Supporting information for:

Uridine phosphorylase from *Trypanosoma cruzi*: kinetic and chemical mechanisms[†]

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Stationary-point transition structure coordinates with arsenate as nucleophile

opt=(calcfc,ts,noeigentest,nofreeze) freq rb3lyp/6-31g(d,p)

Sum of electronic and thermal Free Energies= -3446.129576

Thermal correction to Gibbs Free Energy= 0.193701

Sum of electronic and zero-point Energies= -3446.076398

C	0.02359000	0.86308800	1.33446000
C	0.41933900	-0.15775100	0.26711400
O	0.08277300	0.18777600	-0.95500800
C	-0.42018900	1.57807800	-1.01133100
C	-0.59345700	2.04964500	0.45783300
C	0.54185400	2.38367600	-1.86430400
O	1.81479900	2.61285200	-1.27055600
O	-1.90107400	2.39166000	0.76029600
O	-0.81562100	0.30842600	2.28458000
N	2.41991200	-0.16044700	0.09050000
C	2.78501300	-0.82229900	-1.04002700
C	4.01772700	-1.35346700	-1.30202800
C	5.05553500	-1.24940300	-0.30617300
N	4.61291200	-0.58344800	0.84492000
C	3.34659800	-0.03124600	1.11017900
O	3.15084400	0.53106200	2.18380200
O	6.21555000	-1.66903700	-0.37708800
O	-3.27228200	0.74540500	-0.57915600
As	-3.24117700	-0.92831000	-0.21470900
O	-4.66547900	-0.95806000	0.94068100
O	-3.55622300	-1.97344100	-1.45934200
O	-1.90477700	-1.33685300	0.76743600
H	0.09405100	3.36986000	-2.03965900
H	0.64956500	1.89229700	-2.84730900
H	2.09871100	1.77812500	-0.86091400
H	-1.40819700	1.47894600	-1.47342800
H	0.37297500	-1.22021600	0.46610300
H	0.93163800	1.21759200	1.82972800
H	-1.44644900	-0.32931700	1.75598400
H	0.04080700	2.93289300	0.61781200
H	-2.51609600	1.67386600	0.33100600
H	4.23578600	-1.85718800	-2.23485600
H	1.98502100	-0.89759800	-1.77394800
H	-4.84100200	-0.00516900	0.93756600
H	5.28811600	-0.47285800	1.58988400

Stationary-point transition structure coordinates with phosphate as nucleophile

opt=(calcfc,ts,noeigentest,nofreeze) freq rb3lyp/6-31g(d,p)

Sum of electronic and thermal Free Energies= -1553.799969

Thermal correction to Gibbs Free Energy= 0.196954

Sum of electronic and zero-point Energies= -1553.747563

C	-0.37782100	0.64923800	1.34252200
C	0.08254700	-0.25425900	0.20050000
O	-0.24363000	0.17980100	-0.99375700
C	-0.80632900	1.54636000	-0.94051400
C	-1.04508000	1.87315200	0.55825900
C	0.14436800	2.46511800	-1.68664200
O	1.38812600	2.68885800	-1.03358600
O	-2.37792000	2.10470100	0.84682900
O	-1.19737300	-0.02934200	2.22401000
N	2.09386700	-0.16393800	0.07059000
C	2.50752500	-0.72229300	-1.09810800
C	3.76658900	-1.18080400	-1.37258200
C	4.78050600	-1.10944500	-0.34957900
N	4.28897400	-0.55079400	0.83815900
C	2.99546900	-0.07279700	1.11630000
O	2.75637600	0.40011500	2.22369100
O	5.95863800	-1.47414000	-0.42670400
O	-3.59458400	0.39511100	-0.54792800
O	-4.87033600	-1.40364200	0.65937300
O	-3.67557100	-2.00910900	-1.57353400
O	-2.28585100	-1.53110900	0.56501100
H	-0.33967400	3.44470400	-1.78694800
H	0.30041200	2.07016100	-2.70605300
H	1.70043100	1.83050300	-0.69986600
H	-1.77268900	1.45237500	-1.44440900
H	0.08125600	-1.33137800	0.30755100
H	0.50481900	1.00701700	1.88041300
H	-1.80517800	-0.63741300	1.62944000
H	-0.47178100	2.77528400	0.81530900
H	-2.92916400	1.36108900	0.37034700
H	4.02321000	-1.60327700	-2.33544600
H	1.72519700	-0.77484400	-1.85290200
H	-5.16650700	-0.48966600	0.76448300
H	4.94515800	-0.46861600	1.60353500
P	-3.50833400	-1.15789300	-0.33832500