-5.1833007146,-1.4012999415,-2.6349467085
H,0,-7.3171093001,-2.1265861012,-2.3833779694
H,0,-6.3879887089,1.0421035535,-3.0974494256
H,0,-4.8950865148,3.1225600002,-3.2578467262
H,0,-1.1957023778,-1.9258824469,-1.805715524
H,0,-0.0983609301,3.1752782401,-2.7989455453
H,0,3.6289259364,0.2152726831,-3.7537155909
H,0,3.8470776032,-1.5507974419,-3.731367129
H,0,3.9227604961,-0.1699404838,-1.0663187429
H,0,2.9174626963,-2.7860328641,-1.9990409858
H,0,3.404318453,-3.2813510261,0.0807513469
H,0,0.679885953,-2.2989242022,-1.6546413669
H,0,0.0355814765,-1.8724299613,0.6128627424
H,0,0.6257396429,0.391168789,-0.4418428099
H,0,7.1564158951,3.3016587496,-3.0575784686
H,0,-3.9178274898,6.2647174352,-0.1365328251
H,0,-8.512318298,-6.2331997342,-2.2690738097
H,0,-3.1400823191,-5.6414926095,-1.7416008445
Mg,0,2.6237485971,-1.6178781067,1.7217401642
O,0,4.5842476926,-1.4761938353,2.6334263698
H,0,4.9093965146,-2.3892815459,2.8352611095
H,0,5.2913214062,-1.0794299532,2.0731821799
H,0,1.1263821099,2.0244088679,-2.4966252543
H,0,4.1297655441,-0.4968593993,4.6297340035
O,0,-0.7691197987,3.4185397843,4.3266083204
H,0,-0.175328972,3.5598277386,5.0818229296
H,0,-1.6888214284,3.5430829293,4.6610141283
H,0,0.1098090604,-1.0564660755,3.4163287267
H,0,7.7198200831,-0.7616164274,1.4429429787
H,0,9.0634165361,-3.5434555108,-2.4763494019
H,0,8.1852397719,-2.1318026877,-3.7104288428
H,0,1.4697357353,7.6301221504,-3.9918801095

Pocketrafcutcut2*6*.log

Fixed bonds at

C-N = 1.73

C-O = 2.60

B3LYP/6-31G* Lanl2DZ Mg

Zero-point correction=1.306299 (Hartree/Particle)

Thermal correction to Energy= 1.419023

Thermal correction to Enthalpy= 1.419968

Thermal correction to Gibbs Free Energy=1.150528

Sum of electronic and zero-point Energies=-6563.155811

Sum of electronic and thermal Energies= -6563.043087

Sum of electronic and thermal Enthalpies=-6563.042142

Sum of electronic and thermal Free Energies=-6563.311581

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	890.451	409.957	567.082

C	6.13	2.93358	-3.15529
N	5.48111	2.8025	-1.85538
C	6.09652	2.33429	-0.78075
N	7.38825	1.88838	-0.88717
N	5.51962	2.36581	0.43161
C	-3.4792	5.86172	-0.99237
N	-2.10928	5.43912	-0.78399
C	-1.75199	4.5044	0.09792
N	-0.45944	4.17859	0.2292
N	-2.67709	3.92743	0.89401
C	-7.88239	-5.89371	-3.18737
C	-7.0918	-4.64911	-2.79057
O	-7.77995	-3.64666	-2.40965
O	-5.83811	-4.69179	-2.88257
C	-2.80631	-4.6016	-1.99188
N	-3.84535	-3.66155	-1.50597
C	1.75686	6.69721	-3.52814
C	0.66993	6.11493	-2.62892
O	-0.34426	6.79733	-2.38074
O	0.8759	4.92805	-2.16994
O	9.46355	-2.69303	-2.87682
O	6.81655	-0.81125	1.01844
O	-8.12823	0.59293	-4.44706
O	5.20025	-4.17142	2.61553
O	-8.61884	-2.81511	0.00361
O	7.83704	-4.69766	-1.94509
O	6.37871	-3.58693	0.30377
O	2.75614	3.12799	-1.78065
O	-3.36875	3.00977	5.34941
O	-1.67785	0.89713	5.40648
O	-4.25738	-3.8999	1.18594
O	0.27807	-4.39757	3.19849
O	2.58538	-3.70252	2.0394
O	-2.26299	1.61003	2.50449
P	-3.57707	0.84592	2.6487
O	-4.4318	1.09384	3.86235
O	-3.23374	-0.76644	2.58518
P	-1.83726	-1.55307	2.28215
O	-1.35174	-1.29343	0.86592
O	-0.85765	-0.77473	3.35964
O	-2.03064	-2.98949	2.71098
O	-4.40196	1.11518	1.28452
C	-5.83882	0.94453	1.28435
C	-6.30891	0.42979	-0.05833
C	-5.62738	-0.85453	-0.54751
O	-6.03409	-2.02861	0.10619
C	-5.89781	-0.76919	-2.07142
O	-7.23692	-1.08976	-2.37567
C	-5.72738	0.74016	-2.31479
O	-6.05054	1.3966	-1.09193
N	-4.36572	1.15743	-2.71788
C	-3.13187	0.56691	-2.56573
C	-2.19952	1.58034	-2.81375
N	-2.8227	2.76831	-3.12375
C	-4.09746	2.47354	-3.05346
N	-2.82443	-0.71697	-2.25623
C	-1.52925	-0.90938	-2.13345
N	-0.53331	-0.01044	-2.30377
C	-0.82304	1.29336	-2.6247
N	0.12945	2.21624	-2.71928
O	7.09314	-1.76358	-4.20681
P	6.27963	-1.58458	-2.84461

O	7.20106	-0.97116	-1.77503	H	-7.21717	-6.71784	-3.45276
O	5.50502	-2.83526	-2.44488	H	-8.5315	-5.65697	-4.03781
O	5.22508	-0.39942	-3.26711	H	-2.64658	-4.45006	-3.06109
C	3.83313	-0.64251	-3.44347	H	-1.87522	-4.44837	-1.44065
C	3.10807	-0.67305	-2.0908	H	-3.9755	-3.75867	-0.45841
O	1.92048	0.1812	-2.16246	H	-4.76744	-3.90241	-2.00159
C	2.60536	-2.02687	-1.55673	H	-3.60307	-2.6821	-1.71236
O	3.34096	-2.38287	-0.38493	H	1.9576	6.01518	-4.36213
C	1.10229	-1.79415	-1.20953	H	2.68941	6.79881	-2.96015
O	0.80863	-2.23806	0.08793	H	9.31648	-2.05411	-2.15682
C	0.92928	-0.29372	-1.42443	H	6.9687	-0.81083	0.00833
O	2.38408	0.14685	0.80704	H	-8.91129	1.00158	-4.04815
P	2.12689	1.4858	1.56747	H	-7.92962	-0.15251	-3.84051
O	2.79722	2.68811	0.92714	H	5.77275	-4.72628	3.16615
O	0.64873	1.67907	1.95977	H	5.6093	-4.14135	1.70097
O	2.94631	1.20196	3.01801	H	-8.60688	-3.57569	0.60552
P	2.2244	0.25536	4.12063	H	-8.53131	-3.21335	-0.89877
O	1.7767	-1.05739	3.41375	H	7.04024	-4.31427	-2.36476
O	1.09705	0.98733	4.80248	H	7.66078	-4.51293	-1.00261
O	3.43603	-0.07384	5.12003	H	5.9342	-3.34673	-0.55859
Mg	-0.56344	1.41162	3.61563	H	6.67218	-2.70782	0.62418
H	5.54294	3.63356	-3.75347	H	2.62745	3.00303	-0.80859
H	6.17586	1.97082	-3.67619	H	2.2414	3.9536	-2.00284
H	4.45714	2.99971	-1.81307	H	-3.97552	3.41183	5.98819
H	7.77661	1.58618	-0.00229	H	-3.91641	2.42528	4.74664
H	7.52995	1.15734	-1.58902	H	-2.40188	1.52287	5.63487
H	4.52619	2.63287	0.56648	H	-2.07367	0.01394	5.34559
H	5.85524	1.68646	1.10302	H	-4.90551	-3.16628	1.19687
H	-4.11004	5.04443	-1.36795	H	-3.52697	-3.6458	1.79383
H	-3.46653	6.64999	-1.74708	H	-0.57495	-3.98195	2.90672
H	-1.37677	5.90854	-1.36645	H	0.31678	-4.1939	4.14556
H	-0.16741	3.42645	0.84981	H	3.34602	-4.13241	2.48259
H	0.18134	4.49975	-0.5091	H	1.72464	-4.03145	2.4399
H	-3.64659	3.99023	0.62259	H	-6.14499	0.23326	2.05651
H	-2.43301	3.08911	1.428	H	-6.29749	1.91344	1.50641

H	-7.39299 0.2571 0.01226	
H	-4.55175 -0.76061 -0.37143	**nofixNCbound.log**
H	-7.01388 -2.19448 0.01635	
H	-5.20246 -1.36544 -2.66898	no fixed bonds
H	-7.33709 -2.09133 -2.42637	C-N = 1.47
H	-6.40434 1.08487 -3.10123	C-O = 3.10
H	-4.90905 3.16544 -3.23593	
H	-1.21546 -1.90481 -1.84635	B3LYP/6-31G* Lanl2DZ Mg
H	-0.11227 3.20698 -2.77647	Free Energy = -6563.344432
H	3.44998 0.20577 -4.01574	Zero-point Energy = -6563.193803
H	3.6661 -1.56069 -4.01523	Potential Energy = -6564.50414103
H	3.74337 -0.21296 -1.33332	Nimag = 1 (16.7727 cm-1)
H	2.73507 -2.81617 -2.29829	
H	3.22135 -3.33772 -0.22478	Charge = 0 Multiplicity = 1
H	0.49805 -2.33079 -1.94787	C 5.92561 2.78147 -3.03668
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H	1.46094 7.67442 -3.91428	O 9.62376 -2.04393 -1.73232

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NofixOCbound.log

No fixed bonds
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C-O = 1.45

B3LYP/6-31G* Lanl2DZ Mg

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Zero-point Energy = -6563.189679
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