

Transition States of *Plasmodium falciparum* and Human Orotate  
Phosphoribosyltransferases<sup>†</sup>

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## Supporting Information

**Reference 48.** M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2002.

## Optimized Geometries

### OMP as the substrate

C	-1.00350200	-0.82877200	0.15713000
C	-0.64429500	-1.62793200	-1.10698400
C	0.70023200	-2.25026300	-0.67841600
C	1.30454000	-1.20319900	0.28452300
C	2.45679200	-0.38528700	-0.29505100

H	-2.41699500	-2.42631500	-0.88657300
H	2.04947200	0.39872500	-0.94898600
H	-1.50428500	-1.49511900	0.86216600
H	-0.49450100	-0.94015400	-1.94515300
H	1.36358700	-2.43484400	-1.53616800
H	1.67423800	-1.72750400	1.17296700
H	3.09817300	-1.04786200	-0.89225000
O	-1.59484200	-2.62830300	-1.41917900
O	0.43341000	-3.46591800	0.00928500
O	0.20328800	-0.34244900	0.69320100
P	4.79669800	0.63892800	0.40909300
O	5.41964200	1.00840600	1.71688900
H	-0.43255900	-3.73210200	-0.35890600
N	-1.94776100	0.28899200	-0.06864700
C	-1.48493000	1.40023100	-0.78608700
O	-0.46640900	1.42103600	-1.45970600
N	-2.29926000	2.52153800	-0.68621600
C	-3.23374400	0.26391400	0.46692200
C	-3.56219800	2.63073300	-0.08399300
C	-3.90816000	-1.07812000	0.90332200
H	-1.95040400	3.33659500	-1.17259100
O	-4.16926000	3.70231700	-0.11821000
O	-4.73608000	-0.98137800	1.81936500
O	3.22372100	0.17928200	0.75707400
C	-4.00794200	1.38428400	0.48726600
H	-4.99422600	1.32042400	0.92319600
O	5.38691500	-0.34421800	-0.57604800
O	4.51607900	2.03566900	-0.48512100
O	-3.60025700	-2.09755800	0.21475800
H	4.75574400	1.76191700	-1.38028900

End

### Orotate dianion at the transition state

N	0.10991300	1.23642000	-0.08464500
C	-1.24771600	1.27542300	-0.08715800
O	-1.94811700	2.30977600	-0.17562300
N	-1.93756600	0.04452800	0.02647300
C	0.71596000	0.02627500	-0.02170400
C	-1.37774400	-1.24010800	0.08940000
C	2.28360100	-0.01055500	-0.00132000
H	-2.94720200	0.09857500	0.03338000
O	-2.14141000	-2.23492200	0.17095700
O	2.86424100	0.94518300	0.57053400
O	2.80274400	-1.02851400	-0.54422500
C	0.04387000	-1.19761400	0.04626500
H	0.61327600	-2.11792300	0.04778300

End

### 5'-phosphate ribooxacarbenium with PA at the *Pf*OPRT transition state

O	0.84678000	0.88778900	1.44191100
C	-0.09965000	1.66279600	1.07176200
C	-0.01476900	1.99005900	-0.40751000

C	0.75310800	0.74346700	-0.93997300
C	1.66167900	0.40395700	0.24019500
C	3.01361800	1.15314400	0.28980000
O	4.04011700	0.38874100	0.85314700
H	0.71936300	2.81821200	-0.41632000
O	-1.13670500	2.44558700	-1.06664900
O	-0.09665800	-0.35514000	-1.22101100
H	1.82512900	-0.66689700	0.36745200
H	3.27411100	1.48930800	-0.72552000
H	2.88674500	2.05465000	0.90627000
H	1.34687100	0.99919800	-1.82432200
H	-0.94664900	-0.03676400	-1.59040600
H	-1.84311100	1.74086700	-1.05195600
H	-0.56088600	2.28387100	1.82771100
P	-2.67386300	-0.22190900	0.36770200
O	-1.97434600	0.66636600	1.41109300
O	-2.75218300	0.35003700	-1.04675400
O	-2.03720600	-1.71707400	0.35402200
H	-1.16192500	-1.66525600	-0.07731200
C	-5.35403100	-0.89002600	-0.04420400
O	-5.59408800	-1.98021400	-0.51420800
P	4.65527400	-0.78799600	-0.22369300
O	5.79570600	-1.39971100	0.80077700
H	6.61687100	-0.94774700	0.56440200
O	5.33831700	-0.05134500	-1.34127000
O	3.55556200	-1.78929500	-0.42750500
O	-5.99082100	0.23450600	-0.46075200
H	-6.54709500	-0.04626200	-1.20619700
C	-4.35378800	-0.58930500	1.03924600
H	-4.26427600	-1.45233600	1.70059600
H	-4.65910600	0.29118300	1.60714800

2 19 2.1500 F  
1 5 6 12 -136.8 F

End

### 5'-phosphate ribooxacarbenium with PA at the *Hs*OPRT transition state

O	0.84348600	0.88562400	1.44242700
C	-0.10357600	1.66164500	1.07377800
C	-0.01540400	1.99448000	-0.40434800
C	0.75351900	0.75023100	-0.94017600
C	1.65901900	0.40501300	0.24066600
C	3.01222000	1.15167200	0.29487200
O	4.03666200	0.38348800	0.85694100
H	0.71836100	2.82285700	-0.40872400
O	-1.13610300	2.45205100	-1.06460400
O	-0.09624100	-0.34687400	-1.22860900
H	1.82082700	-0.66659000	0.36384000
H	3.27495900	1.49115200	-0.71875900
H	2.88581000	2.05101100	0.91457300
H	1.34937500	1.00944800	-1.82206000
H	-0.94443700	-0.02606500	-1.59947000
H	-1.84318400	1.74831900	-1.05168500

H	-0.56059700	2.28462600	1.83076800
P	-2.67072300	-0.21927000	0.36259100
O	-1.96947700	0.66806600	1.40666600
O	-2.75446900	0.35673200	-1.04954000
O	-2.03152200	-1.71294200	0.34403300
H	-1.15795700	-1.65844200	-0.09072100
C	-5.35001800	-0.89696800	-0.03893000
O	-5.58712000	-1.98920400	-0.50561800
P	4.65185800	-0.79006600	-0.22322300
O	5.79116800	-1.40589500	0.80011300
H	6.61266500	-0.95329900	0.56611600
O	5.33631700	-0.05011200	-1.33779500
O	3.55187200	-1.79016600	-0.43133300
O	-5.99292300	0.22396300	-0.45571000
H	-6.55090200	-0.06079200	-1.19837100
C	-4.34721600	-0.58965500	1.04039300
H	-4.25294900	-1.45025500	1.70425900
H	-4.65347100	0.29171500	1.60641500

2 19 2.1400 F  
1 5 6 12 -136.8 F

End