Supporting Information for:

Density Functional Studies on Diimine Chelated Palladium Complex Catalyzed Suzuki-Miyaura Cross-Coupling Reaction: The Impact of Lewis Base Employed in Transmetallation Process

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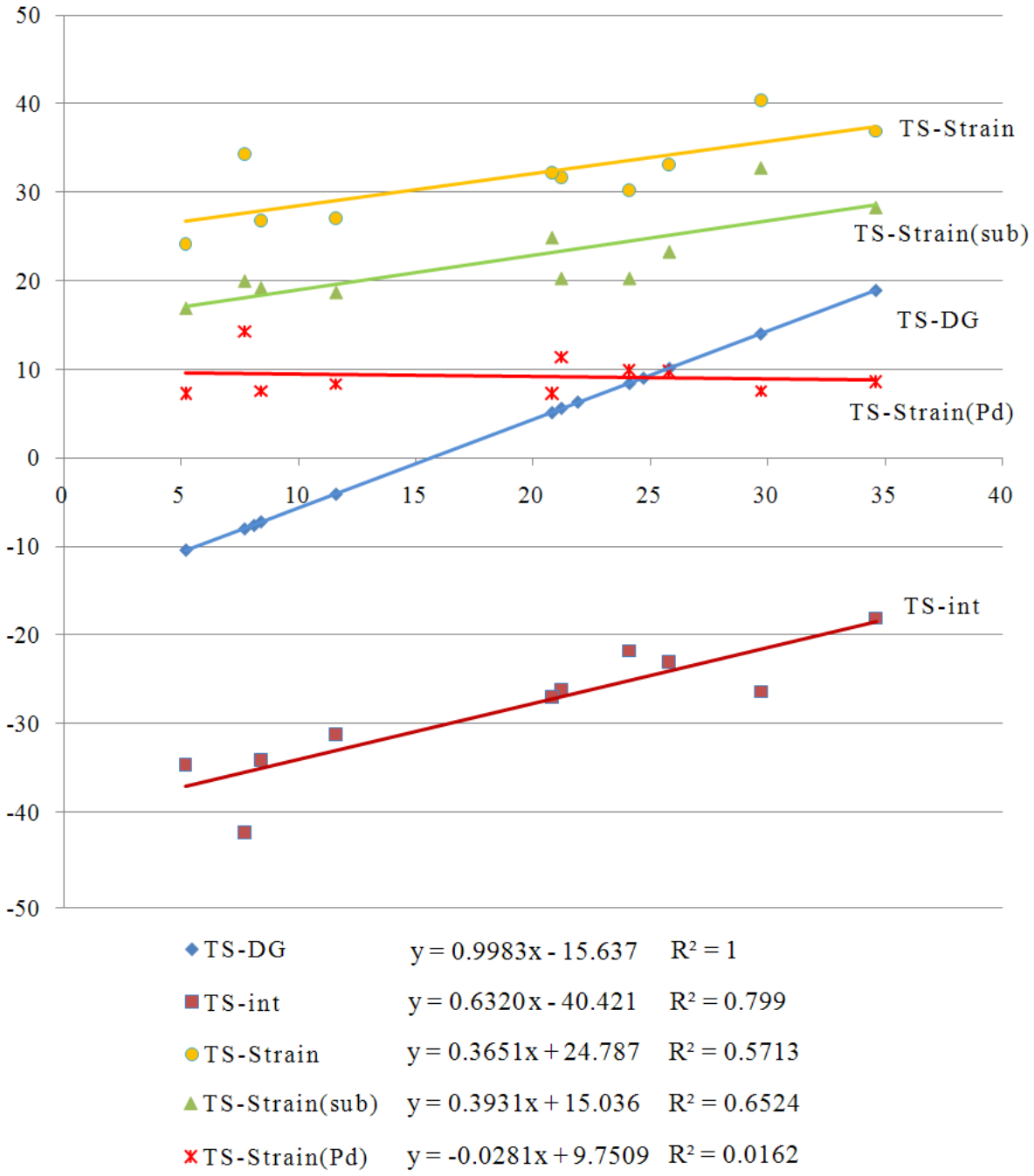

Diagram S1 Plot of $\Delta G^{\ddagger}_{TS}$ (Horizontal) against various free energies ($\Delta G^{\ddagger}$, $\Delta G^{\ddagger}_{int}$, $\Delta G^{\ddagger}_{strain}$, $\Delta G^{\ddagger}_{strain,B}$, $\Delta G^{\ddagger}_{strain,Pd}$) from **Table 2**

Cartesian coordinate for optimized geometries in gas phase and free energies take into account of solvent effect of THF at B3LYP level of theory (LANL2DZ(f) for Pd and 6-31+G(d) basis set for the other atoms)

IMH4 thermal Free Energies = -1030.413904 A.U.

C	-2.04766800	-3.38891400	0.10606200	H	6.61292700	1.60469200	-0.52828700
Pd	-1.32299600	-0.56945600	-0.15440100	C	5.65057700	1.12331200	-0.36846300
C	-1.84891100	1.35486900	-0.06595800	C	5.12392800	1.00749700	0.92170900
C	-3.29976200	-2.61376800	0.23200300	C	4.92437300	0.62018300	-1.45310000
C	-1.32257400	2.16594900	0.95278800	C	3.88488900	0.38744000	1.12099800
C	-1.69610200	3.51334600	1.04933800	H	5.67776200	1.40189400	1.77166800
C	-2.59462400	4.06507300	0.13099100	C	3.68692100	0.00392000	-1.23837700
C	-3.12009100	3.26321500	-0.88682100	H	5.31923800	0.71343700	-2.46305800
C	-2.75281800	1.91398700	-0.98299500	C	3.13569800	-0.13723400	0.05211900
H	-0.62334500	1.75042500	1.67545200	H	3.47988900	0.31390900	2.12840200
H	-1.28088800	4.12995300	1.84370900	H	3.12970600	-0.36311700	-2.10090400
H	-2.87990500	5.11165900	0.20503600	B	1.71201800	-0.89057900	0.29550700
H	-3.81315000	3.68606900	-1.61141500	O	1.20814700	-0.89369700	1.65930600
H	-3.16176500	1.31082200	-1.79163900	O	0.64292100	-0.07596600	-0.51570400
N	-0.99963200	-2.68842300	-0.10875800	O	1.70040500	-2.27456200	-0.22713900
N	-3.19172300	-1.32979800	0.13686900	H	1.62338300	-1.60538500	2.16562500
H	-4.25566700	-3.10800900	0.40784300	H	0.80109900	0.87792200	-0.43690500
H	-2.05850500	-4.47597200	0.21288500	H	2.41194000	-2.41790800	-0.86574300
H	-4.04984800	-0.78736900	0.23848400	H	-0.05044900	-3.08702900	-0.17650000

IMH4TS thermal Free Energies = -1030.385859 A.U.

C	1.58172700	3.32943200	-0.63664900	C	1.27614600	-2.53273800	-2.12402600
Pd	0.04072700	0.84321000	-0.19252100	C	-0.12744700	-3.37173600	-0.33197900
C	-1.79655900	0.11488900	0.13078800	C	1.49208900	-1.36315000	-1.39153400
C	0.16224600	3.71703100	-0.75339300	H	1.73997500	-2.66554400	-3.09927200
C	-2.65027200	-0.21369200	-0.93234200	C	0.07772300	-2.18819200	0.37259100
C	-3.98812100	-0.55797300	-0.69065300	H	-0.76212300	-4.15385900	0.07920200
C	-4.48724400	-0.57699800	0.61520000	C	0.91997400	-1.14853400	-0.10937900
C	-3.63920200	-0.25219400	1.67955500	H	2.16013400	-0.60671700	-1.79908000
C	-2.30147900	0.08979500	1.44031300	H	-0.40019700	-2.06268100	1.34109100
H	-2.27620800	-0.22202100	-1.95394200	B	2.25944800	-0.65160400	1.25389400
H	-4.63577900	-0.81833600	-1.52580400	O	3.29522800	0.11884100	0.59884400
H	-5.52378700	-0.84750200	0.80242500	O	1.46404700	0.06659900	2.21514600
H	-4.01566400	-0.26864100	2.70072200	O	2.82913700	-1.89701800	1.66991100
H	-1.64774200	0.32363300	2.27804500	H	4.04035400	-0.47222800	0.41459900
H	0.30865200	-4.46275000	-2.14621700	H	1.99257900	0.20919800	3.01721400
C	0.47058800	-3.54292300	-1.58810700	H	2.18463000	-2.46171400	2.11661100
H	2.74910800	1.73092400	-0.26519900	N	-0.70070700	2.78141400	-0.55006300
H	-0.11960700	4.74764200	-0.97654900	N	1.80193000	2.08088000	-0.45968700
H	2.36236900	4.09346500	-0.6675210	H	-1.68424500	3.04597300	-0.61507200

IMH4' thermal Free Energies = -1030.3906 A.U.

Pd	-0.15109300	0.39871000	-0.49936200	C	2.70565800	0.64569300	-1.17281500
N	0.07750600	2.48575000	-0.34763700	H	1.65294400	-0.07487000	1.98541000
N	-2.73068500	2.56520000	0.65448800	H	4.08780700	0.02963000	2.39810300
C	-1.73463200	3.19560300	1.13325900	H	5.66268100	0.50815300	0.52788900
C	1.81422100	0.36733700	-0.12518300	H	4.76733000	0.89308000	-1.76612300
C	-0.49400700	3.40239300	0.34233200	H	2.33500200	0.80135300	-2.18540200
C	2.32520600	0.15008700	1.16108000	H	2.14638400	-3.78062200	0.57786300
C	3.70573700	0.20208700	1.39381000	C	1.24444900	-3.18891100	0.44242500
C	4.59147800	0.47220100	0.34528400	C	0.42312000	-2.89335900	1.55189300
C	4.08822300	0.69230300	-0.93990600	C	0.89985100	-2.71764700	-0.81237200
O	-3.27084000	-0.47561600	1.07116200	C	-0.73163300	-2.13979200	1.39551700
H	-2.66079100	1.08109400	-0.56670600	H	0.69993900	-3.26789800	2.53565900

H	-4.12442200	-1.40299900	-1.40409000	C	-0.28810400	-1.96045300	-0.97927300
H	-3.97206200	-1.09920300	1.30593200	H	1.52444400	-2.93858700	-1.67445800
H	-1.71752100	3.64422000	2.13580500	C	-1.15256200	-1.68078200	0.11885700
H	-0.03850000	4.39553100	0.41463500	H	-1.36529500	-1.92130000	2.25196600
H	-3.49442200	2.45834200	1.32663100	H	-0.64084300	-1.75727800	-1.98949300
H	0.94421600	2.80083600	-0.78755300	B	-2.61722500	-0.96071000	-0.15645500
O	-2.24938500	0.28807100	-0.96728400	O	-3.42730800	-1.88043000	-0.93019700

IMH4'TS thermal Free Energies = -1030.384869 A.U.

Pd	0.47075500	-0.31954000	-0.35124100	H	-3.14093700	-2.58381900	2.53340300
N	1.15812400	-2.27612800	-0.68584300	H	-4.67281500	-3.07765200	0.63070600
N	3.78598800	-1.28609900	0.30001800	H	-4.04879800	-2.34632500	-1.66918700
C	3.36921200	-2.48968000	0.37049700	H	-1.93211400	-1.14094500	-2.06262000
C	-1.30387000	-1.18279100	0.01161000	H	-3.60695800	3.60987900	-0.13711800
C	2.17365600	-2.98671500	-0.35369100	C	-2.65622400	3.08292900	-0.09311000
C	-1.66930700	-1.59637900	1.30306400	C	-2.16944300	2.62122200	1.13622900
C	-2.87445800	-2.27534500	1.52418200	C	-1.92337000	2.86614800	-1.26583700
C	-3.73598300	-2.55341800	0.45746400	C	-0.95217500	1.94346000	1.18762800
C	-3.38344300	-2.14515200	-0.83164600	H	-2.74482400	2.78707000	2.04441900
C	-2.17611300	-1.46557800	-1.05256600	C	-0.70228600	2.19338800	-1.19884300
H	-1.01776000	-1.38413000	2.14818300	H	-2.30577700	3.22077800	-2.22060200
H	2.02267900	3.44843100	-0.94752300	C	-0.16626100	1.72641500	0.03035500
H	2.27205100	2.37010100	2.12459700	H	-0.57078200	1.59270800	2.14347900
H	3.87936700	-3.26272700	0.96002200	H	-0.13291300	2.04614900	-2.11591600
H	2.17620500	-4.06160100	-0.55978200	B	1.70502400	1.91301700	0.29576300
H	4.61362500	-1.14002400	0.88398700	O	2.21054700	0.91576000	-0.68156100
H	0.42527700	-2.82999800	-1.13446800	O	2.02966600	3.26859200	0.00198800
H	2.94293700	0.37304700	-0.32122300	O	2.01894600	1.56781800	1.64540600

IMH5' thermal Free Energies = -1030.430725 A.U.

C	0.08619600	2.22365400	1.36756500	Pd	0.03693800	-0.39044600	-0.05893900
H	0.24651700	4.06427100	2.48194500	N	-0.02221300	-2.59976700	-0.13877400
C	-0.36644300	2.44713000	-0.98832500	N	2.80081200	-2.93459100	0.60323200
H	-0.55214300	4.46659000	-1.72948900	C	1.93676900	-3.87491800	0.62324600
C	-0.12752500	1.60938600	0.11816700	C	-1.96703100	-0.44821500	-0.07564000
H	0.26683800	1.61263200	2.24982400	C	0.53561000	-3.71493600	0.16597000
H	-0.56249100	2.01234800	-1.96571600	C	-2.74884700	-0.23199200	1.07310200
B	3.30403300	0.55911100	-0.42276800	C	-4.13545800	-0.42556000	1.05138800
O	2.30816700	-0.33791100	-0.09869900	C	-4.77703900	-0.83112400	-0.12412500
O	3.03785900	1.85078900	-0.76584200	C	-4.01808200	-1.03757600	-1.27876400
O	4.60683700	0.10902200	-0.39775500	C	-2.62801900	-0.84728700	-1.25334600
H	2.61024000	-1.25767300	0.12840400	H	-2.27756600	0.10260500	1.99368600
H	2.09303000	2.08418400	-0.70961500	H	-4.71668400	-0.25077300	1.95489200
H	5.22823300	0.81357500	-0.63323600	H	-5.85485800	-0.97484500	-0.14113000
H	2.18256500	-4.88556600	0.97085100	H	-4.50385900	-1.33841900	-2.20529700
H	-0.02757300	-4.65196400	0.10944000	H	-2.06398100	-0.99481500	-2.17346500
H	3.71547900	-3.23220000	0.94962100	H	-0.15667600	5.51668600	0.49644700
H	-0.99667800	-2.74114700	-0.42095800	C	-0.14983600	4.43439200	0.39154300
C	-0.36956700	3.84386500	-0.85586000	C	0.07546700	3.61731200	1.50441200

IMH5 thermal Free Energies = -1030.438014 A.U.

C	-0.90949400	-1.42290300	-1.38447000	Pd	0.67831100	0.76496600	-0.11210300
H	-2.15313000	-2.88374300	-2.38057600	C	2.38745700	-0.28252300	0.07604800
C	-0.32064200	-0.98290300	-0.17855700	C	0.70892500	3.74768600	-0.15874900
H	-0.11585900	-1.46593200	1.92112500	C	3.18710400	-0.05765600	1.21290000
H	-0.72749500	-0.87595700	-2.30822600	C	4.44420900	-0.66221200	1.35013000
B	-4.35219200	0.08538900	0.34496800	C	4.93347900	-1.50333300	0.34640400
O	-5.27281400	1.03637000	0.70594900	C	4.15046700	-1.73951700	-0.78790300
O	-3.38116600	0.49377700	-0.54558300	C	2.88910300	-1.14405500	-0.91552200
O	-4.45038000	-1.17527200	0.88116800	H	2.82981300	0.59006300	2.01225900

H	-5.91347200	0.68284500	1.33970700	H	5.03827500	-0.47590600	2.24319900
H	-2.74312300	-0.20143300	-0.79361900	H	5.90910600	-1.97283100	0.44923300
H	-3.73259100	-1.79204600	0.65615400	H	4.51643700	-2.39787100	-1.57371400
N	1.53738400	2.77052700	-0.06002200	H	2.29234100	-1.36214700	-1.79769700
N	-1.01173800	2.14746700	-0.28428000	H	-2.58950800	-4.19760900	-0.30339900
H	2.52283900	3.02941200	0.00600800	C	-1.97096500	-3.30377200	-0.26838000
H	1.01247300	4.79703900	-0.16835900	C	-1.38511400	-2.88974100	0.93573200
H	-1.47260300	4.19061000	-0.31973500	C	-1.72076600	-2.56808900	-1.43298600
H	-2.00711200	1.89939200	-0.35408700	C	-0.56911000	-1.75124200	0.97548100
C	-0.72415600	3.39647300	-0.26422900	H	-1.55537400	-3.46148800	1.84607100

IMMe4 thermal Free Energies = -1108.97811 A.U.

C	5.06835000	-0.41088900	-1.25115300	C	-3.24396400	-2.45235500	0.12419300
C	3.76965800	0.09205600	1.16221100	Pd	-1.29885500	-0.28464500	-0.22447300
H	5.57607000	1.12447100	1.74236600	C	-0.90188800	1.67124300	-0.21272400
C	3.76593000	-0.87469100	-1.03331000	C	-3.91259000	-1.20372900	0.49818500
H	5.56665500	-0.60914900	-2.19837500	C	-0.16202100	2.22986800	0.84012000
C	3.08158900	-0.64052300	0.17775700	C	0.09275600	3.60819400	0.86329000
H	3.26421900	0.29614400	2.10368300	C	-0.37522600	4.43448900	-0.16358400
H	3.26852300	-1.42817500	-1.83075500	C	-1.09653200	3.87659800	-1.22339300
B	1.58588500	-1.22767000	0.44834500	C	-1.36029700	2.49957300	-1.24860000
O	0.94866800	-0.78549700	1.68210100	H	0.23127500	1.58617400	1.62262900
O	0.68190500	-0.63973500	-0.72476600	H	0.66916500	4.03218500	1.68293300
O	1.51418200	-2.68785900	0.37703600	H	-0.16940700	5.50206700	-0.14464900
H	0.96538200	-1.51852000	2.31290200	H	-1.45182400	4.50819000	-2.03528300
H	1.07854400	0.18734700	-1.04001300	H	-1.91783300	2.08165600	-2.08494100
H	2.30223700	-3.05610200	-0.04462100	H	6.74066200	0.67323200	-0.41309200
N	-2.02553800	-2.38361100	-0.27046800	C	5.72808700	0.31008800	-0.25077100
N	-3.27494300	-0.08982900	0.36900300	C	5.07198900	0.56160900	0.95876400
H	-4.93680600	-1.22813600	0.87745800	H	-1.06283300	-3.45887700	-1.75311800
H	-3.79390600	-3.39678200	0.18225500	H	-0.33583800	-3.57753300	-0.16007400
C	-1.29868200	-3.56630300	-0.68741800	C	-3.92115800	1.15846300	0.75763600
H	-1.87381300	-4.48784200	-0.52314500	H	-3.32573300	1.62891000	1.54538200
H	-4.94686100	0.98927100	1.10755400	H	-3.92065900	1.84015200	-0.09700500

IMMe4TS thermal Free Energies = -1108.943214 A.U.

C	1.05996700	3.46986900	-0.54571900	C	-1.72524700	-0.32715000	0.03041300
Pd	-0.00905400	0.67447600	-0.13360100	C	-0.38894400	3.58612900	-0.38330000
H	2.64868700	-0.34804100	-1.24014300	C	-2.44077600	-0.67586000	-1.12313800
H	-0.43818500	-2.53324400	0.80625600	C	-3.72935300	-1.21874600	-1.01860000
B	1.84669400	-0.83071600	1.66742300	C	-4.31006700	-1.42191100	0.23742500
O	2.94322500	0.07809300	1.46283100	C	-3.58817000	-1.09024900	1.38929900
O	0.73579300	-0.29145600	2.42400200	C	-2.29831800	-0.54995500	1.29005500
O	2.37874200	-2.08430300	2.13020100	H	-1.99835600	-0.53998800	-2.10741200
H	3.75913700	-0.43898100	1.54313200	H	-4.27336500	-1.48882200	-1.92177100
H	1.06674100	-0.04061400	3.30179400	H	-5.30894800	-1.84419400	0.31778000
H	1.67847400	-2.69401600	2.39831300	H	-4.02495500	-1.25751300	2.37223100
N	-1.10231800	2.52684300	-0.24110800	H	-1.72691300	-0.32297900	2.18571200
N	1.60993400	2.31242900	-0.52995200	H	1.41412600	-4.18840100	-2.68857000
C	-2.54316100	2.67096700	-0.07306900	C	1.31614200	-3.37595800	-1.97154100
H	-2.83172900	2.23405300	0.88701900	C	2.10646800	-2.22986000	-2.09674000
H	-2.85215800	3.72317400	-0.11744700	C	0.40200800	-3.47767800	-0.91465000
H	-3.05191900	2.09466100	-0.85045600	C	1.98317900	-1.20128400	-1.15903900
C	3.05078000	2.23431200	-0.70942600	H	2.82312000	-2.14730900	-2.91144700
H	3.44637000	1.61739300	0.10241400	C	0.27559700	-2.43001900	-0.00617100
H	3.25786100	1.72512400	-1.65800100	H	-0.21279500	-4.36930500	-0.81108600
H	3.52162900	3.22727600	-0.72596700	C	1.07514600	-1.25336800	-0.06950300
H	1.64113000	4.38846400	-0.68183400	H	-0.84183500	4.58196100	-0.38859700

IMMe4' thermal Free Energies = -1108.958618 A.U.

H	-1.66970500	2.57023800	2.65733900	Pd	0.17655600	-0.17433900	-0.48550700
C	-0.30091800	2.52448600	-0.97652900	N	0.35368600	-2.21352400	-1.05271700
H	-2.17168400	3.45321600	-1.52809200	N	2.71143500	-1.89137100	0.78667800
C	0.53245500	2.02236500	0.06389100	C	1.89464900	-2.86388800	0.74047000
H	0.60029100	1.66205700	2.18871900	C	-1.70357900	-0.57563900	0.07124100
H	0.10387400	2.56534400	-1.98476900	C	1.04064700	-3.10706900	-0.44679600
B	2.15560200	1.72967900	-0.21757100	C	-1.94744300	-1.22952400	1.28889200
O	2.19642400	0.40164200	-0.97941100	C	-3.25381800	-1.54492500	1.68507700
O	2.65812000	2.81382900	-1.03357900	C	-4.33740600	-1.22010100	0.86267000
O	2.90864100	1.50249300	1.02605200	C	-4.10350600	-0.57620800	-0.35559000
H	2.72514600	-0.25082000	-0.47889400	C	-2.79624200	-0.25625200	-0.74890800
H	3.47409800	2.54068100	-1.47889400	H	-1.12044900	-1.48414500	1.94927000
H	3.33772400	2.33237500	1.27721400	H	-3.42242800	-2.04160700	2.63870600
H	1.81097400	-3.60918000	1.54780300	H	-5.35165200	-1.46450000	1.16907600
H	1.00117400	-4.14438400	-0.80227500	H	-4.93800000	-0.31615600	-1.00412600
C	3.52510200	-1.68743800	1.96947900	H	-2.64044600	0.25656500	-1.69509700
H	4.58071100	-1.76846500	1.68394300	H	-3.03496000	3.50074000	0.80170400
H	3.36526800	-0.65430300	2.29842700	C	-2.05325100	3.08066300	0.59480100
H	3.30682100	-2.39863000	2.78118600	C	-1.28318600	2.55939100	1.64094200
C	-0.39935900	-2.60118900	-2.24684400	C	-1.56888700	3.05198100	-0.71642200
H	-0.27056800	-3.66549800	-2.48304100	C	-0.01915600	2.03162900	1.37512700
H	-1.45667100	-2.37805600	-2.08211000	H	-0.04707000	-1.99339400	-3.08615800

IMMe4'TS thermal Free Energies = -1108.952938 A.U.

H	-3.18225600	2.25371100	2.31080500	Pd	0.30058800	-0.14364200	-0.46293300
C	-1.48351500	2.04682100	-1.16927800	N	1.40520800	-1.89291100	-1.03693600
H	-3.38372600	2.68844100	-1.97219500	N	3.49397300	-0.39048500	0.54984000
C	-0.70747600	1.73149200	-0.02210600	C	3.27661900	-1.64349100	0.53541400
H	-0.80637300	1.56114700	2.12441100	C	-1.19570100	-1.32178300	0.16349700
H	-1.01645100	2.00787800	-2.15298100	C	2.50381100	-2.31619000	-0.53403500
B	1.09388700	2.34792500	-0.00396800	C	-1.05554300	-2.05066500	1.35646500
O	1.75237800	1.39782900	-0.93441300	C	-2.06442000	-2.91875700	1.79505200
O	1.05991300	3.69856600	-0.45455100	C	-3.23404000	-3.07620800	1.04493800
O	1.59517800	2.24477900	1.33344300	C	-3.38730800	-2.35263100	-0.14147900
H	2.55558700	1.01047900	-0.52471800	C	-2.37930700	-1.48083500	-0.57592100
H	0.98363700	3.76075600	-1.41597300	H	-0.15873400	-1.93730800	1.96308200
H	1.63087900	3.13406600	1.71525600	H	-1.93551000	-3.46866900	2.72558700
H	3.69657100	-2.31747300	1.29915900	H	-4.01844800	-3.74856600	1.38437800
H	2.92153900	-3.26993100	-0.88144000	H	-4.29720900	-2.45720500	-0.72970400
C	4.24909900	0.18457400	1.64798400	H	-2.53160300	-0.91314500	-1.49070100
H	5.12471700	0.70303100	1.24006600	H	-4.46791700	2.82868200	0.26223500
H	3.61000500	0.94162100	2.11633300	C	-3.42811700	2.51887900	0.18214000
H	4.57380300	-0.55908900	2.39172700	C	-2.70336700	2.19864000	1.33567700
C	0.79370500	-2.67954000	-2.10974800	C	-2.81798100	2.44049600	-1.07648200
H	1.38264600	-3.57411000	-2.35204100	C	-1.37075400	1.80019700	1.22687000
H	-0.21557700	-2.96359800	-1.80122100	H	0.70966100	-2.04442300	-2.99738800

IMMe5' thermal Free Energies = -1108.999281 A.U.

Pd	-0.07566500	-0.19364200	-0.25375100	H	0.01657900	3.91422800	2.83825800
N	0.17692700	-2.36644200	-0.87333800	C	-0.60567000	2.69343600	-0.78519300
N	2.55247300	-2.25692400	0.96718600	H	-0.83385400	4.78151300	-1.29137200
C	1.76349400	-3.23979200	0.78492100	C	-0.34019500	1.73781500	0.21541400
C	-2.04216800	-0.43267200	0.05305100	H	0.06567600	1.50402300	2.32911300
C	0.82789800	-3.33883800	-0.35788700	H	-0.81275800	2.37172000	-1.80479000
C	-2.48304000	-1.18126800	1.16013500	B	3.10468100	1.03481400	-0.79198800
C	-3.84123500	-1.47102900	1.34800200	O	2.19052700	0.04601300	-0.50013800
C	-4.79362400	-1.01469600	0.43153600	O	2.71608500	2.27934500	-1.19190600
C	-4.37345100	-0.25921800	-0.66745500	O	4.44451600	0.73253300	-0.68335300
C	-3.01505900	0.03352800	-0.84824500	H	2.53639100	-0.77747200	-0.06727200
H	-1.76500600	-1.54291700	1.89375200	H	1.75818900	2.43820600	-1.10048800

H	-4.15375700	-2.04966000	2.21568200	H	4.99742400	1.50131100	-0.88700100
H	-5.84840700	-1.23608100	0.57718700	H	1.77899500	-4.11638400	1.45035200
H	-5.10405200	0.11439500	-1.38273800	H	0.69960300	-4.35686800	-0.75049500
H	-2.71921600	0.64312400	-1.69890800	C	3.45165800	-2.26883900	2.10877700
H	-0.42392100	5.57773500	1.03562100	H	4.48006800	-2.15737100	1.74790500
C	-0.40189800	4.51481300	0.80736200	H	3.23166400	-1.39526400	2.73325600
C	-0.15333700	3.57851500	1.81682000	H	3.36859100	-3.18210900	2.71588400
C	-0.63042200	4.06679900	-0.49605900	C	-0.66830700	-2.66848400	-2.02837400
C	-0.12294000	2.20987700	1.52329800	H	-0.59771500	-3.72119500	-2.33525900
H	-0.35959600	-2.02123500	-2.85578500	H	-1.70277600	-2.41547400	-1.78080000

IMMe5 thermal Free Energies = -1109.01258 A.U.

C	0.18124800	3.51205300	0.42118900	H	-0.91447700	-1.72551200	-0.96213700
Pd	0.80521400	0.60771100	0.25886500	B	-4.48431500	-0.10772100	-1.53319100
C	2.06044300	-0.86502400	-0.28925800	O	-3.67933900	0.25872400	-0.48883700
C	1.51148700	3.45249500	-0.20103200	O	-5.50362500	0.72671400	-1.93931500
C	3.01309700	-1.39648500	0.59824400	O	-4.28968900	-1.29674400	-2.19287200
C	3.98074700	-2.31109000	0.16125200	H	-3.00887200	-0.41223800	-0.25377900
C	4.01099700	-2.72495600	-1.17428900	H	-5.56573300	1.52149900	-1.39023700
C	3.06088900	-2.21851500	-2.06638900	H	-4.93482800	-1.42984600	-2.90234100
C	2.09652200	-1.30158000	-1.62615800	N	2.04330800	2.30469000	-0.41466200
H	3.00055600	-1.10627000	1.64659500	N	-0.40049900	2.41738400	0.75186400
H	4.70591500	-2.70747000	0.86993200	H	2.01504000	4.38771300	-0.46813900
H	4.75795300	-3.43951000	-1.51248300	H	-0.28240600	4.49074400	0.58470000
H	3.06442700	-2.53979500	-3.10662300	C	3.35771300	2.20769300	-1.02457800
H	1.36297300	-0.93160600	-2.34093400	H	3.28155800	1.58430800	-1.92099800
H	-3.02555900	-3.40686700	2.38724000	H	3.77613500	3.19082000	-1.27986900
C	-2.30555200	-2.69540000	1.98999800	H	4.02474700	1.68258000	-0.33319500
C	-1.61183400	-1.83568900	2.84652300	C	-1.72323500	2.45279300	1.35182900
C	-2.05291400	-2.63587900	0.61548200	H	-2.42413100	1.92950000	0.69244400
C	-0.68610800	-0.91773000	2.33160100	H	-1.69547900	1.89456400	2.29307600
H	-1.78798400	-1.87860500	3.92004200	H	-2.07097800	3.47931300	1.53367000
C	-1.11705700	-1.72237100	0.10640400	H	-2.57683800	-3.30229200	-0.06658500
H	-0.15618000	-0.26838100	3.02695500	C	-0.42353200	-0.83244800	0.95061800

IMCy4 thermal Free Energies = -1499.404772 A.U.

C	3.13685900	-2.17137300	-0.60403400	C	-0.82372900	3.12824900	-0.36414800
H	2.28099300	-3.29223800	-2.22604100	Pd	-0.40837200	0.30028100	0.26713500
H	4.21434000	-1.38180000	1.09982200	C	-1.14643200	-1.48538100	0.78041800
B	2.25888600	-0.82690800	-0.88369200	C	-2.14395400	2.49513600	-0.32518400
O	1.21378400	-0.96290000	-1.89076800	C	-1.03303300	-2.58566000	-0.08393800
O	1.49384200	-0.52228200	0.47974300	C	-1.54412500	-3.83471400	0.29509900
O	3.07899600	0.34356500	-1.20133700	C	-2.15660400	-4.00368000	1.54119400
H	1.48811300	-0.47929200	-2.68208100	C	-2.25090700	-2.91652700	2.41515200
H	1.40837400	-1.35024500	0.97752100	C	-1.74966000	-1.66291900	2.03642200
H	4.01191100	0.17549900	-1.01315900	H	-0.52788600	-2.46874400	-1.03921500
N	0.20855400	2.39770300	-0.14068500	H	-1.44971600	-4.67974700	-0.38387100
N	-2.24347300	1.24261300	-0.03055000	H	-2.54446800	-4.97649900	1.83400500
H	-3.01921700	3.10220700	-0.55398400	H	-2.70872500	-3.04048200	3.39472600
H	-0.76904200	4.19611600	-0.58137000	H	-1.82732600	-0.82955900	2.73259200
C	-3.55173600	0.55674600	-0.06435200	H	5.33137600	-5.38122700	-0.01398200
C	-4.77556700	1.43736900	0.23579400	C	4.72462700	-4.49292300	-0.17619000
C	-3.71393400	-0.16304100	-1.42208100	C	3.78768500	-4.45649700	-1.21426400
H	-3.48327400	-0.21299200	0.71034000	C	4.87239900	-3.37634200	0.65270900
C	-6.04822400	0.57096200	0.25777900	C	3.00982100	-3.31150200	-1.41861600
H	-4.90090900	2.21085500	-0.53563100	H	3.66426500	-5.32115900	-1.86399400
H	-4.64380600	1.95334100	1.19649700	C	4.08720000	-2.23799400	0.43628100
C	-4.99827200	-1.00863800	-1.43164800	H	5.59525500	-3.39393000	1.46635400
H	-3.75392100	0.59600600	-2.21811700	H	-2.83778400	-0.79051400	-1.61187700
C	3.57539300	3.27885200	1.40236300	C	-6.23873700	-0.17558000	-1.07249700

H	1.48882000	3.48010000	1.98525900	H	-6.91896700	1.20405100	0.47041700
H	1.99724600	1.80598800	1.68639900	H	-5.97920500	-0.15526100	1.08064600
C	3.78525100	4.67870400	0.80581800	H	-5.12136500	-1.47014300	-2.41960700
H	3.34604000	5.77809500	-1.02269100	H	-4.88692100	-1.83354500	-0.71392700
H	3.81523900	4.09867500	-1.28155400	H	-7.12537200	-0.82018900	-1.01905800
H	3.91646300	3.25283400	2.44554800	H	-6.43111400	0.55624800	-1.87208900
H	4.18733900	2.55122100	0.85178400	C	1.57264500	2.93141200	-0.11402800
H	4.85179500	4.93876300	0.81427200	C	1.75085500	4.34767700	-0.67801300
H	3.27535000	5.42510000	1.43471000	C	2.10417800	2.83710300	1.33690800
H	1.38338300	4.39515500	-1.71270300	H	2.15982900	2.21373800	-0.70526100
H	1.16617500	5.07308900	-0.09068300	C	3.23280900	4.76103300	-0.62564100

IMCy4TS thermal Free Energies = -1499.368212 A.U.

C	-0.85484300	-2.66037200	-0.16350300	Pd	0.07895300	0.20011900	0.02823600
N	-1.47721800	-1.54070000	-0.09395100	C	1.72430300	1.32311200	-0.01827600
C	-3.56907400	-2.41931400	0.99630600	C	0.60565000	-2.69212900	-0.14081700
H	-3.25750700	-0.53708600	0.06191800	C	2.33459100	1.63748500	-1.24072000
C	-5.01284900	-1.93469200	-1.55826000	C	3.58541000	2.27059200	-1.26513800
H	-3.15241800	-3.03615700	-1.72478000	C	4.23309000	2.60149100	-0.07035600
H	-3.03939400	-1.36945300	-2.29564900	C	3.61475000	2.30671500	1.15011600
C	-5.10388000	-2.33981900	0.94688400	C	2.36303800	1.67651900	1.17935700
H	-3.26112600	-3.47095100	0.89558500	H	1.83779300	1.40329900	-2.17939300
H	-3.19490300	-2.05088300	1.95755200	H	4.04672300	2.51213000	-2.22100700
C	-5.65159900	-2.75717200	-0.42740400	H	5.20188200	3.09522100	-0.09034600
H	-5.37129700	-2.28338500	-2.53562600	H	4.10212400	2.57508500	2.08577500
H	-5.32755600	-0.88468800	-1.46647900	H	1.86890200	1.47902500	2.12623200
H	-5.53176800	-2.97070700	1.73673400	H	-1.65762600	4.73884400	-2.89757400
H	-5.41580300	-1.30888900	1.16767400	C	-1.49805900	4.00240400	-2.11269400
H	-6.74345200	-2.64583500	-0.45078900	C	-2.21261400	2.80158800	-2.12115200
H	-5.44221100	-3.82547000	-0.59327100	C	-0.57754200	4.25543800	-1.08685100
C	2.76064300	-1.68995200	-0.04091000	C	-2.01423600	1.87164900	-1.09605300
C	3.27500300	-2.48689700	1.17466500	H	-2.92931500	2.59854700	-2.91450800
C	3.32764200	-2.24919100	-1.36145200	C	-0.37174900	3.30272000	-0.09305500
H	3.11304200	-0.66360300	0.06233200	H	-0.01821900	5.18860700	-1.07545500
C	4.81279500	-2.47832100	1.20329400	C	-1.09819700	2.07935300	-0.03249400
H	2.92039500	-3.52701900	1.12445200	H	-2.61873700	0.96980500	-1.10126700
H	2.86795400	-2.05058000	2.09503000	H	0.34874100	3.51817600	0.69116100
C	4.86517100	-2.24724300	-1.32635800	B	-1.75974900	1.79510800	1.77764600
H	2.96588600	-3.27641000	-1.51849600	O	-2.79547500	0.80179600	1.73007000
H	2.95994400	-1.64520500	-2.19982000	O	-0.57401100	1.41898800	2.51928600
C	5.40579900	-3.01563200	-0.10940600	O	-2.35747700	3.05393600	2.13928400
H	5.16817700	-3.07234400	2.05511500	H	-3.64041200	1.27116600	1.80260600
H	5.16372700	-1.44981800	1.36944700	H	-0.83350600	1.27508200	3.44385300
H	5.25503700	-2.68039100	-2.25658000	H	-1.69211400	3.74012000	2.28189800
H	5.22060200	-1.20755800	-1.29019300	N	1.28097700	-1.59963900	-0.07290700
H	6.50135900	-2.95482900	-0.08139900	H	-1.37323600	-3.62063600	-0.23553800
H	5.15394600	-4.08269000	-0.21153000	H	1.09286000	-3.66913300	-0.17859900
C	-2.95499100	-1.56582600	-0.13146300	C	-3.47695000	-2.00547300	-1.51546900

IMCy4' thermal Free Energies = -1499.387803 A.U.

Pd	-0.53103900	0.41708400	-0.30740800	H	3.10058600	2.25431600	-2.10074400
N	-0.81894100	-1.63483600	0.20795300	H	1.83723100	-2.29329100	2.04062900
N	2.16910400	-1.31026900	0.22418200	H	-0.16880700	-3.39611700	1.05073200
C	1.46333800	-1.95199800	1.06603800	C	3.54920000	-0.90679700	0.49267900
C	-1.71069700	0.88932100	1.23772000	C	4.10914300	-1.17318700	1.89822600
C	0.07366500	-2.37213700	0.75521400	C	4.45115300	-1.53245300	-0.59375400
C	-1.20889200	0.83381800	2.54751200	H	3.53847300	0.17613700	0.29872800
C	-2.02663900	1.13346400	3.64476800	C	5.55267100	-0.64999900	2.01489100
C	-3.36653700	1.48397600	3.45040500	H	4.10607000	-2.25472800	2.10598200
C	-3.87807500	1.53563500	2.15080400	H	3.47697400	-0.69722400	2.66084100

C	-3.05673500	1.24100200	1.05329600	C	5.89775000	-1.03006200	-0.46867400
H	-0.16777300	0.56957600	2.72409200	H	4.42444700	-2.62826600	-0.49095800
H	-1.61350100	1.09437200	4.65100800	H	4.04399100	-1.28427800	-1.57964200
H	-4.00263200	1.71626200	4.30118400	C	6.46449800	-1.26312700	0.94063800
H	-4.91813300	1.81010400	1.98431400	H	5.94356300	-0.86483200	3.01791700
H	-3.47470700	1.30359600	0.05123900	H	5.54906600	0.44472600	1.90783600
H	-2.00418800	5.14220300	0.58048200	H	6.52617300	-1.52593400	-1.21983500
C	-1.40242200	4.37791800	0.09393100	H	5.92158800	0.04475300	-0.69920800
C	-0.17631800	3.99712300	0.64892400	H	7.47531700	-0.84182800	1.01841000
C	-1.86210700	3.76792200	-1.07776300	H	6.56073100	-2.34490800	1.12178100
C	0.59964900	3.02395900	0.01568400	C	-2.15782100	-2.17900000	-0.12897100
H	0.17157000	4.46170000	1.56862300	C	-2.31854100	-2.16888200	-1.66440600
C	-1.08148800	2.79512500	-1.70734400	C	-2.50708900	-3.56116700	0.44433100
H	-2.81889600	4.06141600	-1.50409200	H	-2.85923200	-1.44843800	0.29156100
C	0.19245300	2.40926400	-1.20105600	C	-3.74460100	-2.57488200	-2.06871200
H	1.57397900	2.75780400	0.41839800	H	-1.58835500	-2.86600500	-2.10035400
H	-1.40748500	2.36873500	-2.65276700	H	-2.07249100	-1.17496800	-2.05387400
B	1.24548000	1.50494600	-2.13435900	C	-3.94812800	-3.94313400	0.05639400
O	0.79783500	0.05207600	-1.96890400	H	-1.82335900	-4.32608400	0.04723000
O	1.09094700	1.93811200	-3.50676200	H	-2.40253900	-3.56090800	1.53771000
O	2.62692800	1.55538900	-1.62834600	C	-4.14572600	-3.93056500	-1.46731900
H	1.49608800	-0.46616100	-1.52053000	H	-3.81814900	-2.60429900	-3.16310100
H	1.45307600	1.26542500	-4.10280700	H	-4.45041200	-1.80244300	-1.72889000
H	-5.18964100	-4.16287500	-1.71430900	H	-4.18517800	-4.93328000	0.46570600
H	-3.53209200	-4.72510200	-1.91845900	H	-4.64803600	-3.23544400	0.52415000

IMCy4'TS thermal Free Energies = -1499.381335 A.U.

H	2.13610700	-2.65049000	1.40921800	Pd	-0.48206200	0.44675300	-0.31376400
H	0.20508900	-3.56000800	0.18324000	N	-0.56066000	-1.69308200	-0.22256000
C	-1.85897000	-2.30357600	-0.63635700	N	2.42447300	-1.18423200	-0.04549300
C	-1.70774900	-3.17017500	-1.90127800	C	1.74576300	-2.07525400	0.55978500
C	-2.53943600	-3.08016600	0.50664900	C	-1.87394000	0.54194700	1.12794700
H	-2.50148500	-1.45426400	-0.88158300	C	0.38457300	-2.47995400	0.13594200
C	-3.07672600	-3.70890200	-2.35142400	C	-1.51531800	0.27380600	2.46017800
H	-1.03617900	-4.01668400	-1.69511700	C	-2.47180400	0.28888000	3.48403700
H	-1.24164600	-2.57856900	-2.69892300	C	-3.81034400	0.57295200	3.19439300
C	-3.90555000	-3.61749800	0.04738700	C	-4.17838500	0.85176300	1.87478500
H	-1.90471500	-3.92374300	0.81608300	C	-3.21848300	0.84015500	0.85315400
H	-2.65452800	-2.42128700	1.37407800	H	-0.47894700	0.05624300	2.71275400
C	-3.78370300	-4.47551000	-1.22209000	H	-2.16799900	0.08113000	4.50857200
H	-2.94682400	-4.35317100	-3.23039400	H	-4.55398600	0.58618300	3.98780000
H	-3.70845900	-2.86746900	-2.67246300	H	-5.21380500	1.08886100	1.63647900
H	-4.36319800	-4.19681400	0.85931700	H	-3.52721700	1.08344400	-0.16093500
H	-4.57759600	-2.76879700	-0.14590000	H	-2.87939300	5.57607700	-0.15405200
H	-4.77701000	-4.80439100	-1.55379100	C	-2.18855300	4.74627900	-0.28760100
H	-3.21304200	-5.38829200	-0.99092100	C	-1.23023500	4.46981300	0.69422600
C	3.77081500	-0.80388500	0.39129400	C	-2.26082400	3.95577100	-1.44183600
C	4.31608200	-1.46745800	1.66461400	C	-0.34754700	3.40340100	0.51905600
C	4.73824400	-1.00242800	-0.79583200	H	-1.18196900	5.08068400	1.59305700
H	3.68029400	0.28009400	0.55822400	C	-1.36801800	2.89704300	-1.60544100
C	5.71968100	-0.93035200	2.00032700	H	-3.00734700	4.17117100	-2.20360300
H	4.37879500	-2.55798500	1.52376000	C	-0.36949500	2.59438900	-0.64207600
H	3.63875100	-1.28942600	2.51101500	H	0.40097000	3.19439200	1.27906200
C	6.14759500	-0.48824600	-0.45922300	H	-1.42283800	2.30187500	-2.51660400
H	4.78112900	-2.07438700	-1.04229100	B	1.34332100	2.09414900	-1.30922200
H	4.34116200	-0.48537500	-1.67692300	O	1.10592100	0.70590800	-1.77030700
C	6.69388700	-1.12399200	0.82825500	O	1.65189800	3.02128300	-2.34722300
H	6.09993000	-1.42900100	2.90124300	O	2.28547000	2.16873200	-0.23315800
H	5.64778200	0.14027600	2.24194700	H	1.76279100	0.08583900	-1.38110300
H	6.82301900	-0.68786100	-1.30109600	H	1.19954700	2.80530700	-3.17359700

H	6.11135000	0.60446000	-0.33953400	H	2.81898600	2.96837000	-0.34972800
H	6.85450200	-2.20074200	0.66406500	H	7.67387700	-0.69604800	1.07655800

IMCy5' thermal Free Energies = -1499.501643 A.U.

H	3.37510400	1.71900900	-3.50349800	Pd	-0.62587800	0.62176600	-0.08125800
H	1.94375400	-2.78010000	1.54406200	N	-0.61484500	-1.64242400	-0.20119900
H	0.04210700	-3.56394600	0.19448700	N	2.34796600	-1.26005000	0.18167600
C	-1.89612300	-2.17667900	-0.74188500	C	1.60807100	-2.15333500	0.70914200
C	-1.67486000	-2.95975600	-2.05104000	C	-2.16713400	0.62765200	1.19922500
C	-2.68963600	-3.00465800	0.28742700	C	0.25910200	-2.48851500	0.19354000
H	-2.49221200	-1.29028900	-0.97565500	C	-1.95622400	0.29739200	2.55086500
C	-3.02024500	-3.41503800	-2.64106700	C	-3.02677500	0.17638300	3.44671800
H	-1.04608800	-3.84120400	-1.85539400	C	-4.33915600	0.38830300	3.01211000
H	-1.13072400	-2.33132800	-2.76712600	C	-4.56535000	0.73290800	1.67606900
C	-4.03208700	-3.45663100	-0.31128100	C	-3.49073700	0.85752900	0.78514400
H	-2.11087100	-3.89216300	0.58354400	H	-0.94529800	0.13379600	2.91921900
H	-2.85144700	-2.40168400	1.18766600	H	-2.83230400	-0.07869900	4.48720000
C	-3.83803000	-4.22977300	-1.62568600	H	-5.17112500	0.29801000	3.70677000
H	-2.84309500	-4.00252600	-3.55122100	H	-5.57955700	0.91629600	1.32529500
H	-3.59744300	-2.53053100	-2.94825400	H	-3.69654000	1.14886000	-0.24283500
H	-4.57052000	-4.07315900	0.41976700	H	-0.54169200	6.54532600	-0.25444800
H	-4.65905300	-2.57191300	-0.49296000	C	-0.58891900	5.46056500	-0.19502200
H	-4.81197300	-4.49863800	-2.05481500	C	0.20076800	4.76624400	0.72793500
H	-3.31590200	-5.17642300	-1.41682100	C	-1.44537700	4.74287700	-1.03378100
C	3.69718900	-0.96641500	0.67881200	C	0.14071200	3.36951700	0.80329600
C	4.14127400	-1.65898000	1.97604500	H	0.86622400	5.31360700	1.39324300
C	4.70430100	-1.22845400	-0.46315700	C	-1.50712600	3.34307100	-0.95013300
H	3.68476000	0.12044000	0.85656100	H	-2.07287800	5.26792600	-1.75168600
C	5.55436800	-1.19775600	2.37786400	C	-0.70760100	2.62532600	-0.03872200
H	4.15264800	-2.75025500	1.83297600	H	0.76172900	2.85714200	1.53509400
H	3.43264800	-1.44645000	2.78813800	H	-2.20182300	2.81309300	-1.59977100
C	6.12314300	-0.79403400	-0.06107000	B	1.80557200	1.42670100	-2.38194000
H	4.69497800	-2.30446300	-0.69397700	O	1.20110600	0.60315800	-1.46025600
H	4.37983700	-0.69957800	-1.36583100	O	1.21636200	2.57584500	-2.82178300
C	6.57248700	-1.44854400	1.25455000	O	3.03968700	1.05970000	-2.87809400
H	5.86184200	-1.71355600	3.29637200	H	1.74553900	-0.12935400	-1.06048100
H	5.53002400	-0.12410800	2.61659300	H	0.42230700	2.82750100	-2.31440100
H	6.82368500	-1.03924100	-0.86941500	H	7.56011200	-1.07093800	1.54922300
H	6.14643900	0.30035000	0.04943100	H	6.68402700	-2.53306000	1.1028370

IMCy5 thermal Free Energies = -1499.50964 A.U.

C	0.04683500	-2.74735800	0.38434400	N	-0.61619200	-1.75970100	-0.09809100
Pd	0.60087100	0.10813300	-0.21867800	H	2.01505400	-3.43591200	1.09497600
C	1.83731800	1.69981500	-0.18922400	H	-0.40197200	-3.72189500	0.58734200
C	1.47874900	-2.58061900	0.67878800	C	3.47318600	-1.22844400	0.67863800
C	2.37116300	2.26001800	-1.36393000	C	4.17960500	-2.22665500	1.60884300
C	3.33225000	3.27808400	-1.31486200	C	4.20083000	-1.13859100	-0.68220600
C	3.77184500	3.77698700	-0.08423000	H	3.52058100	-0.23001900	1.13240900
C	3.23560900	3.24970800	1.09423400	C	5.64458200	-1.80487300	1.82315100
C	2.27990800	2.22549200	1.03934000	H	4.16816000	-3.23551900	1.16960900
H	2.03152600	1.90844000	-2.33602200	H	3.65554400	-2.28594100	2.57276100
H	3.72953300	3.68895800	-2.24150400	C	5.67413800	-0.74567200	-0.48461100
H	4.51094800	4.57398600	-0.04507000	H	4.13237000	-2.11709000	-1.18159400
H	3.55442500	3.63878900	2.05990300	H	3.69035500	-0.40766800	-1.31639400
H	1.87094000	1.84330700	1.97343200	C	6.39676800	-1.69169100	0.48734000
H	-3.80299400	3.89041700	-1.51683800	H	6.14313600	-2.52590400	2.48361100
C	-2.98585700	3.21214300	-1.28270200	H	5.66985500	-0.83503800	2.34112700
C	-2.28009700	2.57141800	-2.30473700	H	6.18253200	-0.73731100	-1.45730600
C	-2.61453700	2.98300400	0.04792400	H	5.71839000	0.28318300	-0.10051700
C	-1.21763400	1.70935400	-1.99910700	H	7.42343500	-1.34438400	0.66140700

H	-2.54696100	2.74964200	-3.34505800	H	6.47695000	-2.69119600	0.03274800
C	-1.55584800	2.11062700	0.34573600	C	-2.03395000	-1.88386100	-0.46514400
H	-3.13315900	3.49501500	0.85654300	C	-2.13919400	-1.96396900	-2.00537800
C	-0.83988500	1.44603300	-0.66968300	C	-2.81603400	-3.03303700	0.19028300
H	-0.67288900	1.24692400	-2.82053900	H	-2.48683600	-0.93577600	-0.15397300
H	-1.27768800	1.96915700	1.38805900	C	-3.61007900	-1.94108000	-2.45316000
B	-5.15599700	0.95420300	2.26367000	H	-1.65579000	-2.89418500	-2.34094700
O	-4.54853900	0.51759500	1.11790300	H	-1.58864900	-1.12990000	-2.45073100
O	-6.09080000	0.15973900	2.89111900	C	-4.29325800	-2.97705500	-0.23981800
O	-4.84450900	2.17777500	2.80620300	H	-2.40082200	-4.00562700	-0.11363800
H	-3.91195000	1.15628400	0.74388300	H	-2.73450200	-2.96956500	1.28391800
H	-6.24509400	-0.66963200	2.41622400	C	-4.43467800	-3.04298200	-1.76919500
H	-5.35111900	2.36138600	3.61053300	H	-3.66063300	-2.04744500	-3.54460800
N	2.04231800	-1.45259900	0.43872000	H	-4.04006900	-0.95894900	-2.21230600
H	-5.49126600	-2.95541400	-2.05394900	H	-4.84429800	-3.80247200	0.23003100
H	-4.09500500	-4.02831200	-2.12457800	H	-4.73465800	-2.04102800	0.12789600

IMPh4 thermal Free Energies = -1492.353938 A.U.

H	-0.49795800	-4.00250100	1.41420500	C	1.33082900	-2.94801100	0.79850000
H	1.98285600	-3.68849100	1.26801100	Pd	0.06535100	-0.58032700	-0.44389300
C	-2.31597700	-2.49096100	0.46191100	C	-1.57223900	0.47359400	-0.84146000
C	-3.12018100	-2.37930700	-0.68057000	C	-0.10839800	-3.12017500	0.90525900
C	-2.89110700	-2.81446300	1.70109700	C	-2.39095400	0.93175900	0.19529200
C	-4.48768500	-2.63173700	-0.58701700	C	-3.54953700	1.66205500	-0.09830700
H	-2.66847800	-2.09665400	-1.62444300	C	-3.89576900	1.93406600	-1.42478600
C	-4.26518900	-3.04430100	1.78779400	C	-3.06728600	1.48846600	-2.45959100
H	-2.27426500	-2.83963800	2.59533500	C	-1.90013500	0.76940000	-2.16979800
C	-5.06481100	-2.96246700	0.64402900	H	-2.12855800	0.74375800	1.23322100
H	-5.10665200	-2.55146600	-1.47609600	H	-4.17225800	2.02777900	0.71512700
H	-4.71040200	-3.27387100	2.75203900	H	-4.79427100	2.50364000	-1.65002600
H	-6.13476300	-3.13800200	0.71427300	H	-3.31775800	1.71174200	-3.49487400
C	3.17959900	-1.77937400	-0.05567200	H	-1.24820800	0.45762700	-2.98226600
C	4.08165600	-1.96092800	1.00700200	H	-1.58781000	6.12184000	1.60422500
C	3.65469900	-1.38651100	-1.31649900	C	-0.94331800	5.29045300	1.32529600
C	5.44639200	-1.76603300	0.79698300	C	-0.33351600	4.50650400	2.31002700
H	3.70823500	-2.19677400	1.99951300	C	-0.71878000	4.99261500	-0.02322700
C	5.02244000	-1.21665900	-1.52302000	C	0.49624000	3.44038600	1.94314400
H	2.94641500	-1.24733700	-2.12813100	H	-0.50246700	4.72804400	3.36275300
C	5.92155100	-1.40179600	-0.46776900	C	0.10972400	3.92178900	-0.37449800
H	6.13849300	-1.88294400	1.62653500	H	-1.19591600	5.58935900	-0.79871100
H	5.38499600	-0.92118600	-2.50340400	C	0.74201400	3.11993800	0.59548100
H	6.98501300	-1.24507000	-0.62484600	H	0.96727800	2.83372400	2.71354100
O	3.04482500	2.41652500	-0.38299300	H	0.25343700	3.68937900	-1.42850800
H	3.02264200	0.96224100	1.38653900	B	1.78578400	1.94862200	0.19896700
H	1.88581800	0.86270700	-1.55432100	O	2.06196000	1.01532100	1.28158600
H	2.99616000	3.35119100	-0.62348100	O	1.12253200	1.10958000	-1.00579400
N	1.79015700	-1.96631200	0.09725800	N	-0.91340400	-2.26917000	0.34389000

IMPh4' thermal Free Energies = -1492.347521 A.U.

Pd	-0.38955200	0.20897900	-0.27118400	B	0.65112500	0.98033900	-2.77288600
N	-1.05393700	-1.76388700	0.18482100	O	0.18887500	-0.40209700	-2.28222300
N	1.85883300	-1.63339100	0.21792300	O	-0.02200700	1.35858100	-3.99163400
C	1.18745300	-2.63891100	0.65059100	O	2.11403200	0.83267500	-2.89186200
C	-0.90540800	0.86241900	1.54349700	H	0.98226000	-0.95461600	-2.19374900
C	-0.25846100	-2.74801400	0.44433400	H	0.01900300	0.63427400	-4.63324600
C	-0.11907200	0.52594700	2.65469400	H	2.44697800	1.45368200	-3.55466700
C	-0.47136700	0.96515800	3.93789300	H	1.65253000	-3.49924400	1.14832100
C	-1.62060400	1.73858300	4.12786000	H	-0.67969800	-3.75295700	0.53657000
C	-2.41026200	2.07404100	3.02401000	C	3.23941500	-1.50664400	0.44355800
C	-2.05439200	1.64051900	1.73925100	C	3.91047700	-2.07207300	1.54754600

H	0.78301200	-0.06816600	2.52847700	C	3.95721100	-0.73084400	-0.48723100
H	0.15674300	0.70283800	4.78715600	C	5.28357100	-1.88769100	1.69566800
H	-1.89576900	2.07791200	5.12357000	H	3.35600900	-2.61945300	2.30504300
H	-3.30616400	2.67766900	3.15703500	C	5.33552400	-0.57222100	-0.33922900
H	-2.67564200	1.92250400	0.89296800	H	3.42491000	-0.26736500	-1.31643300
H	-0.49874400	5.08158600	0.82954100	C	6.00210300	-1.14770800	0.74750200
C	-0.30579500	4.23565300	0.17384100	H	5.79404500	-2.31144400	2.55667500
C	0.82808700	3.45450800	0.35991300	H	5.88691900	0.01560500	-1.06815900
C	-1.21091300	3.92714500	-0.85864500	H	7.07310000	-1.00703100	0.86785100
C	1.08000600	2.37239800	-0.50441600	C	-2.41448700	-2.07758500	-0.12342300
H	1.52434300	3.68019300	1.16380400	C	-3.45071700	-1.45476400	0.58594300
C	-0.96444200	2.85497100	-1.70748300	C	-2.70796200	-2.99697800	-1.14220200
H	-2.09812800	4.54141000	-0.99869400	C	-4.77489700	-1.77954600	0.29213400
C	0.21022200	2.05634000	-1.58418900	H	-3.21038700	-0.73633500	1.36153700
H	2.01786000	1.82992500	-0.41567100	C	-4.03846900	-3.29985800	-1.43985300
H	-1.63787300	2.64363300	-2.53352600	H	-1.89973400	-3.43042200	-1.72423500
H	-4.26223700	-3.99748000	-2.24247100	C	-5.07442200	-2.69853500	-0.72026600
H	-6.10906600	-2.93488300	-0.95353700	H	-5.57635900	-1.30674300	0.85347300

IMPh4'TS thermal Free Energies = -1492.339393 A.U.

B	0.54664500	1.62674000	-2.31769000	Pd	-0.46567700	0.13586300	-0.30692700
O	0.28349900	0.16641800	-2.36409400	N	-0.59611900	-2.00463500	-0.03725500
O	0.11979100	2.33760300	-3.46856500	N	2.31067500	-1.44934800	-0.07809600
O	1.89110800	1.92524400	-1.95089100	C	1.75284500	-2.42680000	0.53634200
H	1.13419000	-0.30212800	-2.31486800	C	-0.99328200	0.46486800	1.60032100
H	-0.62370100	1.90629400	-3.91062400	C	0.35840900	-2.80785200	0.29207800
H	2.20662700	2.66301700	-2.49316500	C	-0.08393500	0.11960500	2.61398500
H	2.28486400	-3.06612000	1.25340000	C	-0.40249400	0.30378600	3.96617100
H	0.13155800	-3.87010600	0.42897000	C	-1.64282100	0.83440900	4.33210800
C	3.66901300	-1.13500100	0.13039900	C	-2.55295100	1.19027800	3.33247500
C	4.63772700	-2.05884600	0.57397600	C	-2.22886200	1.01347600	1.98071100
C	4.05387500	0.18466700	-0.16727700	H	0.89196400	-0.28700800	2.35751300
C	5.95828700	-1.65187100	0.75290400	H	0.32305700	0.03341200	4.73127500
H	4.37253700	-3.09845600	0.74462800	H	-1.89311100	0.97621500	5.38080900
C	5.37508500	0.58609000	0.03578000	H	-3.51796300	1.61680800	3.60047800
H	3.30800400	0.87100200	-0.55953700	H	-2.94412100	1.32405500	1.22377800
C	6.32947500	-0.32549400	0.49721300	H	-2.46789300	5.44736100	0.37895400
H	6.70293000	-2.37217000	1.08204700	C	-1.95187800	4.55190600	0.03913500
H	5.66190900	1.61135300	-0.18284800	C	-0.63222500	4.31214800	0.43667600
H	7.36090000	-0.01330400	0.63880500	C	-2.60995900	3.64102300	-0.79827800
C	-1.85321000	-2.59483200	-0.38115500	C	0.02543100	3.16263300	-0.00387100
C	-3.03349500	-2.11482300	0.20407100	H	-0.12496400	5.01726900	1.09140200
C	-1.90878900	-3.63859700	-1.31848900	C	-1.93944800	2.49894800	-1.23163500
C	-4.25437400	-2.70262500	-0.12648000	H	-3.63547400	3.82962300	-1.10902900
H	-2.97936100	-1.30406800	0.92170600	C	-0.59377300	2.22695400	-0.86695300
C	-3.13904200	-4.20736100	-1.65635000	H	1.05506000	2.98908100	0.29646200
H	-0.99803700	-3.97099900	-1.80921000	H	-2.45926700	1.81001400	-1.89633600
C	-4.31410800	-3.74654300	-1.05707000	H	-3.17654400	-5.00320500	-2.39552500
H	-5.16445200	-2.33875700	0.34303200	H	-5.27086700	-4.18968100	-1.31990900

IMPh5' thermal Free Energies = -1492.394235 A.U.

H	1.48243400	-0.82108600	-1.31320700	Pd	-0.52429600	0.38168400	-0.09758600
H	0.32723800	1.94823900	-2.99023800	N	-0.88786100	-1.88446000	0.02007600
H	2.77567500	0.08461700	-4.39460400	N	2.05223100	-1.66555600	0.30930600
H	1.66103500	-3.12028400	1.74894300	C	1.30100700	-2.51694700	0.90553700
H	-0.41868200	-3.81412200	0.59695900	C	-1.56451700	0.85461700	1.55375100
C	3.39032300	-1.46572400	0.71833600	C	-0.08036800	-2.77872700	0.47813400
C	4.21951000	-2.50446400	1.17811800	C	-1.13745700	0.30920300	2.77893400
C	3.90425600	-0.16282300	0.60767400	C	-1.85324900	0.52615300	3.96383100
C	5.53606000	-2.23006200	1.54963600	C	-3.01728300	1.30015000	3.95224000

H	3.85046500	-3.52610700	1.20561900	C	-3.44999400	1.85907100	2.74585200
C	5.21456700	0.10568700	1.00144500	C	-2.72643600	1.64685100	1.56500200
H	3.25839200	0.62669300	0.23523300	H	-0.23453000	-0.29776100	2.82085600
C	6.03460100	-0.92513200	1.47306200	H	-1.49683300	0.09099800	4.89600100
H	6.17715400	-3.03936000	1.88917300	H	-3.57429200	1.47116700	4.87053300
H	5.59873200	1.11954400	0.92983200	H	-4.34815100	2.47371500	2.72181400
H	7.06060400	-0.71673300	1.76381900	H	-3.07330100	2.11421000	0.64703100
C	-2.13500000	-2.34248700	-0.49891100	H	0.46863700	6.07401300	-1.36365900
C	-3.31869000	-1.66889900	-0.16096600	C	0.26457100	5.04097000	-1.09258400
C	-2.18135000	-3.44039000	-1.37578600	C	1.01833000	4.40704200	-0.09914900
C	-4.53746000	-2.11987300	-0.66788200	C	-0.76316100	4.33450300	-1.72300500
H	-3.27304700	-0.81545200	0.50559600	C	0.75574000	3.07715900	0.25238100
C	-3.40466200	-3.87069900	-1.89284300	H	1.81149600	4.95172300	0.41003400
H	-1.25822200	-3.92197000	-1.68701100	C	-1.02582700	3.00229800	-1.36681100
C	-4.58730400	-3.21757000	-1.53422400	H	-1.36784400	4.81700800	-2.48878000
H	-5.45224800	-1.60436200	-0.38793600	C	-0.26156200	2.34268700	-0.38261800
H	-3.42951800	-4.70818800	-2.58510200	H	1.34317100	2.61560400	1.04281700
H	-5.53929600	-3.55292900	-1.93698400	H	-1.85135200	2.48403200	-1.85360800
O	0.93461100	1.45083600	-3.56845200	B	1.44107400	0.32358300	-2.99049600
O	2.47000200	-0.36194600	-3.59144700	O	0.93239500	-0.16814800	-1.80539100

IMPh5 thermal Free Energies = -1492.395323 A.U.

O	-6.57814100	-1.31580500	-2.64292400	C	0.79250100	3.09318000	-0.46070400
O	-5.62648000	-3.03256700	-1.30836600	Pd	0.71913200	0.15036800	0.15484000
H	-4.29735500	-1.15454100	-0.37999600	C	1.65644700	-1.61332900	0.39511200
H	-6.53543300	-0.36480000	-2.81908800	C	2.16405700	2.65458700	-0.66128500
H	-6.24244700	-3.57944900	-1.81716500	C	2.46934500	-1.84612200	1.51764900
N	2.47216700	1.40271300	-0.55507800	C	3.23139600	-3.01648800	1.62996100
N	-0.12350600	2.24032500	-0.13461000	C	3.19274900	-3.98527600	0.62250800
H	2.90801800	3.40634500	-0.93649600	C	2.37871000	-3.77434400	-0.49474300
H	0.56157200	4.14791800	-0.62927800	C	1.61511400	-2.60455500	-0.60099100
C	-1.44708300	2.69594900	0.07634700	H	2.51064500	-1.11412900	2.32125300
C	-2.50962100	1.89644300	-0.37157900	H	3.85211900	-3.17172700	2.51063400
C	-1.71626700	3.90901300	0.73751200	H	3.78086900	-4.89586800	0.71120700
C	-3.82484400	2.32832500	-0.20364400	H	2.32938000	-4.52378200	-1.28301600
H	-2.29415600	0.94850800	-0.85114300	H	0.98169300	-2.47301000	-1.47669900
C	-3.03534500	4.32375500	0.91975200	H	-4.13890900	-2.28998400	2.55550800
H	-0.89997200	4.49853500	1.14626300	C	-3.24184600	-1.86571300	2.11040400
C	-4.09181700	3.54065000	0.44137700	C	-2.55720600	-0.82542300	2.74612900
H	-4.63227100	1.69470600	-0.55742700	C	-2.74751000	-2.36728900	0.89978200
H	-3.23763100	5.25161500	1.44850600	C	-1.39504700	-0.29171800	2.17496800
H	-5.11860400	3.86450200	0.58982000	H	-2.92376600	-0.42952100	3.69143700
C	3.82571500	1.01673000	-0.71910800	C	-1.58079800	-1.82918100	0.33672000
C	4.87803300	1.77055100	-0.16823900	H	-3.25295600	-3.19621400	0.40698600
C	4.10989800	-0.15562700	-1.43567200	C	-0.88629400	-0.77433800	0.95386700
C	6.19946100	1.36647700	-0.35988000	H	-0.88471100	0.51594500	2.69608300
H	4.65907800	2.64143100	0.44371900	H	-1.20960600	-2.25898600	-0.58967500
C	5.43451100	-0.53948100	-1.63977200	B	-5.69379100	-1.70646200	-1.66219500
H	3.29202300	-0.75100200	-1.82352800	O	-4.89611900	-0.77613300	-1.05157600
C	6.48261700	0.21687900	-1.10465800	H	5.64622500	-1.44355000	-2.20376500
H	7.00663400	1.94310400	0.08421300	H	7.51248000	-0.09783200	-1.25015200

IMF4 thermal Free Energies = -1228.758138 A.U.

C	-2.11348300	-3.29745000	0.04074900	H	5.38614000	-0.76507600	-2.39995000
Pd	-1.11143200	-0.40659300	-0.16559700	C	3.31103400	0.07213800	0.20709700
C	-1.61281000	1.52139100	-0.20659100	H	3.87723900	1.38902600	1.80899000
C	-3.22184900	-2.39711000	0.33235800	H	3.09839100	-1.16117900	-1.55651700
C	-0.99338300	2.42469200	0.66384300	B	1.84302500	-0.24261000	0.81340500
C	-1.37589300	3.77382600	0.62799500	O	1.44185400	0.61935900	1.90017800
C	-2.35011700	4.21435300	-0.27162000	O	0.82989500	0.08871700	-0.44885400

C	-2.95151800	3.30293000	-1.14508500	O	1.56009300	-1.62301700	1.13992000
C	-2.58754300	1.95071600	-1.11414900	H	1.16505500	0.06677200	2.64483300
H	-0.21787000	2.08698200	1.34722200	H	0.93478800	1.01689500	-0.71656100
H	-0.89895900	4.47784700	1.30603500	H	2.18419000	-2.22894400	0.71896300
H	-2.63669000	5.26275600	-0.29690700	N	-0.98731300	-2.72768000	-0.20685100
H	-3.70610300	3.63818900	-1.85307300	N	-2.98850100	-1.13234900	0.20803900
H	-3.06686000	1.25301300	-1.79582700	H	-4.19905600	-2.76179600	0.63428400
H	6.93993500	0.72806100	-1.14864400	H	-2.24175100	-4.37697100	0.03042600
C	5.93493500	0.54626600	-0.77375000	F	-0.01365600	-3.65969300	-0.52257100
C	5.50210600	1.15279900	0.40965000	F	-4.11945600	-0.38267400	0.51658000
C	5.06191700	-0.29320900	-1.47423300	H	6.17295600	1.81017800	0.95971400
C	4.20844200	0.91518900	0.88795000	C	3.77038000	-0.51959400	-0.98703400

IMF4' thermal Free Energies = -1228.759572 A.U.

C	0.00213100	1.74203500	1.47466400	Pd	0.30670900	-0.08390100	-0.29142400
H	-1.42160800	1.59967000	3.10217900	N	0.78609300	-1.93348300	-1.13051300
C	-0.83449300	2.73167700	-0.57490000	N	2.37756600	-2.00225400	1.22431300
H	-2.88789700	3.37257200	-0.53683900	C	2.22562500	-3.02608500	0.46948400
C	0.26360000	2.16795300	0.13971000	C	-1.58084500	-0.72009100	-0.08288800
H	0.83219200	1.38730400	2.08278200	C	1.56702800	-2.90780500	-0.83192200
H	-0.65675700	3.06550300	-1.59340200	C	-1.97998900	-1.38553900	1.08200300
B	1.83194500	2.24316200	-0.43139500	C	-3.29035600	-1.86884000	1.20127000
O	2.27542900	0.77115000	-0.58836000	C	-4.20334300	-1.69416300	0.15704200
O	1.79702100	2.91125000	-1.70619200	C	-3.79933400	-1.03869600	-1.00977900
O	2.77023900	2.77018300	0.55322900	C	-2.48974000	-0.55475900	-1.13351400
H	2.90177400	0.57251300	0.12693300	H	-1.28498400	-1.52244500	1.90729500
H	2.67390400	2.89469700	-2.11619700	H	-3.59398000	-2.37842100	2.11346000
H	2.77746800	3.73699000	0.54449200	H	-5.22009200	-2.06768500	0.25072500
H	2.59605100	-4.00715000	0.76512600	H	-4.50057400	-0.90168800	-1.83026300
H	1.72292900	-3.69835000	-1.56302400	H	-2.19052200	-0.05215200	-2.04969800
F	3.01246700	-2.41839900	2.40995300	H	-3.26116400	2.66035900	1.81499200
F	0.30028000	-2.11524000	-2.43537900	C	-2.28795300	2.51098800	1.35356600
C	-2.07541100	2.91336100	0.02180500	C	-1.25974200	1.91566100	2.07458200

IMF4'TS thermal Free Energies = -1228.750873 A.U.

C	1.87494300	-1.41974600	1.19529100	Pd	-0.31869000	0.00655200	-0.42609800
H	3.81390800	-1.43226100	2.14144800	N	-1.76239300	1.44455300	-0.98826400
C	1.86920600	-1.69021800	-1.20628400	N	-3.64321100	-0.21548600	0.44048900
H	3.80333500	-1.90360400	-2.14285900	C	-3.71870400	1.05918900	0.37236100
C	1.12754900	-1.53481900	-0.00301500	C	0.87750400	1.50589700	0.16996700
H	1.33540800	-1.29418000	2.13001300	C	-2.94980600	1.78662900	-0.64373400
H	1.33553700	-1.78083000	-2.15149100	C	0.74482900	2.01697900	1.46861500
B	-0.44335500	-2.56904900	0.16304000	C	1.51973700	3.10860100	1.88454400
O	-1.32850400	-1.88420400	-0.83529400	C	2.43779200	3.69499800	1.00838600
O	-0.10996900	-3.91178700	-0.16145300	C	2.57740700	3.18248400	-0.28496600
O	-0.93766000	-2.43340000	1.49184500	C	1.80264200	2.09219000	-0.70301700
H	-2.22447300	-1.82106800	-0.45993300	H	0.04802400	1.56290400	2.17081400
H	-0.02963600	-4.05341800	-1.11411600	H	1.40754000	3.49344400	2.89632500
H	-0.89456100	-3.29022700	1.94046100	H	3.04137400	4.53973100	1.33160900
H	-4.38786000	1.62537600	1.02048900	H	3.29235200	3.62811000	-0.97377300
H	-3.40257300	2.66289100	-1.10501000	H	1.92808100	1.70657800	-1.71163600
F	-1.32622200	2.31167100	-2.01024100	H	5.04520100	-1.74682300	0.00599800
F	-4.48293400	-0.66416100	1.47126500	C	3.95935000	-1.68205600	0.00141000
C	3.26094300	-1.77109500	-1.20942800	C	3.26586800	-1.50715300	1.20510200

IMF5' thermal Free Energies = -1228.8085 A.U.

Pd	-0.01822500	-0.17030300	-0.25237000	C	-0.54157800	4.10611500	-0.35158400
N	0.07867000	-2.30964300	-0.81352800	C	0.32066900	2.20037300	1.49555400
N	2.10377300	-2.56626100	1.17199600	H	0.76044500	3.87401900	2.78307900
C	1.22708700	-3.46962800	0.94400500	C	-0.61089700	2.74006200	-0.66335600

C	-2.01072700	-0.25237600	-0.02436400	H	-0.88584900	4.84112600	-1.07631200
C	0.44521100	-3.42578700	-0.29552700	C	-0.16540300	1.76443500	0.24830500
C	-2.59154400	-0.38310100	1.24748200	H	0.66191100	1.47515300	2.23122900
C	-3.97358500	-0.56579100	1.38997700	H	-1.03069700	2.43977900	-1.62057000
C	-4.80049500	-0.60543400	0.26338900	B	3.18837200	0.84872600	-0.90099200
C	-4.23383000	-0.45978300	-1.00643700	O	2.29433500	-0.07835300	-0.38483100
C	-2.85107900	-0.28239000	-1.14872200	O	2.75951600	2.04654000	-1.38191200
H	-1.97224000	-0.32956700	2.13971400	O	4.51650300	0.50776300	-0.92560700
H	-4.40298600	-0.66472400	2.38522900	H	2.69048200	-0.85176300	0.05520800
H	-5.87405700	-0.73925100	0.37396100	H	1.82104800	2.23688700	-1.19815000
H	-4.86663500	-0.48128300	-1.89167700	H	5.07097500	1.22280600	-1.27123000
H	-2.43552400	-0.17263400	-2.14799700	H	1.07553400	-4.29905000	1.63465400
H	-0.00115100	5.57998200	1.13341000	H	0.15881700	-4.36452800	-0.76683800
C	-0.04762200	4.52181400	0.88772000	F	-0.59996700	-2.58002900	-2.01630000
C	0.37905000	3.56263800	1.81257300	F	2.71273700	-2.81550500	2.41471500

IMF5 thermal Free Energies = -1228.808494 A.U.

H	-2.32110500	3.14046000	-3.13520300	C	-1.35825600	-2.97644300	-1.28980400
C	-0.40190400	2.41479900	0.15843600	Pd	0.27626600	-0.45531600	-0.66065900
H	-0.98240600	4.40266100	0.75795500	C	1.95990400	0.32876600	0.09614700
C	-0.46342300	1.41519300	-0.82999200	C	-0.09265200	-3.48007900	-0.77005700
H	-1.24253500	0.95713100	-2.80475700	C	2.99927700	0.73889500	-0.75123300
H	0.14920900	2.23971200	1.07723300	C	4.23419000	1.13296900	-0.21862400
B	-2.41714300	-0.12602700	2.81158600	C	4.43889400	1.13339400	1.16405300
O	-2.76170500	0.17126200	1.52395500	C	3.39930000	0.74053900	2.01254400
O	-3.36845800	-0.63458500	3.67018500	C	2.16344300	0.34454200	1.48423200
O	-1.13358200	0.05442200	3.27306800	H	2.85527600	0.76187900	-1.82838100
H	-2.05327000	0.58027400	0.99488200	H	5.03179500	1.44801000	-0.88854500
H	-4.24093200	-0.68276300	3.25268500	H	5.39603400	1.44381500	1.57653300
H	-1.05478800	-0.16933800	4.21200400	H	3.54535500	0.74413900	3.09108300
N	0.78655600	-2.59043800	-0.45807300	H	1.36206900	0.05746900	2.16099100
N	-1.45965300	-1.69738900	-1.40188100	H	-2.21366300	4.88262400	-1.35508900
H	0.09333200	-4.54388000	-0.64875000	C	-1.72766900	3.92074400	-1.20987100
H	-2.16953700	-3.64628400	-1.56285900	C	-1.78743400	2.94266500	-2.20780100
F	1.94418500	-3.18912200	0.03371100	C	-1.03728300	3.65008600	-0.02587800
F	-2.71109200	-1.34489800	-1.90729100	C	-1.16864500	1.70242300	-2.0160170

Cl thermal Free Energies = -460.392104 A.U.

Cl	0.00000000	0.00000000	0.00000000	

3 thermal Free Energies = -1468.603969 A.U.

C	4.30692900	1.43280900	0.79225400	C	1.62171700	2.17311000	0.00555100
C	5.28111200	-0.65785800	-0.78777800	N	2.03638300	0.94803700	-0.03034000
H	3.21704300	-0.99610300	-1.34055400	Pd	0.22345900	-0.46358700	-0.01442800
C	5.67003200	1.14272300	0.78395600	C	-1.47834700	-1.49749000	-0.02369300
H	3.92161600	2.21074700	1.44576200	C	0.19774100	2.44392000	0.04412000
C	6.16288300	0.10393600	-0.01451100	N	-0.66049300	1.46852500	0.06401000
H	5.65604000	-1.47719600	-1.39473200	Cl	1.33578100	-2.50720100	-0.08375700
H	6.34556500	1.71752100	1.41193100	C	-2.30813200	-1.43682700	-1.14959600
H	7.22593700	-0.12160400	-0.01769500	C	-3.52812400	-2.12630600	-1.16363600
C	-2.04452500	1.81066300	0.06054600	C	-3.92667200	-2.87662300	-0.05371500
C	-2.89876400	1.23577300	1.01129800	C	-3.09064700	-2.94734300	1.06555200
C	-2.55104600	2.71789000	-0.88376500	C	-1.86394500	-2.27088200	1.07833500
C	-4.24482300	1.59824600	1.03590300	H	-2.01324200	-0.86139200	-2.02398700
H	-2.50311600	0.51679500	1.71892100	H	-4.16301900	-2.07550700	-2.04591600
C	-3.90536300	3.05697500	-0.86435800	H	-4.87261600	-3.41292400	-0.06594300
H	-1.89579900	3.12123100	-1.65122600	H	-3.38155400	-3.54564000	1.92672900
C	-4.75370400	2.50504100	0.09961600	H	-1.20606200	-2.36814700	1.93717800
H	-4.90098400	1.15686700	1.78077200	H	2.31036400	3.02124500	-0.00355300
H	-4.29630200	3.74543500	-1.60880900	H	-0.13885800	3.48109900	0.08009400

H	-5.80773600	2.76866200	0.11308300	C	3.42189600	0.67472500	0.00088500
				C	3.91246400	-0.39075500	-0.77200000

5 thermal Free Energies = -1239.926515 A.U.

H	1.35321700	2.53893900	1.14064100	Pd	-0.53261600	0.38180100	-0.11214600
H	-1.81575400	2.57351600	-1.78360500	N	-0.94493100	-1.88203500	-0.07813800
B	1.65559100	0.55596900	-2.77519500	N	1.99709200	-1.76044400	0.24542200
O	0.93774300	-0.13300200	-1.81124900	C	1.21064300	-2.58627800	0.83212900
O	1.21024500	1.73103700	-3.29532300	C	-1.59030100	0.80766000	1.53871800
O	2.83795100	0.00535800	-3.20419500	C	-0.17020300	-2.80273200	0.38284300
H	1.44999300	-0.81601700	-1.31826700	C	-1.16620000	0.24313900	2.75514900
H	0.48734300	2.12175900	-2.77199400	C	-1.89677700	0.42251900	3.93484100
H	3.25979800	0.59107600	-3.84930700	C	-3.07319100	1.17417400	3.92687500
H	1.53742300	-3.20702100	1.67542900	C	-3.50375000	1.75101900	2.73068300
H	-0.53766300	-3.83024100	0.47970400	C	-2.76584500	1.57809900	1.55443200
C	3.33612900	-1.59657800	0.66192300	H	-0.25217500	-0.34678500	2.79191100
C	4.10293800	-2.61736400	1.25090800	H	-1.54291300	-0.02573600	4.86143500
C	3.91920100	-0.34159500	0.42390200	H	-3.64265000	1.31461500	4.84239600
C	5.42113800	-2.36740500	1.62438700	H	-4.41264100	2.34931800	2.71153700
H	3.68469800	-3.61138900	1.37959600	H	-3.10989100	2.05948300	0.64273400
C	5.23141400	-0.09462300	0.81935400	H	0.53897400	6.10780900	-1.11406200
H	3.32294100	0.42873400	-0.05372200	C	0.31925500	5.06707600	-0.88985000
C	5.98595100	-1.10493500	1.42085500	C	1.05569300	4.38188900	0.07964700
H	6.01313700	-3.16366200	2.06701900	C	-0.70896200	4.40309300	-1.55976000
H	5.66862000	0.88444600	0.64638600	C	0.77515700	3.04292900	0.37003400
H	7.01453100	-0.91627500	1.71475800	H	1.85148900	4.89372700	0.61732100
C	-2.19073100	-2.30003600	-0.63071900	C	-0.99222000	3.06160800	-1.26450700
C	-3.36191500	-1.59205800	-0.32355600	H	-1.29923900	4.92635000	-2.30929800
C	-2.24636000	-3.39437700	-1.51027900	C	-0.24525000	2.34977000	-0.30408000
C	-4.57732400	-2.00496800	-0.86581600	H	-1.32957100	-3.90280900	-1.79494100
H	-3.30909600	-0.74576300	0.35120400	C	-4.63564600	-3.09702800	-1.73605100
C	-3.46538400	-3.78479600	-2.06267100	H	-5.48381300	-1.46361000	-0.61004200
H	-5.58525100	-3.40202100	-2.16667600	H	-3.49653300	-4.62015700	-2.75666600

PhB(OH)$_3$ thermal Free Energies = -484.168617 A.U.

O	2.10954200	-0.75878100	-1.17172700	C	-0.83030900	1.20778300	-0.00009500
B	1.58110600	-0.01807800	0.00000200	C	-2.20708900	-1.20903700	0.00002800
O	2.03669000	1.40709800	-0.00082900	H	-0.25549700	-2.12257900	0.00002200
H	3.00478300	1.37080000	-0.00067800	C	-2.23269800	1.20267000	-0.00004000
O	2.10939300	-0.75733400	1.17272300	H	-0.29510000	2.15532500	-0.00017700
H	1.81886500	-0.28394500	1.96430800	C	-2.93162600	-0.00916300	0.00002000
H	1.81920600	-0.28632800	-1.96394100	H	-2.73731600	-2.16237000	0.00006700
C	-0.07351000	0.01983500	-0.00006800	H	-2.78187500	2.14542200	-0.00005100
C	-0.80845600	-1.18424900	-0.00000500	H	-4.02145900	-0.02083800	0.00005500

B(OH)$_3$ thermal Free Energies = -252.496383 A.U.

B	0.00002800	-0.00004100	0.00000000	H	-1.84166100	-0.66921300	0.00002600
O	1.33852800	-0.30560500	-0.00000300	O	-0.40457400	1.31193900	-0.00002100
H	1.50069700	-1.26017800	0.00001500	H	0.34106900	1.92963400	-0.00003800
O	-0.93398400	-1.00633900	0.00002300				

PhB(OH)$_2$F thermal Free Energies = -508.223891 A.U.

H	-0.30231100	2.14118100	-0.11582700	H	-4.02056100	-0.03633000	0.05562700
H	-0.25631700	-2.13683600	0.01941000	C	-2.93112900	-0.02423900	0.02872200
B	1.56656700	-0.01179500	-0.03327800	C	-2.23431700	1.18715200	-0.02656600
O	2.12335300	-0.48047700	1.26218900	C	-2.20557600	-1.22296300	0.04477300
O	2.05527500	-0.89405600	-1.08360700	C	-0.83273500	1.19209200	-0.06327200
H	2.09276900	0.25831800	1.88618900	H	-2.78386800	2.12924200	-0.04532300
H	2.96924900	-1.11648400	-0.85089300	C	-0.80756900	-1.19801200	0.00908700
F	2.03322000	1.37265000	-0.22063400	H	-2.73441400	-2.17609600	0.08410200

				C	-0.07623900	0.00570200	-0.04438400

$B(OH)_2F$ thermal Free Energies = -276.529534 A.U.

B	-0.01638700	0.01665200	0.00000300	O	-1.37311400	-0.02357300	0.00000500
H	-1.71873600	-0.92808900	-0.00000900	O	0.73423600	-1.12592600	-0.00000900
F	0.58034100	1.22254400	-0.00000300	H	1.68862900	-0.96207400	0.00006200

4_F_1 thermal Free Energies = -1516.40996 A.U.

C	1.42514300	-2.87187700	0.83457900	Pd	0.10040300	-0.55601400	-0.44579800
H	3.12711400	1.05902900	1.20576400	C	-1.56528800	0.42964200	-0.89552000
H	1.86309400	0.94541300	-1.59385200	C	-0.01039700	-3.07844700	0.94091800
N	1.86087200	-1.88658500	0.12405200	C	-2.41345700	0.89679400	0.11218600
N	-0.83558900	-2.26044000	0.36044800	C	-3.59252600	1.57269400	-0.22670000
H	-0.37869800	-3.96105600	1.46479800	C	-3.92738900	1.78072400	-1.56752900
H	2.09411900	-3.59267700	1.31093400	C	-3.06795800	1.32652000	-2.57276100
C	-2.23234900	-2.51713200	0.47826500	C	-1.88080200	0.66098500	-2.23902700
C	-3.03451800	-2.45159000	-0.66921000	H	-2.15979300	0.76120700	1.16011600
C	-2.80271500	-2.83049400	1.72231300	H	-4.23926500	1.94789200	0.56313700
C	-4.39482400	-2.73984400	-0.57478000	H	-4.84138300	2.30932300	-1.82734100
H	-2.58736100	-2.17667600	-1.61746600	H	-3.30964900	1.50134000	-3.61925800
C	-4.17023800	-3.09592900	1.80924900	H	-1.20666800	0.34083000	-3.02991200
H	-2.18895300	-2.81952500	2.61895200	H	-1.96031300	5.83371100	1.77023700
C	-4.96721000	-3.06023000	0.66119500	C	-1.24578200	5.07527900	1.45582000
H	-5.01231100	-2.69531800	-1.46733100	C	-0.64178400	4.23882800	2.39926600
H	-4.61284400	-3.31708000	2.77660600	C	-0.91887000	4.93149400	0.10234500
H	-6.03216100	-3.26370100	0.73163400	C	0.28110000	3.26962500	1.98646000
C	3.24492200	-1.66847400	-0.03688500	H	-0.88387200	4.34603100	3.45558900
C	4.15532800	-1.81181200	1.02432600	C	0.00077600	3.95716200	-0.29513900
C	3.70451700	-1.27915700	-1.30495800	H	-1.38287800	5.57808100	-0.64039200
C	5.51360500	-1.58124100	0.80630300	C	0.62326400	3.10248500	0.63332300
H	3.79232900	-2.04471600	2.02131700	H	0.75638500	2.62841100	2.72543000
C	5.06634700	-1.07331800	-1.51903300	H	0.23966200	3.85366900	-1.35167300
H	2.98980800	-1.17280900	-2.11602200	B	1.73247800	2.02932400	0.17479300
C	5.97404500	-1.21934100	-0.46453200	O	2.16491500	1.15347400	1.24406100
H	6.21155000	-1.66879100	1.63448600	O	1.11744500	1.16415400	-1.01099400
H	5.41742800	-0.78250000	-2.50498800	H	7.03208800	-1.03499300	-0.62768600
F	2.86868400	2.61811300	-0.47435800				

$4'_F$_1 thermal Free Energies = -1516.402717 A.U.

H	1.65471300	-3.60569600	0.85237300	Pd	-0.40480900	0.21214800	-0.28477500
H	-0.70019900	-3.79133600	0.32590400	N	-1.06431500	-1.78302800	0.09413600
C	3.22256300	-1.54481800	0.33530500	N	1.83793600	-1.64889600	0.12783700
C	3.91397800	-2.21586400	1.36535900	C	1.17813900	-2.69800600	0.46128400
C	3.92282900	-0.68273400	-0.53031500	C	-0.80145400	0.75777200	1.59123800
C	5.28998800	-2.04579300	1.50408300	C	-0.27243600	-2.78597000	0.28105400
H	3.37309800	-2.83463200	2.07647500	C	0.06895300	0.38862900	2.62682600
C	5.30387100	-0.53877100	-0.39414900	C	-0.19873200	0.76478500	3.94993400
H	3.37354700	-0.14920900	-1.30416300	C	-1.34517400	1.50423700	4.25625700
C	5.99069800	-1.21618800	0.61888100	C	-2.21820700	1.87051600	3.22795800
H	5.81661300	-2.55110000	2.30958200	C	-1.94804000	1.50094100	1.90299700
H	5.84230100	0.11625800	-1.07389900	H	0.97021600	-0.17944300	2.41061200
H	7.06397900	-1.08696900	0.73161200	H	0.49385800	0.47930200	4.73941600
C	-2.43717400	-2.06848800	-0.18716300	H	-1.55401600	1.79337200	5.28338900
C	-3.44246700	-1.47654700	0.58985600	H	-3.11340200	2.44799000	3.45121300
C	-2.77429100	-2.92905600	-1.24292300	H	-2.63385100	1.80651400	1.11694300
C	-4.77911700	-1.77380500	0.32486200	H	-0.70357700	5.07735500	1.00079000
H	-3.16796200	-0.80425400	1.39498000	C	-0.46580800	4.25564200	0.32923100
C	-4.11724000	-3.20398600	-1.51072700	C	0.75605400	3.59529400	0.44130600
H	-1.99146100	-3.33891600	-1.87471900	C	-1.39524300	3.85607100	-0.64416300
C	-5.12209900	-2.63390600	-0.72485400	C	1.06547600	2.54925300	-0.43951100

H	-5.55630900	-1.32601200	0.93844100	H	1.47133100	3.89423000	1.20349700
H	-4.37489400	-3.85519200	-2.34163400	C	-1.08900300	2.81106100	-1.51097500
H	-6.16634500	-2.84863300	-0.93494300	H	-2.34899000	4.37284000	-0.72675800
F	0.10543800	1.62032300	-3.92627300	C	0.16731400	2.13867800	-1.46189900
O	0.04418000	-0.21199500	-2.37743800	H	2.04747100	2.08576200	-0.39676400
O	2.08634600	0.97525000	-2.79424900	H	-1.79195300	2.53607800	-2.29367400
H	0.74735200	-0.87206300	-2.48218100	B	0.64178800	1.14334600	-2.70386700
H	2.41197300	1.41902900	-3.58987200				

4'TS$_{F}$_1 thermal Free Energies = -1516.388439 A.U.

O	0.81006400	-0.05470800	-2.35781400	C	0.83810000	-2.92347200	-0.07906200
H	2.50166500	2.65508500	-2.79005200	Pd	-0.30368600	0.21721800	-0.45424600
H	0.19183500	-0.32428300	-3.05485100	C	-1.19915500	0.73909900	1.25489500
N	-1.27209700	-1.72423700	-0.38767500	C	-0.60870800	-2.82990000	-0.28654400
N	1.52518600	-1.96694800	0.42920000	C	-0.68423500	0.26588800	2.47143400
H	-1.13391300	-3.78277200	-0.39865100	C	-1.33399100	0.54532600	3.68102900
H	1.28598100	-3.88763100	-0.35445900	C	-2.50787300	1.30489400	3.69300000
F	0.06658000	2.00828400	-3.23730300	C	-3.02383700	1.78465300	2.48569900
C	2.92029200	-2.07440400	0.53931800	C	-2.37158800	1.50829700	1.27643000
C	3.72475300	-2.69690300	-0.43501100	H	0.22476300	-0.33095800	2.47936600
C	3.52883200	-1.47697200	1.65828400	H	-0.91881300	0.16849200	4.61423600
C	5.10855800	-2.74578000	-0.26868700	H	-3.01201500	1.52328800	4.63156400
H	3.27091800	-3.09019700	-1.34022100	H	-3.93398300	2.38160800	2.48039200
C	4.90987500	-1.55376900	1.82976000	H	-2.78906100	1.89989100	0.35202600
H	2.90041300	-0.97211300	2.38595600	H	1.74382500	5.37908700	1.30464000
C	5.70470600	-2.18739800	0.86744400	C	1.44676300	4.47297800	0.78099400
H	5.72491200	-3.20805000	-1.03533500	C	2.22286500	3.31199700	0.89283500
H	5.36921900	-1.10495800	2.70652800	C	0.29028300	4.46603200	-0.00574100
H	6.78352900	-2.22730700	0.99147800	C	1.83962100	2.15592700	0.21446000
C	-2.68921900	-1.79545200	-0.50602700	H	3.12163600	3.31474200	1.50586700
C	-3.44528200	-2.70232800	0.25465900	C	-0.08947700	3.29784100	-0.67068600
C	-3.33784900	-0.91756500	-1.38745200	H	-0.31438800	5.36603500	-0.09369200
C	-4.83244300	-2.74845300	0.10712800	C	0.67789400	2.11155500	-0.59967200
H	-2.95583300	-3.33155000	0.99258600	H	2.46858600	1.27191900	0.28751800
C	-4.72163500	-0.98343300	-1.54329800	H	-0.98609800	3.31184500	-1.28486600
H	-2.74659300	-0.19354100	-1.94047700	B	1.03701800	1.37922800	-2.45582600
C	-5.47390600	-1.89875000	-0.79870900	O	2.36972400	1.69982100	-2.71023800
H	-5.41258900	-3.43860800	0.71382400	H	-6.55417600	-1.93550700	-0.90977400
H	-5.21453900	-0.30930700	-2.23854200				

5'$_{F}$_1

C	0.97899900	-2.44767100	0.86669600	Pd	-0.49917500	0.48955100	-0.30234600
C	3.70370600	-0.24033400	0.90511800	C	-1.10704700	1.00949300	1.53093900
C	5.24298300	-2.54985800	1.24604100	C	-0.43724400	-2.56830400	0.50044100
H	3.45669800	-3.64183300	0.73635000	C	-0.21850800	0.99680000	2.61876700
C	5.04678400	-0.13842900	1.26469400	C	-0.67031000	1.25336300	3.92002700
H	3.09315900	0.64604600	0.76309900	C	-2.01936200	1.53399700	4.15798200
C	5.82262200	-1.29090900	1.43438400	C	-2.91092900	1.55800400	3.08141800
H	5.84527500	-3.44854200	1.35286100	C	-2.45776000	1.30187700	1.78012400
H	5.49171500	0.84355200	1.40187300	H	0.83720700	0.79358400	2.45763500
H	6.87373900	-1.20845300	1.69729000	H	0.03811900	1.24127200	4.74656900
C	-2.51470800	-1.88511000	-0.29581700	H	-2.36944900	1.73836100	5.16721200
C	-3.35333800	-2.51268800	0.63769900	H	-3.96347200	1.77912800	3.24977800
C	-3.03131300	-1.46935700	-1.53265500	H	-3.17152600	1.32992400	0.95965800
C	-4.69456600	-2.74390900	0.32248100	H	1.05886700	6.01439300	-1.80075100
H	-2.97000300	-2.77125800	1.62073800	C	0.77049000	5.01707700	-1.47686000
C	-4.36630900	-1.72221800	-1.84516400	C	1.70900400	3.98395800	-1.44818800
H	-2.37644400	-0.96760200	-2.23800900	C	-0.54446000	4.75519700	-1.07439100
C	-5.20314100	-2.35874800	-0.92062000	C	1.32956300	2.70029100	-1.02432700
H	-5.34364900	-3.21311100	1.05722600	H	2.73936900	4.17167800	-1.74521300

H	-4.75679900	-1.41295600	-2.81110600	C	-0.91675200	3.47455900	-0.65173300
H	-6.24714700	-2.53852200	-1.16273400	H	-1.28370100	5.55414000	-1.08492400
N	-1.14324700	-1.62297200	-0.01343000	C	0.00560900	2.41037000	-0.62779900
N	1.74631100	-1.53926400	0.38991500	H	2.09437500	1.92467700	-0.98880400
H	-0.89315400	-3.54433100	0.69831600	H	-1.94079800	3.30715500	-0.32855100
H	1.33888800	-3.20323600	1.57905200	B	1.17324600	-0.86250800	-2.92479200
F	2.41157400	-0.51721700	-3.34189900	O	0.79268200	-2.16486400	-2.88675000
C	3.10709600	-1.50425600	0.74997300	O	0.27325900	0.10622700	-2.57764400
C	3.89276700	-2.66172900	0.91087300	H	1.49894500	-2.76865600	-3.15782000
				H	0.60919900	1.01871300	-2.66165100

4$_{F}$**_2** thermal Free Energies = -1516.413845 A.U.

B	2.07590300	1.70589300	-0.24349100	C	0.57404600	-3.42316400	-0.48509900
O	1.27152100	0.88430500	0.80628100	Pd	-0.09004600	-0.59178600	0.22298100
O	3.44936300	1.59873400	0.22425200	C	-1.51853600	0.64577200	0.83431900
H	1.92630800	0.53483500	1.43173000	C	-0.85591600	-3.23908200	-0.64555300
H	3.87471100	2.46462800	0.26120800	C	-2.31370800	0.27459400	1.92449500
N	1.31798400	-2.40311600	-0.20532600	C	-3.31907200	1.13730700	2.38201600
N	-1.40931000	-2.08785900	-0.41188700	C	-3.53501500	2.36439300	1.74850700
H	-1.45480900	-4.07452600	-1.00987800	C	-2.73209800	2.73276500	0.66467000
H	0.98808000	-4.41997600	-0.65255300	C	-1.71704700	1.88068100	0.21003500
C	-2.81810000	-1.97414700	-0.61432900	H	-2.16173600	-0.67856600	2.42573600
C	-3.31789900	-0.90464900	-1.36899300	H	-3.93078300	0.84501200	3.23312400
C	-3.69453200	-2.92752000	-0.07369400	H	-4.31519100	3.03327700	2.10386300
C	-4.68807600	-0.81443900	-1.60908600	H	-2.87626900	3.69448200	0.17774300
H	-2.63360100	-0.16215700	-1.76303400	H	-1.07735300	2.20069900	-0.60641600
C	-5.06731700	-2.81533500	-0.30201200	H	0.41222700	6.97762500	-0.68304800
H	-3.30754500	-3.72549000	0.55444700	C	0.72405900	5.93884800	-0.59586600
C	-5.56663300	-1.76420600	-1.07589600	C	0.90569500	5.35971100	0.66513000
H	-5.07104000	0.01029900	-2.20337100	C	0.94719200	5.16932700	-1.74192200
H	-5.74462500	-3.54425400	0.13473300	C	1.30587500	4.02380500	0.77005500
H	-6.63531500	-1.67654600	-1.25107800	H	0.72970300	5.94768200	1.56408600
C	2.70439400	-2.57298800	-0.00090800	C	1.34877500	3.83327900	-1.62191100
C	3.23046700	-3.72352900	0.62313100	H	0.81069100	5.60993200	-2.72797700
C	3.56196100	-1.54393300	-0.42112100	C	1.53627700	3.22498900	-0.36669000
C	4.60646100	-3.84553700	0.79864900	H	1.42527100	3.58531000	1.75964900
H	2.56404200	-4.48904600	1.01158300	H	1.51836200	3.24380200	-2.52037300
C	4.93927500	-1.68628900	-0.25161400	H	5.59329200	-0.88329000	-0.57754700
H	3.14807300	-0.65501500	-0.88320400	H	6.53814300	-2.92860900	0.49721300
C	5.46534700	-2.83159100	0.35260400	F	1.89662700	0.99589200	-1.48138800
H	5.00925400	-4.72226800	1.29891300				

4'$_{F}$**_2** thermal Free Energies = -1516.392642 A.U.

Pd	-0.34571500	0.21898900	-0.22621200	N	-0.98931500	-1.79405600	0.08314500
C	3.27444500	-1.42025100	0.43545700	N	1.88952300	-1.53930700	0.24579000
C	3.97960200	-2.11093100	1.44119000	C	1.28062400	-2.65183100	0.42502500
C	3.95545300	-0.53488000	-0.42181200	C	-0.92466500	0.73860000	1.59088500
C	5.35566500	-1.92854100	1.57363800	C	-0.16596600	-2.77776000	0.22112500
H	3.44591500	-2.75209600	2.13822600	C	-0.14185000	0.37893100	2.69492200
C	5.33654500	-0.38502000	-0.29524000	C	-0.54849400	0.73112200	3.98896800
H	3.39497100	-0.00834400	-1.19316600	C	-1.74150400	1.43270800	4.18814800
C	6.03920500	-1.07371600	0.70033700	C	-2.52340200	1.78657700	3.08449800
H	5.89440000	-2.44657900	2.36296500	C	-2.11743600	1.44282900	1.78750000
H	5.86466400	0.28230600	-0.97130400	H	0.79006500	-0.16269000	2.55564600
H	7.11228600	-0.93617200	0.80536000	H	0.07194700	0.45531700	4.83925000
C	-2.34629700	-2.10634500	-0.24563600	H	-2.05742600	1.70245100	5.19288000
C	-3.38655300	-1.66018800	0.58067400	H	-3.45268200	2.33475100	3.22653100
C	-2.62867400	-2.84748300	-1.40283300	H	-2.72991400	1.73572500	0.93879500
C	-4.70463800	-1.98412300	0.25817700	H	-0.86898200	4.99178300	1.00811200
H	-3.15598300	-1.07532800	1.46405500	C	-0.59181600	4.18910000	0.32874000

C	-3.95409000	-3.14998400	-1.72404700	C	0.58515800	3.48048400	0.53127400
H	-1.81780000	-3.14090300	-2.06347000	C	-1.43195800	3.86349800	-0.75342300
C	-4.99414700	-2.72620300	-0.89281600	C	0.94822000	2.45598200	-0.36595200
H	-5.50933700	-1.64963800	0.90755600	H	1.23300800	3.71942900	1.37091000
H	-4.17039600	-3.70970500	-2.63008300	C	-1.07901500	2.84785800	-1.63301000
H	-6.02441900	-2.96287900	-1.14428400	H	-2.35341600	4.42161200	-0.90649300
F	0.29724100	-0.26490000	-2.28421500	C	0.14256300	2.12638300	-1.49055300
H	0.34138100	0.90372000	-4.64067300	H	1.92146400	1.98217100	-0.26660400
H	2.50015500	1.77312100	-3.32255800	H	-1.70565600	2.62579600	-2.49241300
H	1.80276600	-3.58388700	0.67619000	B	0.70677300	1.14757400	-2.70208400
H	-0.55718700	-3.79832700	0.18378000	O	0.05599800	1.49682600	-3.93003800
				O	2.15909000	1.06614200	-2.75734500

4'TS$_F$_2 thermal Free Energies = -1516.380696 A.U.

Pd	-0.47508200	0.14586800	-0.29835500	O	-0.05396500	2.56162900	-3.39568100
N	-0.77239300	-2.00454200	-0.17263400	O	1.77604600	1.68939900	-2.19559700
N	2.10054300	-1.52838300	-0.10970000	H	-1.00261300	2.51277900	-3.57105900
C	1.58181000	-2.69929000	-0.08195200	H	2.15321800	2.44584300	-2.66828500
C	-0.67744200	0.42237100	1.65997200	H	2.18350900	-3.61553700	-0.01607500
C	0.13692500	-2.92063100	-0.18400700	H	-0.17133800	-3.96730600	-0.26768700
C	0.37523600	0.05020300	2.50848200	C	3.48377200	-1.33716900	0.02501100
C	0.25268600	0.19001200	3.89735300	C	4.32112400	-2.17840900	0.78612200
C	-0.92229400	0.70093400	4.45661400	C	4.02495600	-0.20776400	-0.61714500
C	-1.97054000	1.08134300	3.61393100	C	5.68517900	-1.90486200	0.87481600
C	-1.84846000	0.94988700	2.22378500	H	3.90059200	-3.01450400	1.33858000
H	1.29686800	-0.34367200	2.09047800	C	5.39545600	0.04005400	-0.54149600
H	1.08157100	-0.10096500	4.53988600	H	3.35292100	0.43923900	-1.17557500
H	-1.01655600	0.80850200	5.53453500	C	6.22866600	-0.80329100	0.20205700
H	-2.88663100	1.49298100	4.03341900	H	6.32444500	-2.54495200	1.47760500
H	-2.66698000	1.27396600	1.58763300	H	5.81342500	0.90285300	-1.05371600
H	-1.76092600	5.67639500	0.74687100	H	7.29312400	-0.59524400	0.27324200
C	-1.41347100	4.72492500	0.35016500	C	-2.12274800	-2.42823600	-0.37961700
C	-0.09336200	4.31614900	0.56886300	C	-3.11330600	-2.05376700	0.53988000
C	-2.28919900	3.90971000	-0.37961700	C	-2.46058000	-3.20111300	-1.50130900
C	0.34881100	3.09631300	0.05468000	C	-4.42747900	-2.47931200	0.34720000
H	0.58254400	4.94657400	1.14238000	H	-2.84220100	-1.44646900	1.39663800
C	-1.83383500	2.69272100	-0.88448200	C	-3.78405600	-3.60554500	-1.69398500
H	-3.31657100	4.22671500	-0.54666800	H	-1.69840600	-3.44545300	-2.23615100
C	-0.49512700	2.25167400	-0.70599900	C	-4.76945900	-3.25274600	-0.76858900
H	1.37904300	2.79082000	0.21707500	H	-5.18903200	-2.20038100	1.07071800
H	-2.52538600	2.07227800	-1.45461700	H	-4.04256200	-4.18970300	-2.57330000
B	0.38529000	1.67303200	-2.40021200	H	-5.79808000	-3.56910900	-0.91914500
F	-0.14110200	0.32961700	-2.52880400				

5'$_F$_2

O	2.00047100	0.18673200	-3.28594900	Pd	-0.42685000	0.35173400	-0.24664800
O	1.95668100	-2.18563700	-3.20910900	N	-1.59717300	-1.48101300	0.33007000
H	1.54654700	0.98116700	-2.94432800	N	1.23993100	-1.80883600	0.72899700
H	2.79590700	-2.07046600	-3.67828100	C	0.35176300	-2.47911700	1.37217200
H	0.60743200	-3.13509800	2.21402700	C	-1.06803800	1.54727300	1.23132600
H	-1.66601400	-3.30344600	1.31127700	C	-1.05836900	-2.45295100	0.98773500
C	2.57380900	-1.80725100	1.17626200	C	-0.73804800	1.20864900	2.55277300
C	2.92360700	-1.73446000	2.53676800	C	-1.24919900	1.93918700	3.63133000
C	3.58685200	-1.83695200	0.20274100	C	-2.09809300	3.02469300	3.40832800
C	4.26578300	-1.70984000	2.91161000	C	-2.42292900	3.37865300	2.09754100
H	2.14407800	-1.65415800	3.28920900	C	-1.90516100	2.65390600	1.01815500
C	4.92452900	-1.83786600	0.58821700	H	-0.07701700	0.36832700	2.75222500
H	3.30091100	-1.89166300	-0.84285000	H	-0.98028400	1.65741800	4.64754400
C	5.26938500	-1.77084600	1.94170400	H	-2.49548500	3.59264600	4.24583200
H	4.52830600	-1.63521100	3.96341100	H	-3.07348700	4.23023400	1.90883500

H	5.70218800	-1.87753500	-0.16949600	H	-2.15054900	2.96370900	0.00626500
H	6.31441700	-1.75102000	2.23785400	H	2.96177100	4.70411200	-2.38794100
C	-2.94335000	-1.62076500	-0.10173300	C	2.31940700	3.93721000	-1.96261800
C	-3.80109200	-0.51255700	-0.02635100	C	2.69558400	3.26736600	-0.79526200
C	-3.41569900	-2.83286400	-0.63381900	C	1.10597800	3.61687100	-2.57319600
C	-5.12514100	-0.63431000	-0.44279200	C	1.87036200	2.28153200	-0.24667900
H	-3.42374000	0.41981200	0.37873800	H	3.63628200	3.51473100	-0.30776600
C	-4.73722000	-2.93719300	-1.06424400	C	0.27622000	2.63019100	-2.01842600
H	-2.73517100	-3.67101400	-0.75258800	H	0.79546500	4.13671600	-3.47724300
C	-5.59833000	-1.84234500	-0.96246000	C	0.65036500	1.93029100	-0.85278100
H	-5.78861600	0.22252500	-0.36596100	H	2.18053700	1.77972900	0.66584400
H	-5.08973900	-3.87221400	-1.49087400	H	-0.67455400	2.41221100	-2.50182200
H	-6.62788000	-1.92600400	-1.29900900	B	1.40190600	-0.97155400	-2.93582900
F	0.20221300	-0.99293000	-2.29875200				

PhB(OH)$_2$O^{t}Bu thermal Free Energies = -641.297878 A.U.

H	5.07478900	-1.09902900	-0.19733900	C	4.04545000	-0.74534500	-0.14410400
H	-0.41816400	2.72293800	0.06984200	C	3.00646700	-1.62582500	0.17948700
O	-1.07138100	-0.33273600	-0.35976200	C	3.73868600	0.59475800	-0.40871100
C	-2.46782300	-0.43687600	-0.18455500	C	1.68614100	-1.16206500	0.24033100
C	-2.97709900	-1.29716600	-1.35969800	H	3.22627400	-2.67589400	0.37634400
H	-2.44381500	-2.25600200	-1.37686800	C	2.41276600	1.03941900	-0.33940300
H	-4.05635300	-1.49527200	-1.28185900	H	4.53529100	1.29111000	-0.67379300
H	-2.77969800	-0.78526700	-2.30937800	C	1.34506800	0.18279000	-0.00893300
C	-3.20254400	0.92155900	-0.20128400	H	0.88469300	-1.86368400	0.46725500
H	-2.90337700	1.53188300	0.65583100	H	2.18300200	2.07986400	-0.56393400
H	-2.95367200	1.47714000	-1.11032900	B	-0.20039900	0.75423400	0.15382300
H	-4.29137300	0.76309900	-0.15840600	O	-0.45473800	1.09404500	1.60141100
C	-2.77502700	-1.16388200	1.14674400	O	-0.40746800	2.01547600	-0.58932200
H	-2.27471000	-2.14129800	1.16244500	H	0.07013800	0.51437100	2.16950900
H	-2.39899000	-0.56778700	1.98400600	H	-3.85585700	-1.32581500	1.27969500

B(OH)$_2$O^{t}Bu thermal Free Energies = -409.639226 A.U.

B	1.45900800	-0.14491900	-0.00000100	H	-2.22755900	1.23576000	-1.31669700
O	2.51374900	-1.03853600	0.00000000	C	-1.21987900	0.80588700	1.26958800
O	1.62478800	1.23362400	0.00000000	H	-2.22756800	1.23573400	1.31671600
H	2.53953800	1.54425200	0.00000600	H	-1.07240400	0.18554400	2.16135100
H	3.39623000	-0.64725200	-0.00000500	H	-0.49531600	1.62480400	1.28836800
O	0.22459600	-0.70507200	-0.00000200	C	-2.08304100	-1.19200200	-0.00001200
C	-1.06744900	-0.04355000	0.00000000	H	-1.94833500	-1.82036100	-0.88706600
C	-1.21987300	0.80590700	-1.26957500	H	-1.94834000	-1.82037500	0.88703300
H	-0.49530500	1.62482100	-1.28834100	H	-3.10720000	-0.80148700	-0.00001100
H	-1.07240100	0.18557800	-2.16134700				

4$_{OtBu}$_1 thermal Free Energies = -1649.489281 A.U.

N	-2.30379900	-1.83060700	0.34156300	C	-0.55419000	-3.38815400	0.81398200
H	-2.65487600	-3.56098700	1.43711800	Pd	-0.71242100	-0.70052900	-0.44268600
H	-0.28652200	-4.34352500	1.27194400	C	-1.79931700	0.88996600	-0.92524800
C	-3.67047300	-1.44359300	0.46846900	C	-1.93045100	-2.93306300	0.91746000
C	-4.37854600	-1.05471000	-0.67659300	C	-2.36772500	1.69416500	0.06646000
C	-4.30291800	-1.45341800	1.72157300	C	-3.14662900	2.80113600	-0.29422400
C	-5.72711800	-0.71900300	-0.56972700	C	-3.36084800	3.10617400	-1.64123700
H	-3.86946000	-1.01940200	-1.63278400	C	-2.77609300	2.30944400	-2.63080200
C	-5.64782100	-1.09275000	1.82071700	C	-1.98606600	1.20822800	-2.27515900
H	-3.73317700	-1.69694600	2.61425700	H	-2.19598100	1.48390000	1.11878400
C	-6.36496300	-0.73424500	0.67566300	H	-3.57389600	3.42985600	0.48370600
H	-6.27589500	-0.42658000	-1.46040500	H	-3.96390000	3.96758800	-1.91821000
H	-6.12920900	-1.08081000	2.79477200	H	-2.92029100	2.54968100	-3.68237400
H	-7.41093000	-0.45107100	0.75507800	H	-1.51330900	0.61496300	-3.05430800
C	1.62070300	-3.12389100	-0.02356300	H	0.13346200	5.92638000	1.82351400

C	2.34400500	-3.71169200	1.02990500	C	0.46886200	4.94032200	1.50771800
C	2.23164400	-2.94246000	-1.27442600	C	0.75039200	3.95114500	2.45466800
C	3.65634500	-4.13379100	0.81768100	C	0.61887500	4.64635200	0.14729200
H	1.89768900	-3.78918900	2.01742000	C	1.18419300	2.68576400	2.03887400
C	3.53431500	-3.39055300	-1.48411200	H	0.63399000	4.16493500	3.51615400
H	1.66690000	-2.47319200	-2.07417000	C	1.05122900	3.37857800	-0.25130400
C	4.25106400	-3.98501200	-0.44011000	H	0.39355100	5.40446900	-0.60078600
H	4.21984200	-4.56637200	1.63990900	C	1.35336800	2.36620500	0.67929200
H	3.99766300	-3.25728000	-2.45742800	H	1.39450600	1.91998800	2.78208400
H	5.27464700	-4.31216700	-0.59984400	H	1.15085400	3.16420800	-1.31337500
C	4.43867700	1.34954300	-0.13612400	B	1.88194600	0.90577800	0.21301000
C	4.52662200	2.81533300	-0.60336700	O	1.74774900	-0.04951100	1.31089600
C	4.71863400	1.26091700	1.37579300	O	0.93305500	0.44127900	-0.98605600
C	5.47691100	0.51059600	-0.90182900	O	3.17111100	0.78824400	-0.48201400
H	4.29753000	2.88228900	-1.67363300	H	2.39618200	-0.75509500	1.17576400
H	3.81613600	3.44678200	-0.06383300	H	1.52460900	0.00120800	-1.61913800
H	5.53680600	3.21390900	-0.44102000	N	0.28690900	-2.68891900	0.12873600
H	4.68986200	0.21958300	1.71852200	H	5.42545300	-0.53900400	-0.58810000
H	5.71381800	1.66596300	1.60071600	H	5.27683500	0.55533000	-1.97924800
H	3.98049300	1.82840400	1.94967100	H	6.49504300	0.87899000	-0.72330100

4'$_{OtBu}$ _1 thermal Free Energies = -1649.484838 A.U.

Pd	-0.10488100	-0.42992800	0.20425400	C	-1.33730500	0.06364300	3.87578800
N	-0.35612300	-1.36585300	-1.70082600	C	0.83643100	0.72223800	2.25690300
N	2.15475400	0.09960200	-1.56581100	H	2.03831500	-0.37938100	3.68733100
C	1.86446000	-0.72032800	-2.51072400	C	-1.53547700	0.81284300	2.72414900
C	0.33264600	-2.17914200	1.06015600	H	-2.18162600	-0.18583600	4.51564500
C	0.52545400	-1.29789200	-2.64328900	C	-0.45005400	1.20430000	1.88853100
C	1.57481500	-2.78900700	0.83513300	H	1.70386100	1.07763600	1.70632900
C	1.88046700	-4.02302700	1.42530700	H	-2.52730400	1.17774500	2.47244900
C	0.94384600	-4.66773400	2.23880100	B	-0.62066100	2.33409200	0.67306200
C	-0.29776500	-4.06537900	2.46351200	O	-0.64735700	1.51536300	-0.62616100
C	-0.60074800	-2.82774800	1.88000200	O	-1.83567900	3.06519900	0.93698200
H	2.32145700	-2.30187600	0.21229900	O	0.59569200	3.15764100	0.53149500
H	2.85388700	-4.47663000	1.24856000	H	0.09000900	1.82559800	-1.17566800
H	1.18004100	-5.62620200	2.69467900	H	0.50115000	3.97179600	1.04393000
H	-1.03502100	-4.55409400	3.09776700	H	2.57156700	-0.99502600	-3.30347700
H	-1.56468200	-2.36688800	2.08237500	H	0.27763700	-1.70928800	-3.62563900
H	0.10657900	-0.93992100	5.14403200	C	3.44237400	0.63780700	-1.41079600
C	-0.04219400	-0.36166700	4.23515700	C	4.62157600	-0.00084400	-1.84754100
C	1.03721300	-0.04706400	3.42407200	C	3.52540700	1.87481100	-0.74247300
H	-3.98075700	-4.11954600	-1.08694600	C	5.85818300	0.60801200	-1.64430500
H	-4.16137500	-1.24218000	-4.28697700	H	4.57502400	-0.98359800	-2.30896400
H	-5.20792100	-3.09827100	-2.99798500	C	4.76796400	2.48376900	-0.56389300
C	-2.63509700	3.81569200	0.02164500	H	2.61353200	2.34520500	-0.37818500
C	-1.79367600	4.67844500	-0.93920500	C	5.93470700	1.85631500	-1.01259000
C	-3.53848700	2.85875200	-0.78161800	H	6.76565500	0.10508300	-1.96840500
C	-3.50666800	4.73284500	0.89642900	H	4.82448500	3.44485200	-0.05993000
H	-1.13807300	5.35788400	-0.38235200	H	6.90214000	2.32646200	-0.85666300
H	-1.16678300	4.06093300	-1.58922500	C	-1.66237600	-1.82860200	-2.04925500
H	-2.45093700	5.28626100	-1.57455000	C	-2.26010600	-2.85288000	-1.30166800
H	-4.15206600	2.26054700	-0.09724700	C	-2.34929400	-1.25004400	-3.12826500
H	-4.21097400	3.41788600	-1.44621700	C	-3.52676800	-3.31452700	-1.65862000
H	-2.93249700	2.17475100	-1.38209300	H	-1.72440400	-3.28290900	-0.46305900
H	-4.20068900	5.32373000	0.28533400	C	-3.62526000	-1.70723800	-3.46404200
H	-4.08999000	4.13354800	1.60492300	H	-1.90461700	-0.41742400	-3.66589100
H	-2.87790900	5.42104400	1.47374200	C	-4.21452600	-2.74426900	-2.73612700

4'TS$_{OtBu}$ _1 thermal Free Energies = -1649.475906 A.U.

C	5.49092600	-3.17442200	-0.62657000	Pd	-0.50670000	-0.11256200	0.17455900

H	3.70627100	-3.84061200	-1.60985800	N	-0.93832800	-1.62912800	-1.29019400
C	5.38111700	-1.01420200	0.45910300	N	2.05740000	-1.70570800	-0.97581300
H	3.48703500	0.02178300	0.30737400	C	1.28843000	-2.68772800	-1.27802000
C	6.10615600	-2.15889700	0.11673900	C	-1.44908300	-1.11407900	1.63769100
H	6.05829000	-4.05305400	-0.92261700	C	-0.10212500	-2.51396700	-1.71679000
H	5.85752800	-0.21280000	1.01743200	C	-0.89167800	-2.32153100	2.09149900
H	7.14909200	-2.25398600	0.40733100	C	-1.52272500	-3.08493400	3.08269500
C	-2.19534500	-1.54612100	-1.97067000	C	-2.73051900	-2.65464700	3.64026700
C	-3.39070700	-1.56432300	-1.23907800	C	-3.29393800	-1.45291500	3.20118900
C	-2.22766200	-1.42858400	-3.36927800	C	-2.65735100	-0.68853500	2.21390800
C	-4.60990900	-1.49734500	-1.91339900	H	0.05058000	-2.67742900	1.67797200
H	-3.35374900	-1.64242600	-0.15875900	H	-1.06669400	-4.01446200	3.41878700
C	-3.45406200	-1.34359500	-4.03235000	H	-3.22233400	-3.24460500	4.41011000
H	-1.29685900	-1.36012800	-3.92568700	H	-4.22984400	-1.10069500	3.63140500
C	-4.64817600	-1.38485200	-3.30795200	H	-3.11062400	0.24803800	1.90081700
H	-5.53471100	-1.52752000	-1.34343300	H	-0.84904500	2.67045300	5.13250400
H	-3.47229800	-1.23447100	-5.11348600	C	-0.61597100	2.35912500	4.11637600
H	-5.60203400	-1.31840100	-3.82429100	C	0.48316800	1.52713100	3.87479600
C	0.44709500	4.06524300	-1.64386200	C	-1.41352200	2.79383100	3.05060200
C	1.76597500	3.89825100	-2.41892800	C	0.77810300	1.13745600	2.56790100
C	-0.74025600	3.55368100	-2.47977400	H	1.09991900	1.18407000	4.70262000
C	0.23647800	5.54581000	-1.29177300	C	-1.10727200	2.39329600	1.75064900
H	2.61526500	4.24368200	-1.81845100	H	-2.26413900	3.44581300	3.23817000
H	1.94002600	2.85226000	-2.68804600	C	0.00575900	1.56523000	1.45775700
H	1.73866300	4.48918800	-3.34342700	H	1.64756800	0.50927900	2.39093400
H	-1.67550300	3.67952900	-1.92118000	H	-1.71319300	2.76463700	0.92859000
H	-0.82489000	4.11563800	-3.41911800	B	1.00910600	2.09219100	-0.13003700
H	-0.61939500	2.49280700	-2.71470600	O	0.72330800	1.07774000	-1.16290000
H	0.15460900	6.15817700	-2.19834800	O	0.47741100	3.38215000	-0.37722700
H	-0.68061000	5.66821700	-0.70457700	O	2.39254900	1.99833000	0.24114600
H	1.07481100	5.92007400	-0.69285400	H	1.47212500	0.45894300	-1.25784800
H	-0.44022900	-3.23974700	-2.46398400	H	2.66105600	2.80159400	0.70838500
C	3.41416700	-1.91583000	-0.63913500	H	1.63422200	-3.72952400	-1.28651700
C	4.15492400	-3.05879700	-1.00397600	C	4.04668300	-0.88030100	0.07190900

5'$_{OtBu}$_1

Pd	-0.32897000	-0.46257600	0.41429900	H	1.71072500	-1.82705200	-3.30612200
N	-1.02009700	-0.81408000	-1.71525000	H	-0.66429400	-1.38302900	-3.67070900
N	1.90317800	-0.30879200	-1.88924700	C	3.31720800	-0.33144900	-1.88824600
C	1.22608800	-1.10227400	-2.64065300	C	4.09520000	-0.74586800	-2.98693600
C	-0.63501800	-2.33982300	1.05260500	C	3.95505100	0.13077700	-0.72438000
C	-0.23904500	-1.09060900	-2.70431000	C	5.48629300	-0.73096600	-2.90108500
C	0.10092000	-3.37501000	0.44987800	H	3.62094000	-1.04301200	-3.91791100
C	-0.13835300	-4.71795400	0.77056900	C	5.34747000	0.12418300	-0.64141200
C	-1.11967700	-5.05504100	1.70715300	H	3.35141600	0.49043800	0.10220200
C	-1.84855700	-4.03513500	2.32647400	C	6.11760700	-0.30778500	-1.72524200
C	-1.60151500	-2.69290100	2.00980600	H	6.07993700	-1.03917800	-3.75781500
H	0.87584100	-3.14249200	-0.27821400	H	5.82990400	0.47093200	0.26830200
H	0.44739800	-5.49900900	0.28883300	H	7.20253300	-0.29814100	-1.66376200
H	-1.30613200	-6.09652600	1.95867200	C	-2.41516600	-0.72243100	-1.98410500
H	-2.60562100	-4.28047000	3.06917200	C	-3.32793300	-1.31956100	-1.10054500
H	-2.16186900	-1.91869100	2.52742500	C	-2.88820300	-0.01196000	-3.10129200
H	1.59035100	0.98814600	5.82439500	C	-4.69604800	-1.23479900	-1.35858700
C	1.23014700	0.68955000	4.84245800	H	-2.95435900	-1.85962500	-0.23780000
C	2.07365400	0.01496600	3.95421700	C	-4.26055500	0.08269200	-3.33950000
C	-0.08668200	0.96140300	4.45958900	H	-2.18523100	0.50101400	-3.75206300
C	1.60556100	-0.37604200	2.69366900	C	-5.16857700	-0.53469900	-2.47426000
H	3.09604600	-0.21920600	4.24614900	H	-5.39584200	-1.71529300	-0.68002500
C	-0.55077800	0.56738400	3.19755100	H	-4.61834100	0.64908800	-4.19542500
H	-0.75860300	1.47541300	5.14488700	H	-6.23657800	-0.46130600	-2.66129600

C	0.29143700	-0.08998100	2.28301100	C	-1.38151400	4.11493100	0.15656200
H	2.27357700	-0.92271100	2.03200100	C	-1.53848000	4.18973000	-1.36899300
H	-1.58464900	0.77895700	2.93183100	C	-2.30882800	3.05738100	0.76583600
B	0.78498300	2.77855800	0.09487200	C	-1.64603000	5.48633200	0.78958500
O	0.31156700	1.67966300	-0.60014300	H	-0.84277800	4.92577500	-1.78946500
O	0.00133500	3.82012400	0.49303900	H	-1.34496800	3.21825400	-1.83254900
O	2.13428900	2.83533000	0.36973600	H	-2.55845300	4.49800400	-1.62781800
H	1.02252900	1.12469600	-1.00665700	H	-2.15026900	2.99289300	1.84729400
H	2.36071300	3.64143400	0.85643700	H	-3.35646300	3.32702600	0.58532900
H	-1.49376900	5.44185200	1.87353800	H	-2.12999000	2.07030500	0.33002000
H	-0.96345900	6.23813700	0.37755200	H	-2.67571100	5.80801600	0.59542000

4$_{OtBu}$ **_2** thermal Free Energies = -1649.487421 A.U.

C	-1.96860500	3.10513400	0.26350500	H	-2.27878400	4.14087000	0.41876300
Pd	-0.71797800	0.45231200	-0.40945100	C	-3.69060300	-0.14538400	0.51513900
C	-1.12117200	-1.39711200	-1.01177200	C	-3.38854300	-1.27667100	1.28417800
C	-2.94764000	2.06317900	0.49602500	C	-4.99008100	0.04570800	0.02118000
C	-1.97963400	-1.57908000	-2.10213400	C	-4.39584100	-2.19230600	1.58439200
C	-2.28723300	-2.87470100	-2.53977000	H	-2.37698700	-1.42374600	1.64379400
C	-1.74489100	-3.98591900	-1.88755900	C	-5.98640600	-0.88893600	0.30979500
C	-0.88061800	-3.79618600	-0.80485700	H	-5.20700900	0.89817300	-0.61697800
C	-0.55843200	-2.50377100	-0.37042500	C	-5.69433600	-2.00549000	1.09772500
H	-2.41448600	-0.72592500	-2.61756800	H	-4.16037700	-3.06257300	2.19051200
H	-2.95185400	-3.00966100	-3.39068900	H	-6.98656100	-0.74716000	-0.09076400
H	-1.98569500	-4.99056200	-2.22682000	H	-6.46963100	-2.73337600	1.32045300
H	-0.43638300	-4.65330400	-0.30308000	C	0.15904500	3.81724900	-0.39059300
H	0.14329900	-2.35874100	0.44437500	C	-0.24716900	5.02221200	-1.00234700
H	5.50631000	-4.45589400	-1.68695800	C	1.51435300	3.60690100	-0.09208900
C	4.89144900	-3.63030600	-1.33479100	C	0.69061000	6.01577400	-1.27223800
C	3.59906700	-3.44376700	-1.83481100	H	-1.28077200	5.16009500	-1.30757400
C	5.38570600	-2.73536300	-0.38140100	C	2.44045300	4.61845300	-0.35169200
C	2.81304800	-2.37879400	-1.38050400	H	1.85226300	2.66503800	0.32910700
H	3.20314400	-4.12562900	-2.58545400	C	2.03675900	5.82271500	-0.93528500
C	4.58656400	-1.67569000	0.06273300	H	0.37516000	6.93424000	-1.76018100
H	6.39133800	-2.86104500	0.01600400	H	3.48487100	4.44929300	-0.10521400
C	3.27433300	-1.46580400	-0.41188500	H	2.76633200	6.59966000	-1.14802900
H	1.81805500	-2.24500700	-1.79349600	C	1.88215500	-0.65121600	2.63218800
H	5.00235500	-0.99940200	0.80919200	C	2.15943600	-2.15669900	2.81973100
B	2.37225400	-0.19892200	0.10510200	C	3.09109800	0.17268200	3.11468400
O	1.26589900	0.08633300	-0.99118800	C	0.64918300	-0.25598300	3.46619800
O	1.52325400	-0.37083700	1.27961700	H	1.28344400	-2.74662100	2.52367900
O	3.19128400	1.01918000	0.18360200	H	3.00803500	-2.48275700	2.21217900
H	1.60046200	0.79500900	-1.56092500	H	2.38089600	-2.38284900	3.87107200
H	4.04023100	0.89563600	-0.26171900	H	2.92382300	1.24047400	2.94359700
N	-0.76179500	2.79067100	-0.08199900	H	3.25038900	0.00696300	4.18822100
N	-2.66898500	0.81825100	0.25158800	H	4.00754400	-0.10843700	2.58939000
H	-3.91754700	2.33947000	0.91116000	H	-0.23306400	-0.80937500	3.12299700
H	0.44442400	0.81560200	3.35647000	H	0.80211600	-0.47501900	4.53041300

4'$_{OtBu}$ **_2** thermal Free Energies = -1649.47571 A.U.

C	-3.02056400	-0.57173500	-1.83324300	Pd	0.43036400	0.21940000	0.34373900
C	-3.74817400	-0.14420900	-2.96507500	N	1.28962100	-0.24533000	-1.61058100
C	-3.70678500	-1.05608700	-0.70316000	N	-1.62250400	-0.51687000	-1.73014500
C	-5.13786000	-0.23461900	-2.97226000	C	-0.86784900	-0.52059600	-2.76720000
H	-3.23465800	0.29086400	-3.81816600	C	0.30209400	2.13338500	-0.23868200
C	-5.09794100	-1.16233200	-0.73328000	C	0.58849300	-0.45522700	-2.67819600
H	-3.13102200	-1.34347100	0.17612000	C	-0.80859300	2.58026200	-0.96878800
C	-5.81655300	-0.75543200	-1.86197600	C	-0.90682400	3.91687600	-1.37723200
H	-5.69579100	0.11091600	-3.83886600	C	0.10603600	4.82899900	-1.06926800
H	-5.62310500	-1.55139500	0.13519200	C	1.21097700	4.39448200	-0.33383500

H	-6.90130900	-0.82456900	-1.87369400	C	1.30436600	3.05994700	0.08350400
C	2.70577700	-0.39462000	-1.73409600	H	-1.61697300	1.89825700	-1.20590400
C	3.56064900	0.51805600	-1.10135700	H	-1.78463400	4.24176400	-1.93255700
C	3.25525900	-1.46288600	-2.46522200	H	0.03102800	5.86507800	-1.39036800
C	4.94267800	0.38681900	-1.23199400	H	2.00462300	5.09240200	-0.07397400
H	3.13345100	1.33639300	-0.53740900	H	2.15973900	2.76328900	0.68338200
C	4.63994600	-1.59523800	-2.57975900	H	-0.15181900	4.10898400	3.62129700
H	2.60327300	-2.21546000	-2.89918300	C	-0.22970300	3.07827100	3.28306100
C	5.48946000	-0.66776600	-1.97073200	C	-1.46099600	2.58642600	2.81797000
H	5.59455800	1.11089500	-0.75058500	C	0.89275100	2.25322800	3.29895600
H	5.05255200	-2.43555000	-3.13170300	C	-1.56757200	1.26571000	2.39943600
H	6.56726300	-0.77420400	-2.05751300	H	-2.32864600	3.24162100	2.79199100
C	0.69017600	-3.09994500	1.08477900	C	0.78098400	0.92245500	2.86959900
C	0.26961000	-4.10941000	2.16738300	H	1.84844700	2.63708800	3.64932400
C	-0.05070300	-3.42754400	-0.22143700	C	-0.46060500	0.37058500	2.43730200
C	2.21125300	-3.18670900	0.88789300	H	-2.52495800	0.87313000	2.06574900
H	0.75601600	-3.89680000	3.12191200	H	1.64677400	0.26643900	2.94873000
H	-0.81033600	-4.09257100	2.33093000	B	-0.68927100	-1.28909300	2.44200700
H	0.55595000	-5.11745100	1.84005800	O	0.40676400	-1.73214000	1.47558100
H	0.27585800	-2.77092200	-1.03343200	O	-0.54741900	-1.80364800	3.79980100
H	0.14340100	-4.46522200	-0.52318300	O	-2.00515800	-1.69304300	1.95881400
H	-1.12742600	-3.29557600	-0.08444600	H	0.14498400	-1.35318300	4.30038600
H	2.50296300	-4.18746500	0.54420400	H	-2.50675100	-2.01405400	2.72208000
H	2.55788100	-2.45842500	0.14878500	H	-1.25523600	-0.62612700	-3.78840900
H	2.72800600	-2.98500000	1.83341100	H	1.11346000	-0.61745000	-3.62320600

4'TS$_{OtBu}$_2 thermal Free Energies = -1649.471383 A.U.

Pd	0.46343900	0.19697300	0.02042100	H	3.38626300	3.96594100	1.24522200
N	0.82941400	-1.81683300	-0.76649400	C	0.45559600	2.18352800	0.88744900
N	-2.06668600	-1.37728900	-0.78414100	H	-1.31362400	2.99091800	-0.04459800
C	-1.50220400	-2.40989300	-1.29352600	H	2.40810100	1.74542800	1.72433800
C	0.69833100	0.96572200	-1.81705800	B	-0.53751200	1.31830500	2.29814200
C	-0.05903100	-2.63588200	-1.22656700	O	0.01884700	-0.03409200	2.20974600
C	-0.33070600	0.82226800	-2.76097200	O	-0.25277300	2.08609500	3.47413700
C	-0.19372400	1.33254300	-4.05903600	O	-1.93028400	1.38124300	1.99506100
C	0.97566500	1.99648400	-4.43962300	H	-2.30103100	2.16841100	2.42035400
C	2.00095900	2.15618700	-3.50359000	H	-2.06215500	-3.21577200	-1.78619600
C	1.86065500	1.65231500	-2.20374200	H	0.27034900	-3.60541500	-1.61143900
H	-1.25521100	0.32445000	-2.48632700	C	-3.44974600	-1.16315100	-0.88250200
H	-1.00918000	1.21239600	-4.77006900	C	-4.27360800	-1.72236400	-1.88287400
H	1.08234500	2.39193700	-5.44696400	C	-4.00934400	-0.29634900	0.07532800
H	2.91261100	2.68468700	-3.77652800	C	-5.63834000	-1.44380700	-1.89611200
H	2.66133300	1.82299700	-1.48907800	H	-3.84594000	-2.34013300	-2.66765700
H	2.00702000	5.71451300	0.13320500	C	-5.38143900	-0.04254000	0.06417000
C	1.58118300	4.73426200	0.33617800	H	-3.34917800	0.16451500	0.80680400
C	0.25939100	4.45614100	-0.03062500	C	-6.19929300	-0.61383500	-0.91595900
C	2.35729100	3.75066300	0.96385200	H	-6.26603700	-1.86421500	-2.67780100
C	-0.28339100	3.19843800	0.23354800	H	-5.81031600	0.61680800	0.81435200
H	-0.33818600	5.21826700	-0.52591600	H	-7.26501000	-0.40034600	-0.93156700
C	1.80026900	2.49803100	1.22237700	C	2.17032300	-2.30618700	-0.68315400
H	2.06258100	-0.86756100	3.67464600	C	3.23297000	-1.49273000	-1.10302000
H	1.03789000	0.12684400	4.73984700	C	2.43980600	-3.58716500	-0.17016400
H	1.13242100	-1.62794000	4.98383900	C	4.54166700	-1.97051500	-1.04092000
H	-2.24867400	-1.04458300	3.33672200	H	3.01868100	-0.50823700	-1.49972200
H	-1.45396100	-1.72014100	4.77900000	C	3.75513400	-4.05055900	-0.09603600
H	-1.49892400	0.03727600	4.52455900	H	1.62751200	-4.20110900	0.20796800
H	-0.02690800	-3.20179800	3.33312300	C	4.81050900	-3.24751200	-0.53607200
H	-0.78659200	-2.53490000	1.86939600	H	5.35549300	-1.33866800	-1.38682900
H	0.98440000	-2.50160100	2.05534700	H	3.95242700	-5.03588200	0.31813200
C	-1.40314600	-0.92812000	4.02098000	H	5.83370600	-3.60860400	-0.47689400

C	0.03169400	-2.40202000	2.58477500	H	0.68618700	2.28174600	3.58538400
C	1.11480400	-0.83537500	4.22490100	C	-0.06967700	-1.03351200	3.26434900

5'$_{OtBu}$_2

Pd	-0.30093800	-0.27741700	0.48080000	C	3.79319200	0.77986600	-1.40323000
N	-1.25529200	-0.60088400	-1.54836200	C	5.07203900	-1.16217600	-2.96173700
N	1.63327200	-0.14598700	-1.89609600	H	3.11328100	-1.97665500	-3.30720500
C	0.85068900	-0.59276400	-2.81156400	C	5.18059900	0.79791700	-1.54546400
C	-0.21144600	-2.23475000	0.93216400	H	3.28083700	1.50351300	-0.77682200
C	-0.59934600	-0.70066800	-2.65853800	C	5.82514100	-0.16834000	-2.32525800
C	0.58356100	-3.08058100	0.14204600	H	5.56975000	-1.93563800	-3.54118800
C	0.60387100	-4.46459600	0.36229000	H	5.76180200	1.55876200	-1.03093400
C	-0.16904400	-5.02979500	1.38029300	H	6.90788200	-0.16208900	-2.41935400
C	-0.95314600	-4.19562700	2.18272800	C	-2.67447100	-0.72236400	-1.62747000
C	-0.96690200	-2.81139500	1.96716300	C	-3.34610900	-1.49371100	-0.66570400
H	1.19961900	-2.66647100	-0.65169300	C	-3.41173100	-0.07388900	-2.63402900
H	1.22956000	-5.09853000	-0.26366900	C	-4.73201000	-1.63690600	-0.73415300
H	-0.15253900	-6.10337200	1.55278300	H	-2.77110400	-1.99068600	0.10734900
H	-1.54885800	-4.61812300	2.98983900	C	-4.80043200	-0.20872500	-2.68328700
H	-1.56191500	-2.18215000	2.62346100	H	-2.90454000	0.56651100	-3.35027000
H	2.23490800	0.90370900	5.71005400	C	-5.46530000	-0.99566900	-1.73840100
C	1.76789800	0.65213300	4.76069200	H	-5.24015400	-2.25127000	0.00441000
C	2.51246500	0.04906000	3.74399900	H	-5.36199500	0.31113700	-3.45520500
C	0.41121300	0.92047500	4.54747300	H	-6.54621000	-1.10047300	-1.77836600
C	1.90470200	-0.28139300	2.52403100	H	1.65649900	1.77156800	1.27119600
H	3.56581300	-0.17648400	3.89891400	C	-1.77853300	3.22730300	0.11118400
C	-0.18991900	0.59476200	3.32610700	C	-2.84886700	2.32213800	0.72669800
H	-0.18212500	1.38325400	5.33412600	C	-1.74170100	4.56505200	0.86586500
C	0.54590400	0.00102800	2.28094500	C	-2.02990500	3.43660100	-1.38744900
H	2.49733700	-0.77549400	1.75766800	H	-2.86809000	1.34181400	0.24270100
H	-1.24706100	0.81170600	3.18998000	H	-2.65829300	2.17445600	1.79469900
B	0.73414200	3.08046500	0.10987300	H	-3.83853300	2.77933600	0.61260400
O	-0.50773500	2.51614400	0.30182100	H	-1.00651500	5.25058400	0.43698600
O	1.84724500	2.53111900	0.68762800	H	-2.72684600	5.04352900	0.81428200
O	0.90366600	4.20307400	-0.67363800	H	-1.50013100	4.40073800	1.92238300
H	1.83181400	4.48020200	-0.67741700	H	-3.01330000	3.89672400	-1.54262500
H	1.22447400	-0.92530700	-3.78914000	H	-1.26830700	4.08614300	-1.82673800
H	-1.13842500	-0.94376700	-3.57963800	H	-2.01812600	2.47577000	-1.91168700
C	3.02773500	-0.19064200	-2.07575200	C	3.68329800	-1.17712600	-2.84213400

PhB(OH)$_2$CO$_3$ thermal Free Energies = -672.281764 A.U.

H	4.83936600	0.86313000	-0.00000600	H	1.74990100	-2.15369100	-0.00056700
C	3.78304100	0.58704700	-0.00000900	B	-0.57197700	-0.58405200	0.00006600
C	2.78645900	1.57219200	0.00023300	O	-0.82079900	-1.37845800	-1.23443500
C	3.39690700	-0.76115000	-0.00027800	O	-0.82080700	-1.37779600	1.23499100
C	1.43205900	1.20920800	0.00022400	H	-1.79217600	-1.47118700	-1.22602600
H	3.06878400	2.62779800	0.00042300	H	-1.79219100	-1.47043900	1.22660300
C	2.03863700	-1.10361000	-0.00029000	C	-2.77951200	0.59942700	-0.00013600
H	4.15988600	-1.54361900	-0.00049100	O	-3.40532500	1.69407200	-0.00055800
C	1.01345000	-0.13550600	-0.00002700	O	-3.30208400	-0.57416800	0.00037800
H	0.65798600	1.97446700	0.00037600	O	-1.40822500	0.67236900	-0.00024500

B(OH)$_2$CO$_3$ thermal Free Energies = -440.635451 A.U.

B	1.13484900	-0.10123500	-0.00000700	O	-0.06489100	-0.76375900	-0.00010200
O	2.28935000	-0.88477000	0.00002300	C	-1.35259200	-0.07835600	-0.00000900
O	1.26853000	1.26274800	0.00004200	O	-1.29068600	1.18577900	-0.00003600
H	0.31274300	1.58120700	-0.00000500	O	-2.31785500	-0.83941300	0.00007800
H	3.05297600	-0.28958300	0.00004900				

4$_{CO3}$_1 thermal Free Energies = -1680.48428 A.U.

H	2.77064200	0.18446300	2.11224900	C	-0.41180100	-3.38322300	0.72463000
H	1.96213700	0.71024500	-1.90232400	Pd	-0.52234800	-0.54298500	-0.20780800
N	0.48882400	-2.55244200	0.29788000	C	-1.58064100	1.10665000	-0.57496100
N	-2.14054500	-1.82211600	0.21574900	C	-1.79796300	-2.99390400	0.68048300
H	-2.55966800	-3.72210900	0.96399700	C	-2.46854300	1.62753200	0.37703300
H	-0.16988600	-4.39976100	1.04491800	C	-3.22808400	2.77192200	0.09922500
C	-3.53110400	-1.53646500	0.11933700	C	-3.11546100	3.40806100	-1.13992900
C	-4.03224500	-0.98726200	-1.06958600	C	-2.21910100	2.90332800	-2.08919700
C	-4.40316500	-1.79250800	1.18960200	C	-1.44582700	1.77185500	-1.80293000
C	-5.39788500	-0.73759900	-1.19710600	H	-2.57001300	1.15220700	1.35015600
H	-3.34223500	-0.75493200	-1.87302900	H	-3.90157800	3.16773100	0.85804000
C	-5.76759900	-1.52218800	1.05986700	H	-3.70216300	4.29887600	-1.35616400
H	-4.00571100	-2.16467200	2.13017800	H	-2.10023300	3.40616900	-3.04775100
C	-6.27112300	-1.00248500	-0.13595500	H	-0.71527800	1.42474200	-2.52759100
H	-5.77709700	-0.31372400	-2.12319500	H	1.17397600	6.11439800	2.30638900
H	-6.43285300	-1.70673800	1.90002400	C	1.35388100	5.10660800	1.93391400
H	-7.33217100	-0.78702200	-0.23415600	C	0.77883700	4.00074500	2.56942100
C	1.84595500	-2.91035400	0.26540800	C	2.16460200	4.89766800	0.81210900
C	2.41702300	-3.81681400	1.18217400	C	1.01698300	2.71006000	2.08205600
C	2.65214700	-2.31668600	-0.71887300	H	0.14352400	4.14517400	3.44370100
C	3.76929600	-4.13464000	1.09030500	C	2.39185200	3.59988400	0.33969300
H	1.82214000	-4.21871600	1.99789900	H	2.62387500	5.74755700	0.30738300
C	4.00327400	-2.64888300	-0.81151100	C	1.82667000	2.46607800	0.95519600
H	2.21119000	-1.58361800	-1.38258400	H	0.56383000	1.85927400	2.58881200
C	4.56403300	-3.55892200	0.08857800	H	3.03735400	3.46254700	-0.52556700
H	4.21279400	-4.81167300	1.81715000	B	2.04508000	0.93073700	0.39829600
H	4.62035800	-2.15220100	-1.55466800	O	2.06338500	-0.04643300	1.49341000
H	5.62408900	-3.79478800	0.03398200	O	1.07295100	0.55654700	-0.61529400
C	3.83218200	0.78305500	-1.51233500	O	3.47575200	0.90529100	-0.25136800
O	2.82803200	0.72873000	-2.42599800	O	5.00119300	0.70749100	-1.88268100

4'$_{CO3}$**_1** thermal Free Energies = -1680.490033 A.U.

Pd	-0.46153700	0.19628100	0.16835700	C	-1.21924200	-1.46913600	-2.30590900
N	-1.60990200	-0.55519700	-1.48445600	C	-0.43633400	-2.38645400	1.66203200
N	1.02065700	-1.68500200	-1.48777100	C	-0.97290900	-3.42896200	2.42993600
C	0.09605900	-2.11213600	-2.26515300	C	-2.30519400	-3.38355900	2.85302700
C	-1.21824000	-1.27604500	1.30403900	C	-3.09483200	-2.28390200	2.50074600
C	3.36092900	-1.39848000	-1.11599700	C	-2.55568200	-1.24396200	1.73161700
C	3.84739800	-4.11807400	-1.63649500	H	0.60452100	-2.43894400	1.35331700
H	1.71652700	-4.30470000	-1.89015900	H	-0.34344700	-4.27599600	2.69968700
C	4.66273800	-1.90192100	-1.08621600	H	-2.72111400	-4.19111100	3.45234400
H	3.15122000	-0.34632700	-0.90084800	H	-4.13266500	-2.23015800	2.82699000
C	4.91185000	-3.25460900	-1.34387100	H	-3.18866400	-0.39636300	1.47611000
H	4.03348100	-5.17614100	-1.80683200	H	0.06132800	0.14471200	5.08890400
H	5.48298400	-1.23040400	-0.84570200	C	0.30997100	0.49419000	4.08873600
H	5.92739200	-3.64146200	-1.30024900	C	1.51677800	0.08938700	3.48323400
C	-2.88542800	0.04866400	-1.67906700	C	-0.56167800	1.33002400	3.40542000
C	-2.97100700	1.45008000	-1.63526100	C	1.84267300	0.53319700	2.20964200
C	-4.03591600	-0.72502600	-1.89493500	H	2.19561200	-0.56762500	4.02457100
C	-4.20420900	2.06615100	-1.84599000	C	-0.22551600	1.78806400	2.11305500
H	-2.06744100	2.02829000	-1.45467500	H	-1.49456100	1.64625300	3.86744000
C	-5.26859200	-0.09448600	-2.08474700	C	0.99850500	1.42329100	1.48420500
H	-3.97122400	-1.80937100	-1.86790600	H	2.78680600	0.25034300	1.75084000
C	-5.35570900	1.30032000	-2.06874600	H	-0.84280800	2.55016600	1.64249900
H	-4.26389300	3.15115200	-1.82748300	B	1.52375500	2.20890500	0.11992100
H	-6.16154000	-0.69742400	-2.23137000	O	0.32353500	1.85349500	-0.92029800
H	-6.31587600	1.78849600	-2.21590500	O	1.50253700	3.62279300	0.35678900
C	2.24239300	4.55262500	-0.40928900	O	2.72095400	1.63531500	-0.42730200
O	3.15242500	4.06763600	-1.16115600	H	0.80451400	1.55476900	-1.70959100
O	1.92634900	5.74099200	-0.24845300	H	3.17088300	2.44411600	-0.82101600

C	2.29730500	-2.25970100	-1.45095500	H	0.24990300	-2.92058000	-2.99294100
C	2.54427000	-3.62695400	-1.69643100	H	-1.87398400	-1.76110100	-3.13285200

4'TS$_{CO3}$_1 thermal Free Energies = -1680.480196 A.U.

O	-2.73672800	-0.89195400	-1.00464600	Pd	0.44758700	-0.23639000	-0.11236100
H	-0.92827600	-0.49799700	-2.35831700	N	1.79551300	1.05090900	-1.18554400
H	-3.50695300	-1.54781800	-1.05144000	N	-0.72084600	2.41651500	-0.84956800
H	0.30562800	4.02429200	-1.71529400	C	0.31005200	2.98626700	-1.35317500
H	2.33741500	2.80239500	-2.12412600	C	1.22296400	0.41774700	1.62353600
C	-1.93579900	3.08493500	-0.65099400	C	1.56778800	2.26440400	-1.56117900
C	-2.04210900	4.47292900	-0.41938000	C	0.68582900	1.54138100	2.27567300
C	-3.09261100	2.28070200	-0.64701400	C	1.25910500	2.04198400	3.45214800
C	-3.29504800	5.04915900	-0.21779600	C	2.38847700	1.42865200	4.00447200
H	-1.14769400	5.08756400	-0.35588900	C	2.93192200	0.30745800	3.36932400
C	-4.34208700	2.87665800	-0.46733800	C	2.35331400	-0.19202500	2.19443300
H	-2.99100700	1.20232400	-0.79175000	H	-0.19780200	2.02916500	1.87142000
C	-4.44954500	4.25520400	-0.25318000	H	0.81575200	2.90926600	3.94010600
H	-3.37234900	6.11593000	-0.01972300	H	2.83327300	1.81347000	4.92026000
H	-5.23227600	2.25307200	-0.47841700	H	3.80618300	-0.18762300	3.79024200
H	-5.42481900	4.70951200	-0.09430100	H	2.78954300	-1.07265000	1.72813400
C	3.05386000	0.46626900	-1.50751600	H	-0.73914900	-3.24471600	4.36445000
C	3.06701000	-0.81770500	-2.07650300	C	-0.77027700	-2.83078600	3.35791200
C	4.25983500	1.13518500	-1.25018000	C	-1.62658100	-1.76219500	3.06873500
C	4.28453300	-1.40380900	-2.42060700	C	0.03885800	-3.37661300	2.35330700
H	2.12357400	-1.32869700	-2.24949600	C	-1.66602700	-1.23956200	1.77598500
C	5.47446600	0.52812900	-1.58073100	H	-2.25993100	-1.34557500	3.84978600
H	4.24515300	2.10011400	-0.75107400	C	-0.01520100	-2.84986700	1.06364700
C	5.49129800	-0.73693400	-2.17414100	H	0.69210700	-4.21795000	2.57725000
H	4.28874800	-2.39203200	-2.87307500	C	-0.87605800	-1.76970300	0.72457600
H	6.40710900	1.04131700	-1.35912000	H	-2.35399800	-0.43147800	1.54126000
H	6.43735800	-1.20795000	-2.42900900	H	0.57090200	-3.31579600	0.27495400
C	-3.05977200	-3.79568500	-1.31792100	B	-1.61868700	-1.76412500	-0.96622700
O	-4.08296700	-3.05816800	-1.13594000	O	-0.48236400	-1.16024800	-1.80495200
O	-2.99976000	-5.01536100	-1.51450600	O	-1.80142100	-3.13035000	-1.30968900

5'$_{CO3}$_1

Pd	-0.30291500	-0.57866400	0.41925400	N	-0.69542300	0.48837200	-1.52491800
C	3.68164800	0.33616400	-1.42805300	N	2.29001400	0.54759800	-1.37083300
C	4.26454500	-0.71790100	-2.15389100	C	1.58401900	0.45198100	-2.43655100
C	4.49940200	1.19963400	-0.67776900	C	-1.18630300	-2.23747100	-0.26786900
C	5.65061200	-0.88713300	-2.14579900	C	0.12970300	0.67127600	-2.49327800
H	3.62962700	-1.42342400	-2.68334000	C	-0.51385100	-3.08353600	-1.17143300
C	5.88384600	1.03583800	-0.69486600	C	-1.14451900	-4.19620800	-1.74548800
H	4.03404700	1.99996600	-0.10800700	C	-2.47221800	-4.49638200	-1.42485800
C	6.46518300	-0.00745400	-1.42586000	C	-3.15440900	-3.67258200	-0.52267600
H	6.09301100	-1.71589100	-2.69351000	C	-2.51831200	-2.56359700	0.04946100
H	6.50983500	1.71683000	-0.12393800	H	0.52406900	-2.88007500	-1.43187300
H	7.54370400	-0.14375300	-1.41993700	H	-0.59390500	-4.83082400	-2.43964000
C	-2.07034700	0.79530400	-1.75496700	H	-2.96525500	-5.36101100	-1.86542100
C	-2.73844000	1.59129800	-0.81183600	H	-4.18704100	-3.89536300	-0.25712000
C	-2.74796600	0.31010700	-2.88415800	H	-3.06923300	-1.94730400	0.75551500
C	-4.07031700	1.94084400	-1.03556200	H	0.83612600	-3.00619300	5.70712200
H	-2.21465000	1.96598100	0.06378000	C	0.61159700	-2.59789600	4.72316600
C	-4.09133700	0.63992800	-3.07792200	C	0.91364400	-3.32515200	3.56766600
H	-2.24179900	-0.36330500	-3.57081100	C	0.01508800	-1.33850500	4.59731300
C	-4.75191100	1.46461200	-2.16176800	C	0.61594600	-2.80094500	2.30236400
H	-4.56268900	2.58996700	-0.31690400	H	1.37647200	-4.30841000	3.64795500
H	-4.62214200	0.24107100	-3.93931800	C	-0.26913200	-0.81239300	3.33061300
H	-5.79589900	1.72558800	-2.31870800	H	-0.22740600	-0.75763100	5.48619900
C	-1.32118500	4.33386800	1.53731100	C	0.02979000	-1.53151100	2.15654300

O	-0.45105600	5.23283600	1.39945100	H	0.84228700	-3.39637500	1.42159400
O	-2.53853900	4.37373600	1.69099300	H	-0.71655600	0.17648900	3.26149500
H	0.98571700	4.46454800	0.99657800	B	0.49260100	2.66785100	1.13895000
H	2.05577000	0.28051800	-3.41481100	O	0.81992400	1.30899700	1.04075600
H	-0.23685900	1.03868500	-3.45945500	O	-0.79528800	2.95355000	1.49479200
H	1.61961400	1.18114700	0.49730900	O	1.45538700	3.58877600	0.84851800

4$_{CO3}$**_2** thermal Free Energies = -1680.497407 A.U.

C	2.15645800	2.99837700	-0.53215900	Pd	1.21089500	0.29164500	0.27414000
H	7.10102000	-2.47473300	-1.68181700	C	1.65518100	-1.55821600	0.87431900
C	-0.07831100	3.38649400	0.09993100	C	3.24482100	2.07683300	-0.76379200
C	0.09815700	4.61403800	0.77110700	C	2.69200000	-1.80337800	1.78587900
C	-1.36369900	2.97488000	-0.28425300	C	2.99684400	-3.11292200	2.18273000
C	-1.01106000	5.41106700	1.04832800	C	2.26937500	-4.19101600	1.66941500
H	1.08409900	4.90513600	1.12566800	C	1.22602900	-3.94842200	0.76823900
C	-2.46883200	3.77730900	-0.00302300	C	0.91023300	-2.63998400	0.38042800
H	-1.50384500	2.03943100	-0.81186800	H	3.26988100	-0.97805400	2.19664600
C	-2.29386800	4.99456600	0.66299300	H	3.80315800	-3.28644000	2.89424800
H	-0.87919400	6.34379600	1.59255200	H	2.50445700	-5.20813100	1.97741300
H	-3.45366100	3.40182300	-0.26820900	H	0.64007800	-4.77810400	0.37623400
H	-3.15739700	5.60874300	0.90760900	H	0.07997600	-2.45353900	-0.29556800
H	-6.87100400	-4.55945700	-0.51940100	N	1.00487100	2.52465700	-0.17053800
C	-6.29986100	-3.63274700	-0.47482300	N	3.09711100	0.80800200	-0.50123700
C	-6.43836400	-2.66330000	-1.47669800	H	4.17055600	2.44927700	-1.20555800
C	-5.41150900	-3.39616600	0.57967400	H	2.31817600	4.06355400	-0.71570200
C	-5.69833100	-1.47755900	-1.41291300	C	4.18068700	-0.06618900	-0.79301100
H	-7.12171400	-2.83630600	-2.30858200	C	3.91857500	-1.26977700	-1.46330200
C	-4.67718600	-2.20326300	0.62743900	C	5.49607800	0.25432900	-0.42090900
H	-5.28504400	-4.14475900	1.36209100	C	4.97245200	-2.11938000	-1.79630200
C	-4.79857900	-1.20771900	-0.36170400	H	2.89407500	-1.52305000	-1.71197700
H	-5.80639400	-0.73355000	-2.20058600	C	6.54285600	-0.61361800	-0.74021900
O	-2.74771900	0.01537000	0.63834900	H	5.69045200	1.15905200	0.14910900
O	-3.59589800	0.74483800	-1.59929600	C	6.28637700	-1.79791600	-1.43684900
H	-2.81428500	0.23178900	-1.87211400	H	4.76158800	-3.04631800	-2.32278000
C	-1.52031100	-0.13474600	0.22980400	H	7.55629500	-0.36735000	-0.43262100
O	-1.18622600	-0.39363900	-0.96160100	H	-3.97806300	-2.04217400	1.44630800
O	-0.60665900	0.04655000	1.16507500	B	-4.01149100	0.23536500	-0.31438500
H	-5.23459500	0.91671100	1.12192700	O	-4.81893500	1.27214700	0.32484000

4'$_{CO3}$**_2** thermal Free Energies = -1680.485578 A.U.

Pd	-0.48209300	0.34792300	0.12324400	N	-1.35871600	-1.12233600	-1.17879600
C	3.54209500	-2.78314900	-1.47684500	N	1.53932000	-1.33662100	-1.34058400
C	3.72400700	-0.35585400	-1.30270600	C	0.74118000	-2.10482200	-1.97819600
C	4.93310000	-2.88412400	-1.50486500	C	-0.46213300	-1.04765900	1.57045900
H	2.93154500	-3.68266300	-1.47510400	C	-0.71857600	-1.95276000	-1.92200300
C	5.11369100	-0.47265900	-1.35853100	C	0.70115800	-1.75569400	1.91267800
H	3.23105500	0.61548600	-1.20783400	C	0.66985400	-2.77627700	2.87286800
C	5.72327300	-1.72885800	-1.45869600	C	-0.52873700	-3.11553800	3.50910000
H	5.40128000	-3.86501700	-1.55081600	C	-1.69653400	-2.42266400	3.17251200
H	5.72230500	0.42682300	-1.30697700	C	-1.66103200	-1.40375200	2.21119500
H	6.80765400	-1.81099700	-1.48125100	H	1.64513200	-1.50541600	1.43808300
C	-2.78588400	-1.10814300	-1.26779000	H	1.58910600	-3.30435500	3.12405500
C	-3.51760100	-2.27912900	-1.01995000	H	-0.55232500	-3.90645300	4.25654800
C	-3.44114700	0.09046800	-1.59395700	H	-2.63904600	-2.67128200	3.65903300
C	-4.91296200	-2.25502700	-1.10500100	H	-2.58278100	-0.87797200	1.96992700
H	-2.99756100	-3.18506200	-0.72018500	H	0.16956400	1.09308300	4.86760500
C	-4.83315400	0.09162000	-1.69123100	C	0.32286700	1.37233300	3.82707300
H	-2.85186500	0.98565900	-1.78681800	C	1.60536800	1.25568200	3.24690200
C	-5.57398800	-1.07186400	-1.44589200	C	-0.73670500	1.82192300	3.06042500
H	-5.47864200	-3.15957400	-0.89328500	C	1.80995100	1.61284500	1.92555000

H	-5.33698500	1.01726600	-1.95739300	H	2.43540700	0.89153800	3.85056800
H	-6.65950000	-1.05327900	-1.51141700	C	-0.52401500	2.19990600	1.70876400
C	-0.96399100	2.89284700	-1.50994800	H	-1.73203800	1.90722700	3.49214100
O	-1.96927700	3.40930500	-2.01944300	C	0.76554900	2.14710700	1.11051700
O	-0.71586300	1.59444300	-1.59959800	H	2.80856400	1.55863900	1.49818600
H	1.28184200	1.77247600	-1.74948300	H	-1.32129500	2.72175100	1.18401800
H	2.32974700	4.62692600	-0.47749100	B	1.19112300	3.03650100	-0.23625400
H	1.09433300	-2.90197500	-2.64835100	O	1.94707600	2.27274000	-1.24343600
H	-1.28470700	-2.59470200	-2.60492500	O	-0.07088100	3.63099500	-0.84856800
C	2.92999800	-1.51569900	-1.39213600	O	2.00792700	4.12017700	0.28318300

4'TS$_{CO3}$_2 thermal Free Energies = -1680.475165 A.U.

H	-1.88627600	2.95478900	-0.11842600	Pd	-0.42544700	0.23693600	-0.13634700
B	0.86956100	2.76614400	-1.33058000	N	-1.03366500	-1.74032600	-0.69977800
O	1.87930400	1.81959300	-1.69460500	N	1.88531700	-1.69047300	-0.59242600
O	-0.30478300	2.86545500	-2.22821500	C	1.20654300	-2.71154100	-0.95549700
O	1.43242000	4.06941400	-1.13004300	C	-0.52323700	-0.30253900	1.80098600
H	0.72835200	4.72604300	-1.22439300	C	-0.26199000	-2.72607500	-0.99554500
H	1.67966100	-3.64207900	-1.30271100	C	0.55295300	-0.91891100	2.46337200
H	-0.70984500	-3.65940600	-1.35267900	C	0.42616900	-1.38893800	3.77709800
C	3.28769600	-1.71664900	-0.54549400	C	-0.78587900	-1.25425300	4.46324100
C	4.03121100	-2.86432000	-0.20145800	C	-1.86540600	-0.64191200	3.81860900
C	3.95569600	-0.50407100	-0.80581600	C	-1.73306100	-0.17113300	2.50503700
C	5.42424800	-2.80500900	-0.15208700	H	1.50652900	-1.02718500	1.95365900
H	3.51764900	-3.78404200	0.06704700	H	1.28084000	-1.85564200	4.26621700
C	5.35020600	-0.46663300	-0.77706000	H	-0.88535700	-1.61563700	5.48527800
H	3.36860200	0.38500100	-1.03832800	H	-2.81608400	-0.52543100	4.33800700
C	6.08940700	-1.60998200	-0.45153100	H	-2.58655500	0.30636500	2.02940900
H	5.99087900	-3.68924600	0.13179200	H	-0.61194300	3.92427900	3.86915900
H	5.85861300	0.46904100	-0.99590800	C	-0.40808800	3.48052200	2.89569800
H	7.17549200	-1.56723100	-0.41247800	C	0.84356100	2.90536700	2.63826300
C	-2.44297100	-1.93644100	-0.82719100	C	-1.39979000	3.47612600	1.90857500
C	-3.08614000	-2.95194000	-0.10505900	C	1.09252100	2.33024900	1.39425700
C	-3.17310300	-1.08814700	-1.67538900	H	1.60849700	2.90027500	3.41306200
C	-4.46734700	-3.12575000	-0.23595500	C	-1.12676600	2.91010900	0.65999200
H	-2.51399900	-3.56554200	0.58567600	H	-2.37565800	3.91390100	2.11472800
C	-4.54735100	-1.28850800	-1.80920500	C	0.13436000	2.33272600	0.34391500
H	-2.65414400	-0.30647900	-2.22662000	H	2.07033900	1.89687100	1.19269500
C	-5.20025800	-2.29979600	-1.09230800	O	-1.96587500	1.92201400	-3.39515200
H	-4.96709400	-3.90018600	0.34156400	O	-0.52591600	0.61304400	-2.26340100
H	-5.10844000	-0.63955000	-2.47674600	H	1.38921800	1.05635400	-2.05254400
H	-6.27459800	-2.43573700	-1.19376900	C	-0.98063200	1.77914000	-2.66146000

5'$_{CO3}$_2

H	3.53314600	5.32276200	-0.51412500	Pd	-0.54885100	0.10573500	0.46420400
H	0.73290900	-2.00181300	-3.33366700	N	-1.33047100	-0.01919800	-1.59838700
H	-1.26920900	-0.70996600	-3.54809700	N	1.48465200	-0.96874700	-1.68393200
C	2.70231200	-1.69216500	-1.65483600	C	0.56275600	-1.25848900	-2.54248000
C	2.75396500	-3.08784700	-1.85100500	C	-1.47180700	-1.62541200	0.95118500
C	3.88531200	-0.98060000	-1.37558800	C	-0.75005000	-0.62743500	-2.58775000
C	3.97855100	-3.75774100	-1.78843000	C	-0.77425900	-2.85283800	1.00107600
H	1.83354800	-3.64319200	-2.00142900	C	-1.43787400	-4.06330600	1.24985700
C	5.10489200	-1.65954500	-1.33734300	C	-2.82222700	-4.08300800	1.46356000
H	3.83335500	0.09012800	-1.20278900	C	-3.53303900	-2.87721700	1.42628200
C	5.15893100	-3.04549000	-1.54233600	C	-2.86611500	-1.66838300	1.17546500
H	4.00949600	-4.83552900	-1.91990900	H	0.30222200	-2.86129400	0.85766100
H	6.01494300	-1.10473100	-1.13154700	H	-0.86969900	-4.99119900	1.28692600
H	6.10951100	-3.56823100	-1.49161800	H	-3.33647500	-5.02066000	1.66122300
C	-2.65101800	0.50891600	-1.78336800	H	-4.60845800	-2.87427000	1.59484500
C	-3.64760400	-0.24108700	-2.43416600	H	-3.43995900	-0.74566600	1.15365100

C	-2.94475500	1.78696400	-1.27554300	H	1.60144500	0.73564400	5.98202300
C	-4.92945900	0.29394700	-2.59547500	C	1.19127100	0.59283500	4.98478400
H	-3.43203000	-1.25220100	-2.76372800	C	1.99874400	0.76777000	3.85414700
C	-4.22560900	2.31443700	-1.46078400	C	-0.15112600	0.23364500	4.81417100
H	-2.18249900	2.36358200	-0.75579900	C	1.46799800	0.58726500	2.56868200
C	-5.22047000	1.57644200	-2.11722100	H	3.04306000	1.05152600	3.96923200
H	-5.70050800	-0.29753200	-3.08057700	C	-0.67671600	0.04273400	3.52787400
H	-4.44363600	3.30671000	-1.07915000	H	-0.79188700	0.09582900	5.68336500
H	-6.21668400	1.99103600	-2.24084300	C	0.11693400	0.22074900	2.37529600
C	0.33901300	3.18556900	-0.10670000	H	2.10640000	0.75843600	1.70781200
O	-0.73866900	3.78698800	0.03566600	H	-1.71402300	-0.25800000	3.42173400
O	0.57935500	1.90543100	-0.15196300	B	2.80187400	3.47926100	-0.57439300
H	2.19331100	1.64156700	-0.62160800	O	3.04983800	2.14475600	-0.76676900
O	3.82822300	4.40954200	-0.67694300	O	1.51861800	3.99307600	-0.28685600

4'$_{CO3}$_12 thermal Free Energies = -1680.473795 A.U.

Pd	-0.36108300	-0.07686800	0.17746800	H	1.25521800	0.36416700	4.58836800
N	-0.71208200	-1.03284300	-1.68199100	C	-1.42907000	1.52310600	2.03743500
N	2.15316800	-0.71976500	-1.32859400	H	-2.87870400	1.00241000	3.55785500
C	1.61495400	-1.01990000	-2.44571700	C	-0.06037600	1.63329100	1.66674300
C	-0.52708200	-1.79102000	1.26927300	H	1.93954200	1.23805600	2.36265700
C	0.16320600	-1.17336100	-2.61370200	H	-2.18872400	1.89472700	1.35273600
C	0.58662600	-2.64011800	1.41862000	B	0.39174500	2.47974800	0.26006500
C	0.50776800	-3.83715300	2.14328000	O	-0.07310000	1.69513900	-0.84196100
C	-0.69857500	-4.22570200	2.73662700	O	-0.26510600	3.87259200	0.33111200
C	-1.81871000	-3.39935000	2.59798100	O	1.84075500	2.74524700	0.28256900
C	-1.72906800	-2.20082900	1.87578400	H	-1.23940300	2.59647700	-1.21902700
H	1.53682000	-2.36100700	0.96744600	H	1.96392700	3.69260700	0.43668100
H	1.39204200	-4.46596700	2.24501300	H	2.20475200	-1.14909000	-3.36494900
H	-0.76330900	-5.15454400	3.30074100	H	-0.17482400	-1.42083800	-3.62519100
H	-2.76573900	-3.68367300	3.05653200	C	3.54809000	-0.59737700	-1.22257300
H	-2.61583800	-1.57542100	1.79166600	C	4.42732400	-1.57890700	-1.71647900
H	-1.15621400	0.27537600	5.19682100	C	4.05433900	0.53345900	-0.55403000
C	-0.85659300	0.64494800	4.21774300	C	5.80643000	-1.42635000	-1.55159700
C	0.50356600	0.69798300	3.87501300	H	4.02558600	-2.47277400	-2.18784500
C	-1.82272000	1.04936000	3.29819400	C	5.43505000	0.68357600	-0.42460700
C	0.88596000	1.17104000	2.62244400	H	3.35677200	1.28930900	-0.18994400
H	-4.47462300	0.46776700	-3.85122500	C	6.31543400	-0.29139000	-0.91300600
H	-5.83879500	-1.44052400	-3.00750900	H	6.48061100	-2.19788700	-1.91741200
C	-1.32460000	4.29916500	-0.35463600	H	5.82609600	1.56848500	0.07214100
O	-1.80410200	5.41510500	-0.19873700	H	7.38921400	-0.17182500	-0.78759600
O	-1.84870300	3.42613500	-1.23828400	C	-2.08932500	-1.14798500	-2.04593400
C	-4.02126900	-0.29446000	-3.22272800	C	-2.85528100	-2.20697300	-1.54075000
H	-2.07857100	0.66412800	-3.21127400	C	-2.67060700	-0.18472300	-2.88245400
C	-4.78719300	-1.36078900	-2.74309400	C	-4.19876500	-2.31409000	-1.90338700
H	-4.79064400	-3.14013200	-1.51621400	H	-2.39674100	-2.92083900	-0.86446900

4'TS$_{CO3}$_12 thermal Free Energies = -1680.460439 A.U.

Pd	-0.38627000	0.16512600	-0.20073100	N	-0.87771900	-1.89970300	-0.37945800
H	-0.38522100	-3.81619600	-0.96237000	N	2.14914800	-1.71992500	-0.36802700
C	3.51889600	-1.81637700	-0.07400600	C	1.42903100	-2.79302000	-0.45574800
C	4.07270800	-2.81578600	0.75333700	C	-1.45268800	0.34764600	1.47490400
C	4.36760300	-0.82084800	-0.59912400	C	-0.00969500	-2.84537000	-0.62638100
C	5.44361500	-2.83857400	1.01181100	C	-0.99249000	-0.13746500	2.70752000
H	3.42227600	-3.54748800	1.22500200	C	-1.78500900	-0.02868000	3.85918200
C	5.73863500	-0.86039400	-0.34710400	C	-3.04699400	0.57019000	3.79277000
H	3.94203900	-0.02098400	-1.20031800	C	-3.50692700	1.06232500	2.56586200
C	6.28519300	-1.86880800	0.45513300	C	-2.71607000	0.95496000	1.41479400
H	5.85397700	-3.60742200	1.66294800	H	-0.00849000	-0.59567900	2.78082400
H	6.37935700	-0.08967400	-0.76819200	H	-1.41028100	-0.40981400	4.80865000

H	7.35240400	-1.88682200	0.66240500	H	-3.66247000	0.65693800	4.68648100
C	-2.25339000	-2.25567300	-0.50460500	H	-4.48531800	1.53681500	2.50158200
C	-3.11912700	-1.40018200	-1.20549200	H	-3.07440600	1.34891100	0.46632300
C	-2.74875000	-3.43792700	0.07246300	H	1.61580200	4.43787300	3.12482200
C	-4.45818700	-1.76071500	-1.35838600	C	1.36684500	3.78556900	2.28910700
H	-2.74208000	-0.46527800	-1.61971300	C	2.15447400	2.66133900	2.01476000
C	-4.09664700	-3.77440500	-0.07049900	C	0.25345500	4.06294100	1.48710200
H	-2.09030300	-4.06283200	0.66994500	C	1.82660200	1.83292800	0.93901700
C	-4.95465200	-2.94279600	-0.79626500	H	3.01921700	2.43491100	2.63734400
H	-5.11838800	-1.09877800	-1.91321700	C	-0.07078300	3.21493400	0.42556300
H	-4.47616300	-4.67937400	0.39893100	H	-0.36874100	4.93068100	1.70038600
H	-6.00479300	-3.20358500	-0.90631100	C	0.71422300	2.08531500	0.09664600
C	-1.34976800	2.29015100	-2.55430300	H	2.46920500	0.98192500	0.72651500
O	-1.81878000	1.42810800	-1.72985800	H	-0.94948300	3.43292400	-0.17452600
O	-1.99220000	2.96528100	-3.36625100	B	0.98280900	1.74240200	-1.81536500
H	1.63414600	-0.18916100	-1.69409500	O	0.84138700	0.29285500	-1.98775600
H	2.34976900	3.09272400	-2.25180400	O	0.02566100	2.51822100	-2.51626400
H	1.89939600	-3.78630200	-0.43331100	O	2.33546900	2.14648700	-2.04909600

5'$_{CO3}$_12

Pd	-0.35572500	-0.05979000	0.44558700	H	1.39294300	-1.08428700	2.91625100
N	-0.98266600	-0.80534200	-1.57634600	H	-0.83749100	2.46706100	1.90740200
N	1.98396300	-0.76361000	-1.64788500	B	1.02341100	2.94827200	-0.81456600
C	1.22342000	-1.54178100	-2.33276200	O	0.60970600	1.62368000	-0.87354200
C	-1.05306900	-1.69502700	1.36126800	O	0.22608600	4.02432900	-0.71038900
C	-0.22889200	-1.37615500	-2.45152500	O	2.40445500	3.14414900	-0.95131400
C	-0.33386100	-2.90466800	1.30944200	H	1.32100100	1.00498900	-1.14062200
C	-0.85624300	-4.09211800	1.84095500	H	2.58221500	4.09648500	-0.94773700
C	-2.11748100	-4.09847600	2.44562700	H	1.63810000	-2.36850300	-2.92634100
C	-2.84211100	-2.90324500	2.51556000	H	-0.66661200	-1.78833500	-3.36814600
C	-2.31437700	-1.71890700	1.98543900	C	3.36356700	-1.02221700	-1.53036600
H	0.65507700	-2.92571000	0.85351900	C	3.90867200	-2.32058500	-1.51019100
H	-0.27304700	-5.01122500	1.78565900	C	4.21416700	0.08739400	-1.37260100
H	-2.52576800	-5.01751300	2.86237500	C	5.28592500	-2.49973900	-1.37735800
H	-3.82269700	-2.88889100	2.98983300	H	3.25262900	-3.18571000	-1.55435800
H	-2.89311000	-0.80186900	2.06270000	C	5.59138900	-0.10223600	-1.25835900
H	1.46654700	2.31888300	5.55071200	H	3.78555300	1.08613200	-1.33803300
C	1.12079100	1.84349200	4.63397900	C	6.13384300	-1.39226200	-1.26307000
C	1.52822200	0.54443000	4.31289000	H	5.69578000	-3.50660600	-1.34570000
C	0.26257400	2.52394800	3.76270900	H	6.24063000	0.76227100	-1.14543600
C	1.07672600	-0.06697900	3.13515400	H	7.20617400	-1.53544700	-1.15457100
H	2.19446600	0.00010600	4.98201300	C	-2.37972500	-0.71998200	-1.83732200
C	-0.18395600	1.91561700	2.58158700	C	-3.03201800	0.48533500	-1.52977300
H	-0.06163300	3.53727000	3.99642500	C	-3.10155600	-1.80500800	-2.36273300
C	0.22430600	0.60950100	2.24589800	C	-4.39436900	0.60854000	-1.80587700
C	-1.28701700	4.03383000	-0.77032700	H	-2.48413200	1.32247600	-1.09520600
O	-1.81631400	3.08881000	-0.16416800	C	-4.47004500	-1.67445100	-2.60781300
O	-1.70506300	5.00353600	-1.39827900	H	-2.60710800	-2.75945500	-2.52429500
H	-5.03047900	-2.52469100	-2.99005100	C	-5.11773100	-0.46347300	-2.34209200
H	-6.18356200	-0.36265600	-2.5340840	H	-4.88613800	1.55213500	-1.58534400

4$_{CO3}$_3 thermal Free Energies = -1680.471485 A.U.

N	-1.56431400	-1.55810600	-0.28572400	C	-1.22677000	-2.03141700	0.85220100
H	0.48035700	-3.02188700	1.62425800	Pd	0.11180000	-0.03995100	-0.75138800
H	-1.94387900	-2.55481200	1.49317100	C	1.75801200	1.05499500	-0.94444800
C	-0.14652700	-0.03358500	2.80138200	C	0.21837100	-1.99980600	1.30856400
O	0.35947900	-1.29958400	2.61292900	C	2.25012900	1.32113500	-2.23123200
O	0.43063100	0.69749800	3.60513200	C	3.40794300	2.08913600	-2.40890400
C	2.38037100	-2.00149500	0.25280900	C	4.08936700	2.60079000	-1.29970300
C	3.03741400	-2.51188400	1.40152000	C	3.60403400	2.33387100	-0.01581400

C	3.11196300	-1.99599400	-0.95998300	C	2.44861500	1.56214800	0.16405700
C	4.33441900	-3.02697200	1.31753700	H	1.73200600	0.93557100	-3.10757600
H	2.54491800	-2.46036500	2.36691300	H	3.77487500	2.28512400	-3.41572900
C	4.40860500	-2.49369700	-1.02662700	H	4.99089100	3.19531800	-1.43480900
H	2.63278900	-1.59062800	-1.84548100	H	4.12797600	2.71940900	0.85707200
C	5.03612400	-3.02721200	0.10950700	H	2.09835500	1.35925500	1.17205700
H	4.80761600	-3.40747200	2.22164400	H	-0.09811300	3.81214500	-2.82837300
H	4.93706700	-2.46910000	-1.97830600	C	-0.46609300	3.39343100	-1.89489500
H	6.05122000	-3.41382300	0.05442400	C	-1.21182300	2.20426800	-1.89538400
C	-2.89839400	-1.70502600	-0.75389800	C	-0.20362300	4.02536900	-0.68184800
C	-3.09917500	-2.34293900	-1.98783600	C	-1.67539400	1.67013600	-0.67670000
C	-3.99208300	-1.19465600	-0.03843200	H	-1.49223800	1.73234400	-2.83557100
C	-4.39307700	-2.51327200	-2.48228400	C	-0.65528000	3.47341800	0.52932000
H	-2.23576200	-2.70715700	-2.53823900	H	0.36976300	4.95084900	-0.67064300
C	-5.28257000	-1.35811000	-0.55324400	C	-1.39550700	2.28753400	0.57605700
H	-3.82319700	-0.61669200	0.86840400	H	-2.40378800	0.86665300	-0.70912200
C	-5.49137000	-2.02346300	-1.76468900	H	-0.43873000	3.98304300	1.46546100
H	-4.54327200	-3.02258800	-3.43167700	B	-1.96048600	1.68542600	1.99159100
H	-6.12582800	-0.94544900	-0.00432400	O	-3.37110100	1.38143500	1.86971100
H	-6.49862100	-2.14636700	-2.15617300	O	-1.22559200	0.21996500	2.12740900
H	-0.83981500	2.16116300	3.56430900	O	-1.68008900	2.45734700	3.16773300
N	1.06424300	-1.56516700	0.26618900	H	-3.73716700	1.43550000	2.76544000

4'TS$_{CO3}$_3 thermal Free Energies = -1680.454271 A.U.

C	-1.01571300	-2.58524900	-0.54529800	O	-0.42219500	1.22497500	3.14978900
Pd	0.06604600	0.17898500	-0.45344200	H	-2.70771300	1.73406700	3.21565600
C	1.69371800	1.31281400	-0.39827700	H	0.23037600	0.50244200	3.28827600
C	0.44230200	-2.69029900	-0.48127900	N	1.18979900	-1.66772800	-0.74987700
C	2.00757600	2.10420500	-1.51170700	N	-1.56033600	-1.46403900	-0.87606100
C	3.21166300	2.82030300	-1.55590400	H	0.87645700	-3.66533400	-0.26482400
C	4.10639700	2.76088700	-0.48230700	H	-1.59661300	-3.49663700	-0.40271300
C	3.78590800	1.98174500	0.63503500	C	-0.29304000	-1.56089700	2.20098000
C	2.58540500	1.26172100	0.68152900	O	-0.46000100	-2.75771200	1.76670500
H	1.30956800	2.18137100	-2.34301700	O	0.71978100	-1.16600100	2.83513800
H	3.44197600	3.43235200	-2.42718300	C	2.59834600	-1.83554400	-0.63074400
H	5.03954000	3.32033400	-0.51327000	C	3.15587100	-2.35442000	0.54804300
H	4.47101600	1.93157600	1.47980500	C	3.42522000	-1.45541800	-1.69573500
H	2.34483900	0.66542100	1.55812100	C	4.54034700	-2.52366400	0.63485100
H	-1.87069600	5.20307500	-1.22956100	H	2.50574800	-2.56083900	1.39540000
C	-1.65303800	4.26042500	-0.72888000	C	4.80501900	-1.63777900	-1.60097100
C	-2.36519100	3.10689100	-1.06147500	H	2.97800700	-1.01507200	-2.58178900
C	-0.65782700	4.19973600	0.25830100	C	5.36767100	-2.17636200	-0.43770200
C	-2.08831500	1.90458500	-0.39610800	H	4.97200700	-2.91287300	1.55413400
H	-3.14576700	3.14289600	-1.82020100	H	5.44354200	-1.34414300	-2.43098300
C	-0.37266200	2.98944700	0.88432200	H	6.44515700	-2.30426400	-0.36180800
H	-0.10155800	5.09736700	0.52479500	C	-2.97421100	-1.42024600	-0.97239700
C	-1.08838600	1.78750100	0.60912100	C	-3.55906100	-1.01830900	-2.18373500
H	-2.71428500	1.04771600	-0.62117100	C	-3.78744900	-1.74247000	0.12530700
H	0.38931800	2.95666400	1.65657500	C	-4.94885700	-0.97689400	-2.30863300
B	-1.36023700	0.75223100	2.19301300	H	-2.91381300	-0.74579100	-3.01487600
O	-2.73152200	1.08755600	2.49609800	C	-5.17710500	-1.68386200	-0.00712500
O	-1.30183000	-0.70459100	1.89001700	H	-3.31382200	-1.97236100	1.07436900
H	-5.80178700	-1.91377000	0.85279200	C	-5.76402500	-1.31077600	-1.22051400
H	-6.84666800	-1.26388900	-1.31417500	H	-5.39526100	-0.67463900	-3.25368700

5'$_{CO3}$_3

O	-3.80072000	-2.35060500	2.63835500	C	-1.60029400	-0.44417500	-1.39683200
H	-5.39638300	-0.63883500	3.03064800	Pd	0.98690200	0.56854100	-0.27005600
H	-3.20164100	-2.94094500	2.09537000	C	2.86556900	0.27154800	0.38641100
N	0.45415800	-1.54566400	-0.87999000	C	-0.74826800	-1.62687700	-1.34562300

N	-1.16233500	0.70034500	-0.98686100	C	3.99879300	0.61236700	-0.37280100
H	-1.20411900	-2.56063700	-1.67347500	C	5.28963700	0.26927800	0.04464300
H	-2.61825500	-0.59866900	-1.75431900	C	5.48315400	-0.40854500	1.25008800
C	-3.44292500	-2.79866900	-0.23896100	C	4.37196600	-0.73771600	2.02938200
O	-3.45582100	-2.82760500	-1.47450600	C	3.08294400	-0.40141700	1.60232800
O	-2.70472600	-3.42596500	0.57497900	H	3.87946800	1.15504100	-1.30808500
C	1.18095200	-2.75656300	-0.72954500	H	6.14617300	0.53998600	-0.57150300
C	0.54240000	-3.92453700	-0.27137800	H	6.48603900	-0.67197400	1.58021300
C	2.55201000	-2.77120300	-1.02278100	H	4.50618200	-1.26191700	2.97430400
C	1.28258300	-5.09907200	-0.14092500	H	2.23599500	-0.67776000	2.22620600
H	-0.51150200	-3.89859200	0.00554400	H	1.54602200	6.29987700	1.16494700
C	3.27207200	-3.95806700	-0.90283200	C	1.47803200	5.24331300	0.91360500
H	3.03708900	-1.85493400	-1.33751200	C	2.05590600	4.75597900	-0.26053400
C	2.64212500	-5.12513000	-0.46253600	C	0.81802400	4.35395000	1.76444600
H	0.78954400	-5.99752800	0.22164100	C	1.97170400	3.39527400	-0.57655000
H	4.33282300	-3.96442700	-1.14002900	H	2.58097200	5.43469000	-0.93153900
H	3.21128600	-6.04571300	-0.35668800	C	0.72936300	2.99624400	1.43903900
C	-2.08215900	1.78052700	-0.92786500	H	0.36730200	4.71679500	2.68691300
C	-1.64921100	3.06730600	-1.27891900	C	1.29373300	2.48664000	0.25574700
C	-3.40567900	1.57994000	-0.49470100	H	2.44290500	3.04279000	-1.49204300
C	-2.54479100	4.13402100	-1.23911700	H	0.20573700	2.32845100	2.11935300
H	-0.61711500	3.21781900	-1.57174000	B	-4.50732800	-1.67417100	1.69191500
C	-4.28557400	2.65963500	-0.44240100	O	-5.42069300	-0.70209200	2.06504200
H	-3.73688700	0.59595900	-0.17422300	O	-4.37527400	-1.87157900	0.32941900
C	-3.86381300	3.93626100	-0.82172700	H	-5.30048700	2.49429400	-0.09135800
H	-2.20275100	5.12682800	-1.51968200	H	-4.55365200	4.77553900	-0.77628500

PhB(OH)$_2$PO$_4$ thermal Free Energies = -1050.915822 A.U.

H	2.42803600	-2.13427000	-0.00062100	H	5.35048900	1.05434900	-0.00037800
B	-0.02944400	-0.67173100	0.00035200	C	4.30927600	0.71892100	-0.00027600
O	-0.20426700	-1.48232100	-1.24742300	C	3.25301100	1.64521600	0.00005600
O	-0.20423400	-1.48029900	1.24944500	C	3.99438900	-0.65085000	-0.00050000
H	-1.14147000	-1.29495600	-1.49774300	C	1.92125600	1.20584900	0.00018500
H	-1.14137400	-1.29236900	1.49960900	H	3.47679700	2.71777700	0.00020100
O	-3.13294700	1.82623000	-0.00145100	C	2.65586300	-1.06786600	-0.00038100
O	-2.91073300	-0.43426300	1.30582600	H	4.80233600	-1.39170800	-0.00079000
O	-0.90033500	0.51446400	-0.00057800	C	1.57068700	-0.16222300	0.00000000
P	-2.58943400	0.37264800	-0.00027600	H	1.09535200	1.91730100	0.00040200
O	-2.91102500	-0.43649600	-1.30491900				

B(OH)$_2$PO$_4$ thermal Free Energies = -819.301805 A.U.

O	0.41914900	-0.74508700	-0.08457500	B	1.63698900	-0.04884800	-0.01413300
O	-1.93860700	-0.64822700	-1.14770500	O	2.76913400	-0.95468700	-0.01220900
O	-1.63769500	-0.33123800	1.43525300	O	1.82132200	1.25937500	0.02807700
P	-1.12573800	-0.11032400	0.01894800	H	0.18666700	1.63191600	-0.11535200
O	-0.80846900	1.49556800	-0.23434700	H	3.51579500	-0.33845200	0.02585000

4$_{PO4}$_1 thermal Free Energies = -2059.13244 A.U.

H	1.37085000	0.16376900	-1.23396300	C	-1.20164100	-3.42234000	0.49548100
N	-0.13927100	-2.67556800	0.27097700	Pd	-0.83606800	-0.52436400	-0.08953800
N	-2.66143400	-1.59399000	0.01860300	C	-1.64787200	1.29414000	-0.18745900
H	-3.36096600	-3.53513300	0.39754100	C	-2.49639300	-2.87220200	0.33641000
H	-1.11429200	-4.48383300	0.73919700	C	-2.59409200	1.70427700	0.76515600
C	-3.97720000	-1.14475700	-0.20710100	C	-3.16858600	2.98123200	0.70840100
C	-4.24577600	-0.29695100	-1.29873100	C	-2.81152400	3.86767300	-0.31179300
C	-5.04955600	-1.53411300	0.62214400	C	-1.85845300	3.47188500	-1.25784700
C	-5.54830300	0.11768300	-1.56741800	C	-1.26977900	2.20349600	-1.18873300
H	-3.41844500	0.02711700	-1.91987700	H	-2.88858100	1.02965200	1.56627500
C	-6.35109900	-1.10510800	0.35251000	H	-3.89109900	3.28139300	1.46738800
H	-4.85041100	-2.14285000	1.50030900	H	-3.25006100	4.86381200	-0.35488800

C	-6.61218600	-0.28218700	-0.74775000	H	-1.54289400	4.16517300	-2.03628700
H	-5.73074300	0.77171200	-2.41708100	H	-0.48486300	1.93609600	-1.88905600
H	-7.16069000	-1.40428400	1.01621300	H	1.83361500	6.15470400	1.97964300
H	-7.62490500	0.05757600	-0.95385200	C	1.89468000	5.09623600	1.72167000
C	1.13943000	-3.20303100	0.47300500	C	1.25485800	4.13393100	2.51243800
C	1.40372000	-4.19911200	1.44580500	C	2.61422100	4.67703100	0.59503300
C	2.20450100	-2.71139600	-0.30641900	C	1.33858800	2.77785600	2.17097900
C	2.69614600	-4.69173200	1.60901400	H	0.68850600	4.44091900	3.39376700
H	0.61133000	-4.53039900	2.11266400	C	2.68741600	3.31810000	0.26198600
C	3.50221700	-3.19160200	-0.11779300	H	3.12509100	5.41294000	-0.02785800
H	2.02849300	-1.94792500	-1.06124600	C	2.04641800	2.33163000	1.03802000
C	3.75090700	-4.19044400	0.82881600	H	0.84849700	2.03813300	2.80142100
H	2.89195000	-5.43607500	2.38014400	H	3.26324900	3.00619000	-0.60938200
H	4.29295100	-2.71516900	-0.70053000	B	2.13264400	0.73824400	0.65573400
H	4.76561200	-4.54933800	0.99189100	O	1.97922800	-0.05248100	1.87378800
P	3.75187300	0.23999800	-1.64888400	O	0.94145100	0.43207300	-0.33747100
O	2.39576100	-0.19567500	-2.32060800	O	3.36264400	0.35836900	-0.04658400
O	4.81719300	-0.87148400	-1.75400400	H	2.46258100	-0.87880000	1.73054500
O	4.26048900	1.60543400	-2.14032400				

4'$_{PO4}$_1 thermal Free Energies = -2059.12687 A.U.

Pd	0.50389800	-0.23453500	0.07398100	H	-1.19503100	0.56521900	-1.77413200
N	1.98308800	-0.14234300	-1.45530100	H	-3.90810900	0.81649700	-0.41433100
N	0.77848400	2.48516100	-0.96750700	H	2.27900500	3.10992100	-2.30808700
C	1.81835800	2.28856100	-1.74019400	H	3.15962900	0.96737200	-2.75656500
C	2.00053400	-0.32162800	1.40131100	C	0.27182400	3.75150800	-0.73152100
C	2.37973400	1.00119400	-1.99189300	C	1.03720300	4.94556200	-0.77682500
C	2.69941200	0.83683000	1.78521300	C	-1.10157100	3.84406600	-0.38904400
C	3.76469500	0.77585500	2.69348800	C	0.44377000	6.18056000	-0.51248700
C	4.16533700	-0.45231300	3.23267100	H	2.10399600	4.89423900	-0.98160900
C	3.48349200	-1.61423200	2.85389300	C	-1.68101100	5.08593700	-0.14182700
C	2.41480800	-1.54704000	1.95021600	H	-1.69773300	2.93095200	-0.34798300
H	2.40374700	1.80126300	1.37767800	C	-0.91943800	6.26400500	-0.20118800
H	4.28142800	1.69213200	2.98017200	H	1.05270600	7.08394400	-0.53752400
H	4.99450900	-0.50265000	3.93736600	H	-2.73970000	5.13203500	0.10453900
H	3.78118700	-2.57931200	3.26402700	H	-1.37843600	7.22924300	0.00410100
H	1.89185500	-2.46248000	1.68160600	C	2.60317900	-1.33924300	-1.84665200
H	-0.35926400	-1.50560300	4.76138900	C	1.81901900	-2.50897800	-1.94033600
C	-0.68961800	-1.28896100	3.74622900	C	3.98035200	-1.42482700	-2.14573100
C	-0.62302600	0.00360400	3.25210900	C	2.39127100	-3.71103500	-2.34862800
C	-1.18859100	-2.32664500	2.92953700	H	0.75798100	-2.44031300	-1.71609300
C	-1.06166400	0.27628800	1.93324400	C	4.54593600	-2.63812800	-2.54288800
H	-0.23860700	0.81131900	3.87265900	H	4.61190500	-0.55020000	-2.01699000
C	-1.61897800	-2.06005500	1.63771600	C	3.75810500	-3.78876900	-2.65400700
H	-1.26182800	-3.33758800	3.32990000	H	1.76235400	-4.59490400	-2.42902600
C	-1.59676200	-0.74057700	1.09768500	H	5.61447100	-2.68654900	-2.74746100
H	-1.14236600	1.31131400	1.60844700	H	4.20184500	-4.73325000	-2.96185700
H	-2.07377700	-2.83970100	1.03255100	P	-4.82139600	-1.62884900	-0.62338400
B	-2.34373700	-0.37826100	-0.36436200	O	-5.05513700	-2.43345600	0.67587600
O	-1.11368300	-0.29247000	-1.32624800	O	-5.38949800	-0.18156200	-0.52168800
O	-3.18680800	-1.45317000	-0.80220700	O	-5.32035900	-2.38206800	-1.87037100
O	-2.92835000	0.94907300	-0.34714400				

4'TS$_{PO4}$_1 thermal Free Energies = -2059.119339 A.U.

B	-2.17093500	-0.42626900	-0.73895900	Pd	0.49563500	-0.28403800	-0.06870900
O	-0.94780000	-0.19514900	-1.62356100	N	2.20913200	0.13162900	-1.29710500
O	-2.83297300	-1.60588100	-1.13880000	N	0.68241800	2.61837200	-0.82525800
O	-2.90456400	0.79776900	-0.65538500	C	1.82831600	2.55637600	-1.45349500
H	-0.99810500	0.73255000	-1.90538300	C	1.72326000	-0.43735000	1.51461900
H	-3.86315100	0.52693600	-0.64706600	C	2.54538800	1.34374900	-1.70049900

H	2.28851000	3.45118100	-1.89823100	C	2.21300200	0.72501600	2.14115300
H	3.42361200	1.44915700	-2.34347900	C	3.12235100	0.65748500	3.20460500
C	0.05474600	3.83003000	-0.58043900	C	3.57280600	-0.58287800	3.67214700
C	0.72694900	5.07368300	-0.46047600	C	3.09650100	-1.74890100	3.06299800
C	-1.35116500	3.80486400	-0.40104700	C	2.18373200	-1.67412000	2.00200800
C	0.01419100	6.24470600	-0.20025800	H	1.87578700	1.70020100	1.79518400
H	1.81134800	5.10951400	-0.53064800	H	3.47649700	1.57744700	3.67095100
C	-2.04940700	4.98467100	-0.15558800	H	4.27811000	-0.63946600	4.50063000
H	-1.87566800	2.85106500	-0.47271600	H	3.43193600	-2.72425600	3.41636500
C	-1.37865500	6.21356400	-0.05510800	H	1.82318000	-2.59701800	1.55375600
H	0.55158600	7.18689100	-0.09611600	H	-1.65587800	-1.67603800	4.74741500
H	-3.12965100	4.94052200	-0.03433300	C	-1.58471200	-1.41980700	3.69044800
H	-1.93071400	7.12905500	0.14876000	C	-1.58615000	-0.07757800	3.29519900
C	3.02579900	-0.95299300	-1.65758100	C	-1.50911400	-2.43400200	2.72854200
C	2.41909900	-2.19739800	-1.93072500	C	-1.50738000	0.24030700	1.93745800
C	4.43186500	-0.85769600	-1.74504500	H	-1.65072400	0.71259700	4.04263000
C	3.19069100	-3.29326000	-2.30869900	C	-1.42483500	-2.10248700	1.37655000
H	1.33769200	-2.27247600	-1.85694800	H	-1.54675700	-3.47859200	3.03348600
C	5.19765000	-1.96589100	-2.11224200	C	-1.42499100	-0.75498400	0.92835000
H	4.92440500	0.07177700	-1.47358700	H	-1.54679500	1.28266000	1.63104100
C	4.58596500	-3.18955900	-2.40427900	H	-1.43633100	-2.89219200	0.63070400
H	2.69689100	-4.23766400	-2.52679600	O	-5.16284300	-0.64203600	-0.70182200
H	6.28223600	-1.87554700	-2.14902400	O	-4.87059000	-2.68178200	-2.26166800
H	5.18551400	-4.05238300	-2.68671200	O	-4.52441800	-2.94927400	0.26495600
P	-4.44592100	-2.00208700	-0.94928500				

5'$_{PO4}$_1

H	1.86860200	1.95451300	-3.15890000	Pd	0.86617000	-0.15886800	0.44278200
C	-1.29605600	3.72921200	-0.50942600	N	1.46658400	0.60593700	-1.64695100
C	-0.84262900	5.03775400	-0.24747700	N	-0.45285100	2.69007300	-0.93181900
C	-2.65264100	3.39408400	-0.31870200	C	0.56368300	2.88046000	-1.68947500
C	-1.74465100	6.01422900	0.17661000	C	2.76137600	-0.03721700	1.09050700
H	0.21599700	5.27312000	-0.33198000	C	1.37596300	1.76520900	-2.19512600
C	-3.54244000	4.39052800	0.08846100	C	3.40328700	1.21738200	1.18412600
H	-2.99207700	2.36010400	-0.49874500	C	4.75505100	1.33987900	1.53639300
C	-3.09987300	5.69580600	0.33511300	C	5.52007500	0.19947900	1.80612500
H	-1.38827100	7.01842300	0.39930400	C	4.90736000	-1.05696500	1.72426000
H	-4.58901600	4.13133000	0.22929000	C	3.55413100	-1.16864200	1.38019100
H	-3.80106800	6.45816300	0.66973600	H	2.83537200	2.12541200	0.98383800
C	2.14084300	-0.42288000	-2.35928400	H	5.20900000	2.32961800	1.60357000
C	1.45699700	-1.63670800	-2.54368200	H	6.57043000	0.28796500	2.08165000
C	3.44429600	-0.26325900	-2.85031200	H	5.48449300	-1.95732300	1.93671500
C	2.07209000	-2.66671200	-3.25399600	H	3.10178800	-2.15663300	1.34346200
H	0.45364600	-1.74632400	-2.14019500	H	-1.27566000	-2.28251100	5.54520500
C	4.05839800	-1.31305200	-3.54064600	C	-0.83844700	-1.89603400	4.62461400
H	3.98686600	0.65590400	-2.64473800	C	0.25090100	-1.01878200	4.67200900
C	3.37285500	-2.51248700	-3.75239600	C	-1.36785000	-2.26015000	3.38140800
H	1.53164300	-3.59751100	-3.40540400	C	0.80707300	-0.51407600	3.48740200
H	5.07983700	-1.19508000	-3.89702300	H	0.67240700	-0.71943800	5.63297300
H	3.85291900	-3.32893100	-4.28770900	C	-0.81190100	-1.75499300	2.19848400
P	-4.04549900	-2.82640400	-0.67120700	H	-2.23117000	-2.91811700	3.30524500
O	-4.30574100	-3.27387100	0.75428200	C	0.28404800	-0.86976900	2.23014700
O	-5.13917000	-1.67802400	-1.13762700	H	1.65525100	0.16210200	3.55456200
O	-3.90126100	-3.85668400	-1.77233900	H	-1.27371800	-2.04312400	1.25814000
H	-1.14413500	0.87021400	-0.66605000	B	-2.53515400	-0.51488100	-0.66268900
H	-4.72488400	-0.77357500	-1.02422700	O	-1.13881000	-0.09564900	-0.53826600
H	0.80880200	3.86923600	-2.10628600	O	-2.63421400	-1.89986400	-0.65308400
				O	-3.46585300	0.40347200	-0.80914200

4$_{PO4}$_2 thermal Free Energies = -2059.146521 A.U.

Pd	1.22310500	0.27754300	0.08259400	N	0.30309600	2.40254800	-0.23694400
C	-3.31518800	2.33487800	-0.99277800	N	2.90420700	1.51253600	-0.05744300
H	-1.70038500	0.93051500	-1.12536400	C	1.28926300	3.26217900	-0.26608800
C	-3.71569100	3.61620600	-0.60454900	C	2.22929200	-1.40233700	0.50485100
H	-3.09190400	5.48943000	0.28737300	C	2.63507000	2.80022000	-0.18416500
H	-4.02566000	1.60806700	-1.37964900	C	2.97965800	-1.46199100	1.69029900
H	-4.75912900	3.91238200	-0.69125700	C	3.72108100	-2.60697800	2.01453200
H	-6.06534200	0.43872200	3.78563200	C	3.72309600	-3.70730900	1.15109300
C	-5.65168400	0.06805200	2.84643300	C	2.96323200	-3.65566100	-0.02385800
C	-6.48600200	-0.18869200	1.74999700	C	2.21135600	-2.51805200	-0.34554200
C	-4.27551300	-0.15542800	2.71128600	H	2.99507700	-0.61422900	2.37344000
C	-5.94122300	-0.66311400	0.54971400	H	4.29420100	-2.63544100	2.94177000
H	-7.56186100	-0.01813600	1.83319000	H	4.29425200	-4.60126900	1.40074600
C	-3.74676100	-0.62804000	1.50259100	H	2.92746900	-4.51888400	-0.68751700
H	-3.60797200	0.04418700	3.55103300	H	1.57737200	-2.50282400	-1.23260600
C	-4.55990800	-0.89955900	0.38302000	H	3.44687200	3.51533400	-0.32871700
H	-6.59800100	-0.85594000	-0.29725600	H	1.12464500	4.33013800	-0.43444600
H	-2.67319300	-0.78106500	1.42029800	C	4.26945100	1.13669700	-0.08584000
B	-3.98768500	-1.54524200	-1.02942600	C	4.68173300	0.07737100	-0.91162700
O	-4.81370900	-0.98084700	-2.11771200	C	5.22790600	1.80815000	0.69508400
O	-2.54163100	-1.10664400	-1.27607400	C	6.02723200	-0.28247300	-0.96779700
O	-4.08239700	-3.00767700	-1.03233100	H	3.93550800	-0.45406300	-1.49095300
H	-3.24929600	-3.35900700	-0.65782600	C	6.57324000	1.43462800	0.64044000
O	-0.50257400	-0.65253200	0.06279000	H	4.90667300	2.59675600	1.37078200
H	-4.55112700	-1.46846400	-2.91341700	C	6.98174000	0.39082900	-0.19515600
P	-1.12560900	-1.79193900	-0.95525300	H	6.32728400	-1.10796800	-1.60878400
O	-0.23975100	-1.81747100	-2.20359700	H	7.29884300	1.95274800	1.26493000
O	-1.31571800	-3.10636900	-0.19741600	H	8.02764000	0.09361100	-0.23196700
C	-1.98212200	1.94134800	-0.85502900	C	-1.02840400	2.83620000	-0.33580400
C	-2.77667900	4.50577600	-0.05858900	C	-1.44390100	4.12507800	0.07878400
H	-0.73873600	4.80255700	0.55476500				

4'$_{PO4}$_2 thermal Free Energies = -2059.163591 A.U.

C	0.93851500	2.19839100	-2.05781900	C	4.94664600	-2.19296000	-1.27425500
Pd	1.16573300	-0.29697500	0.34985100	H	2.77331000	-2.07296500	-1.12607000
C	1.55606100	1.06499600	1.81309600	C	6.12279100	-0.07875500	-1.26023100
C	2.19440300	1.46045800	-1.94447800	H	4.87484700	1.68130300	-1.10867500
C	2.10739800	2.34491800	1.61172100	C	6.15034200	-1.47469300	-1.31129300
C	2.36480000	3.22202500	2.67648500	H	4.95764700	-3.28000900	-1.29789600
C	2.07537200	2.83772700	3.98956400	H	7.05107700	0.48969100	-1.26164100
C	1.52132800	1.56977100	4.21404200	H	7.10145100	-2.00126300	-1.36274800
C	1.26553400	0.70252600	3.14533300	C	-1.33039600	2.52460200	-1.56128900
H	2.34095800	2.68511600	0.60334900	C	-1.40394700	3.93203000	-1.61536400
H	2.78766900	4.20824300	2.47626200	C	-2.50915800	1.75335500	-1.55900500
H	2.27032500	3.51449200	4.82145700	C	-2.64848000	4.56007500	-1.68708900
H	1.28129700	1.25551500	5.23063800	H	-0.49425400	4.52456400	-1.54599100
H	0.81899900	-0.27277100	3.32614300	C	-3.74441000	2.39646300	-1.64942800
N	-0.12542300	1.82324500	-1.45414600	H	-2.42654100	0.66188600	-1.50870300
N	2.43613200	0.53213600	-1.07526100	C	-3.82117700	3.79359500	-1.71313700
H	2.96045700	1.70289800	-2.68873900	H	-2.70467700	5.64761700	-1.70034500
H	0.95871700	3.05370400	-2.75314700	H	-4.64920900	1.79421000	-1.63545700
C	3.70072100	-0.12931000	-1.15226200	H	-4.79112100	4.28634900	-1.75437800
C	3.72090500	-1.53457600	-1.18194200	H	-6.44556400	0.54760800	2.24737100
C	4.90010600	0.59738800	-1.18606900	C	-5.71512400	-0.01738900	1.66637600
O	0.00410500	-1.48837200	1.53310200	C	-6.10737700	-0.72578800	0.52343600
O	-2.02948500	-1.36085500	-1.72155700	C	-4.36840300	-0.05004300	2.05296400
O	-1.64209100	-2.94407000	0.12637900	C	-5.15858500	-1.44841000	-0.21444300
O	-3.41213000	-3.35239500	-1.49894500	H	-7.15434000	-0.72011600	0.21192700
H	-1.06006200	-1.42288500	-1.60917800	C	-3.43253400	-0.77605100	1.30542400
H	-2.78151700	-3.72178500	-2.13462900	H	-4.04493700	0.49551400	2.94030600

P	-0.11284200	-2.71291700	0.47925000	C	-3.79711800	-1.49387000	0.14737200
O	0.53726500	-3.99361100	0.94053100	H	-5.47163400	-2.00833700	-1.09410500
O	0.59251600	-2.00432400	-0.78886100	H	-2.39134300	-0.79428300	1.62294900
				B	-2.68766600	-2.29143700	-0.77323700

4'TS$_{PO4}$_2 thermal Free Energies = -2059.11543 A.U.

H	-0.23577700	3.66637700	-1.53471400	Pd	0.60871800	-0.11023500	-0.00683800
C	-3.66225000	1.06110300	-0.31036700	N	0.56065500	1.93906600	-0.76378600
C	-4.55374500	1.97433700	0.27922200	N	-2.28281400	1.30450300	-0.35941000
C	-4.13960700	-0.15350400	-0.83944100	C	-1.85377300	2.37272300	-0.90726900
C	-5.91670800	1.67588400	0.34526800	C	0.19559100	0.54772100	1.87443800
H	-4.16453200	2.88999700	0.71765300	C	-0.43501100	2.69930700	-1.05600800
C	-5.50555000	-0.41913400	-0.78650900	C	-0.94874200	0.05342800	2.53061000
H	-3.40632100	-0.81645600	-1.30652600	C	-1.35015700	0.56193100	3.76931800
C	-6.39959100	0.48226500	-0.19347600	C	-0.61426200	1.57447300	4.39711600
H	-6.59868000	2.37893200	0.82135100	C	0.53201600	2.06548000	3.76880200
H	-5.87685100	-1.35133700	-1.20726700	C	0.92842600	1.55505300	2.52438900
H	-7.46210400	0.25007500	-0.14357700	H	-1.50194800	-0.75852700	2.06108900
C	1.86014000	2.43734400	-1.06391700	H	-2.24231800	0.16173200	4.25251900
C	2.29642100	3.66592000	-0.54660800	H	-0.92724000	1.96866500	5.36424000
C	2.69827200	1.67656600	-1.89727300	H	1.12481800	2.84657100	4.24853500
C	3.57246100	4.14018900	-0.86376300	H	1.83090400	1.95230200	2.05991900
H	1.64946000	4.21885900	0.12901500	H	4.71325500	-2.12413800	2.74747800
C	3.95867200	2.17556500	-2.21668300	C	3.77791100	-2.14004400	2.18607300
H	2.31504900	0.71988800	-2.26197500	C	2.55409800	-2.25296400	2.86260100
C	4.40452800	3.40155100	-1.70491900	C	3.79147000	-2.04227400	0.79557000
H	3.91360200	5.08488800	-0.44421000	C	1.36548100	-2.26394000	2.14072600
H	4.60581900	1.59344000	-2.86905500	H	2.54037500	-2.32637800	3.95047100
H	5.39810700	3.77053500	-1.95249800	C	2.58405800	-2.06811500	0.08143300
B	-0.03154400	-3.11381000	-0.03951200	H	4.74002500	-1.95263100	0.26483100
O	-1.32164100	-2.64503300	0.44270900	C	1.32459800	-2.19604200	0.72151700
O	0.13297300	-3.06159800	-1.49117200	H	0.42159800	-2.36715000	2.66902300
O	0.22338900	-4.45888800	0.48516000	H	2.58327800	-2.01522400	-1.00300400
H	-1.64753400	-2.06052000	-0.28190000	H	-2.53529800	3.10335200	-1.37355200
O	-0.14443000	-2.11304500	-3.86899600	H	-0.68069500	-4.77413200	0.63806400
O	-1.56737600	-1.18820800	-1.86944100	P	-0.21576700	-1.74990400	-2.40642600
O	0.93993800	-0.70630400	-2.00077500				

5'$_{PO4}$_2

C	-2.62846700	4.74011600	-2.30004700	Pd	0.90095500	0.06084700	0.54764300
H	-0.62618600	3.98626500	-2.63971100	N	0.78048200	-0.88866700	-1.51479000
C	-4.20782900	3.13748200	-1.41402100	N	-0.91532500	1.47954700	-1.92281500
H	-3.42769600	1.13879400	-1.06867800	C	-1.20847200	0.29270300	-2.31505300
C	-3.92065300	4.43678500	-1.85009200	C	2.57023700	1.08454700	0.09805400
H	-2.38740800	5.75165400	-2.62379800	C	-0.23768100	-0.81862900	-2.29193600
H	-5.19915200	2.89548400	-1.03562300	C	2.55552700	2.00213300	-0.97786500
H	-4.68721200	5.20918200	-1.82082000	C	3.71069700	2.67757200	-1.39590500
C	1.66815800	-1.99453000	-1.68775900	C	4.93644700	2.45423800	-0.75513400
C	2.99554400	-1.73198600	-2.06182500	C	4.97908600	1.55122200	0.31443800
C	1.23774700	-3.31262700	-1.46774800	C	3.81645100	0.89022600	0.73415700
C	3.88171100	-2.79201700	-2.26362800	H	1.61749200	2.17875400	-1.50008300
H	3.31958800	-0.70221000	-2.17712800	H	3.65337100	3.37957100	-2.22970700
C	2.14323900	-4.36089900	-1.66414700	H	5.83767800	2.97391900	-1.08080200
H	0.22653100	-3.49030100	-1.08534800	H	5.92242400	1.36272500	0.82954600
C	3.45903900	-4.11334600	-2.07067000	H	3.87960700	0.20873900	1.57933800
H	4.90850200	-2.58149700	-2.55816500	H	0.97844200	1.75796400	6.25667900
H	1.81113400	-5.38125700	-1.48047600	C	0.98266800	1.46997200	5.20496400
H	4.15502300	-4.93830300	-2.21708800	C	1.41604500	2.36607400	4.22203000
B	-4.50986300	-1.99991900	1.15059300	C	0.54160800	0.20000400	4.81026200
O	-5.02841000	-1.58886100	-0.05873100	C	1.42516000	1.98823800	2.87093100

O	-3.18745100	-2.13491500	1.42471600	H	1.75226900	3.36552600	4.50348700
O	-5.43090400	-2.28968200	2.16845000	C	0.53711400	-0.16636900	3.45849700
H	-4.22481800	-1.40177400	-0.63655900	H	0.18131100	-0.50751500	5.55816900
H	-6.31385600	-2.11849600	1.81015600	C	0.99032700	0.71411400	2.45189700
P	-1.91948200	-1.99754900	0.29432300	H	1.78007800	2.70433000	2.13445500
O	-1.48980300	-3.41963100	-0.03448200	H	0.13894700	-1.13256500	3.16282500
O	-2.59257200	-1.24312100	-0.91104300	H	-2.16117400	0.05046800	-2.79011900
O	-0.88485600	-1.12196400	1.03414400	H	-0.42658900	-1.61574900	-3.01991900
C	-1.63866900	3.75687900	-2.31728300	C	-1.93423800	2.44029500	-1.91454600
C	-3.22993200	2.14103300	-1.44277800				

4$_{PO4}$_12 thermal Free Energies = -2059.124436 A.U.

O	-2.56780200	-0.46225600	1.73351100	Pd	0.41265000	0.00738500	0.11260300
O	-2.58506200	-2.40887900	0.22717400	N	1.18572300	-1.23529200	-1.35308100
H	-2.00716900	0.63363800	-0.73948500	N	0.62343900	1.45419000	-1.37310400
H	-1.68947300	-2.60405900	0.54798800	C	1.03458600	0.81540100	-2.54045300
H	1.06183000	1.38369300	-3.46668200	C	2.26377700	0.33745300	0.86078900
H	1.49299500	-1.04536000	-3.45944100	C	1.28317000	-0.51733000	-2.53305200
C	0.85203500	2.81036100	-1.20347100	C	3.35631300	0.53590200	0.01519500
C	1.61766500	3.58339600	-2.11994700	C	4.62534300	0.77109100	0.56127800
C	0.26558200	3.50241100	-0.10968900	C	4.80478600	0.80633200	1.94684700
C	1.73918600	4.96800400	-1.97523800	C	3.70244000	0.60500500	2.78347700
H	2.13973800	3.09223700	-2.93464000	C	2.42864800	0.37050300	2.24837200
C	0.41386200	4.87723400	0.02929900	H	3.23542800	0.51033600	-1.06374100
H	-0.28871200	2.92935500	0.62621000	H	5.47174100	0.92470000	-0.10744100
C	1.13891200	5.63724400	-0.90524900	H	5.79191900	0.98839600	2.37008700
H	2.33150700	5.52368500	-2.70301300	H	3.82319900	0.62951700	3.86572100
H	-0.05021400	5.36822300	0.88378100	H	1.58673100	0.21964900	2.91281000
H	1.24103200	6.71505000	-0.79149300	H	-7.89590200	0.39452100	-1.41258100
C	1.79444700	-2.46284700	-1.20412500	C	-6.89898300	0.12411400	-1.06377900
C	1.56379800	-3.25147100	-0.04397800	C	-6.17693700	-0.89630900	-1.69737700
C	2.66055500	-3.01715200	-2.19128500	C	-6.32253600	0.78898400	0.02436700
C	2.13392800	-4.51101000	0.09419500	C	-4.89712400	-1.23649300	-1.24472100
H	0.93564200	-2.84663600	0.74124600	H	-6.61489700	-1.42593000	-2.54449000
C	3.21321800	-4.29093300	-2.03971900	C	-5.04082700	0.43464000	0.46718100
H	2.92135000	-2.43885800	-3.07147300	H	-6.87361000	1.58215700	0.53100700
C	2.95935900	-5.06160400	-0.90152900	C	-4.29175200	-0.58205600	-0.15358000
H	1.92516500	-5.07852500	1.00037100	H	-4.34380800	-2.03362700	-1.73713000
H	3.86781900	-4.67440400	-2.82336800	H	-4.60466100	0.94490500	1.32353800
H	3.39512200	-6.05228600	-0.78548000	B	-2.78188100	-0.98463200	0.32208700
P	-1.11454300	-0.21136500	2.33417400	O	-1.76719200	-0.29635300	-0.60593300
O	-1.09877400	-0.16325100	3.83301600	O	-0.49996000	1.09147400	1.60773500
O	-0.13270600	-1.29372700	1.64141900				

4'TS$_{PO4}$_12 thermal Free Energies = -2059.092733 A.U.

H	-1.87070200	-0.23531600	-1.29598900	Pd	0.43930300	-0.07905500	-0.15807400
H	-1.85194600	-3.66520800	-1.76045600	N	0.30384200	2.07840800	-0.33920500
H	-2.76654000	3.13971700	-1.26827600	N	-2.69417000	1.29246600	-0.30026300
H	-0.53986900	3.54904900	-1.54424900	C	-2.12775400	2.36583400	-0.81561500
C	-4.06536900	1.28327800	-0.08976400	C	1.77041000	-0.00519500	1.32301700
C	-4.82699000	2.43393700	0.23905700	C	-0.74401100	2.67253600	-0.92116600
C	-4.74732200	0.04272400	-0.16134200	C	1.54950000	0.83630300	2.42215600
C	-6.20320700	2.34727500	0.45581600	C	2.46479900	0.87493600	3.48402600
H	-4.32093900	3.38795700	0.36280300	C	3.60812900	0.07035300	3.45583000
C	-6.12159500	-0.03100900	0.05162000	C	3.82052800	-0.77698700	2.36063900
H	-4.17780400	-0.85065400	-0.40482400	C	2.90991400	-0.82378600	1.29718100
C	-6.86616300	1.11789500	0.35912200	H	0.66618800	1.46978100	2.45455100
H	-6.76039000	3.24630900	0.71812200	H	2.28007700	1.53780200	4.32992300
H	-6.61760400	-0.99713100	-0.02184100	H	4.32246000	0.09932400	4.27857300
H	-7.93857800	1.05284700	0.53247300	H	4.70069100	-1.41916500	2.33115900

C	1.50480200	2.82832000	-0.40766500	H	3.07084400	-1.50670900	0.46303800
C	2.69462800	2.24623500	-0.88627700	H	-1.17770300	-3.90808600	3.93114900
C	1.52496100	4.17343200	0.01613200	C	-0.99279800	-3.40327100	2.98230200
C	3.86443400	3.00489300	-0.93551300	C	-1.79591700	-2.32749900	2.58806600
H	2.67655400	1.21520600	-1.23661400	C	0.05952300	-3.81625500	2.15370600
C	2.70646900	4.91790600	-0.02755100	C	-1.54920800	-1.68736800	1.36753500
H	0.61436000	4.61437100	0.41438900	H	-2.61111500	-1.98744300	3.22773300
C	3.88585400	4.33881500	-0.50715000	C	0.31205000	-3.15772600	0.94629300
H	4.77190100	2.53990700	-1.31536600	H	0.69929500	-4.64422900	2.46100300
H	2.70423300	5.94878700	0.32498900	C	-0.50363800	-2.09090500	0.50149200
H	4.80912400	4.91491300	-0.53996900	H	-2.20059200	-0.86778200	1.07279300
P	1.85503600	-2.17826200	-2.15714700	H	1.15384700	-3.45836100	0.32045200
O	2.29573400	-2.21716900	-3.60924700	B	-0.84839600	-2.02403800	-1.42884600
O	1.82474300	-0.63948300	-1.66974100	O	-1.04520600	-0.58677800	-1.68315600
O	2.58775300	-3.06184000	-1.14741800	O	0.23836900	-2.61604000	-2.09045100
				O	-2.08729000	-2.74736300	-1.56225400

5'$_{PO4}$_12

C	0.64581900	2.95534600	1.14925100	Pd	-0.23182200	0.23790000	0.27629900
H	1.34780400	4.93779900	1.60364100	N	-0.74836400	-1.73477000	-0.71408800
C	0.74163700	1.58580500	1.44174200	N	2.26818300	-1.46113100	-0.82889700
H	1.70887800	0.11629000	2.70420500	C	1.55065700	-2.52115300	-1.17283900
H	-0.01252200	3.31419700	0.35484000	C	-1.23739600	-0.23897700	1.93803700
B	0.44180900	1.16144200	-2.81712200	C	0.13637800	-2.60005400	-1.20482300
O	0.95790700	0.80363400	-1.57886000	C	-0.84391600	-1.27533100	2.79835900
O	-0.66042400	1.89846400	-3.00151000	C	-1.62684200	-1.62866000	3.90727400
O	1.15181100	0.70412100	-3.93927600	C	-2.81485000	-0.94201100	4.17840600
H	1.60959900	0.05933800	-1.53680500	C	-3.21135300	0.09653800	3.32563200
H	0.67388000	1.02664600	-4.71787500	C	-2.43182400	0.44582000	2.21646200
H	2.05234700	-3.44648600	-1.48396100	H	0.07773200	-1.82261300	2.60720200
H	-0.24555200	-3.51557700	-1.66669400	H	-1.30506800	-2.44346100	4.55714100
C	3.63304900	-1.58275300	-0.60329600	H	-3.42482700	-1.21376100	5.03961700
C	4.31086400	-2.79840400	-0.32771800	H	-4.13565100	0.63962700	3.52319700
C	4.40476100	-0.39489400	-0.61812700	H	-2.74428800	1.24292300	1.54593700
C	5.69183500	-2.81982600	-0.12467600	H	2.92824300	4.18696100	3.39217700
H	3.74667800	-3.72245000	-0.23892600	C	2.31970000	3.46129300	2.85156200
C	5.78060500	-0.42587300	-0.41469900	C	2.41706700	2.09699500	3.14601000
H	3.88982500	0.54657100	-0.78714800	C	1.43240300	3.87993700	1.85240500
C	6.44315000	-1.63981400	-0.17375400	C	1.62600700	1.17074300	2.45036000
H	6.18384500	-3.76813400	0.09033800	H	3.10390200	1.74787200	3.91828700
H	6.34202600	0.50628700	-0.43514400	C	-4.80414100	-2.95112200	-0.85865000
H	7.51850300	-1.66116700	-0.00831600	H	-5.19128500	-0.87565000	-1.33719200
C	-2.09750500	-2.16242800	-0.73637800	H	-4.08611300	-4.91430300	-0.30158700
C	-3.10236500	-1.21738300	-1.02305500	H	-5.84992900	-3.25150100	-0.90337100
C	-2.47344400	-3.49782700	-0.47132000	P	-1.72919700	2.66291500	-1.84258500
C	-4.43503800	-1.62042100	-1.09841100	O	-3.02807500	2.81352900	-2.61856100
H	-2.81950700	-0.17249500	-1.16793500	O	-1.86798700	1.55345000	-0.72932800
C	-3.81453400	-3.88415900	-0.53047600	O	-0.97083900	3.90581600	-1.40074200
H	-1.71800700	-4.22036600	-0.17353900				

4$_{PO4}$_3 thermal Free Energies = -2059.143648 A.U.

C	-1.37114700	-1.88450000	0.77069100	Pd	0.21096100	0.05638400	-0.73964600
H	0.33563900	-3.05690000	1.48292700	C	1.93902600	1.09471700	-0.77110100
H	-1.82612600	-2.88462300	0.76120400	C	0.13367600	-2.01164900	1.21381600
P	-1.04438300	-0.41041200	2.88886100	C	2.61750100	1.38818100	-1.96858600
O	-1.41697900	-0.53324800	4.33000400	C	3.81887000	2.10974000	-1.97671100
O	0.27758200	-1.28586100	2.48739100	C	4.37631100	2.56042300	-0.77492700
O	-2.07883900	-1.19758300	1.87685900	C	3.71558400	2.27747600	0.42649700
H	-2.16165300	2.98027300	3.57709000	C	2.51674500	1.55324100	0.42709700
H	-3.16302400	0.72017000	1.44485300	H	2.20632900	1.05058600	-2.91997600

C	2.28796800	-2.13254300	0.15301600	H	4.31964100	2.31770100	-2.92356100
C	2.87877800	-2.83836400	1.24197000	H	5.31165300	3.11973400	-0.77439600
C	3.06405200	-2.04651700	-1.03589500	H	4.13552600	2.61991900	1.37237700
C	4.12813400	-3.45006300	1.11724900	H	2.02057000	1.34499300	1.37163200
H	2.36856100	-2.86461300	2.19941700	H	0.30411100	3.76326200	-3.10316400
C	4.31339000	-2.64537400	-1.13923500	C	-0.11835700	3.45968200	-2.14716700
H	2.64780100	-1.49433000	-1.87199500	C	-0.91985400	2.31101900	-2.05726900
C	4.86580200	-3.36991000	-0.06916500	C	0.13537900	4.19727400	-0.99206100
H	4.54125200	-3.97603900	1.97865700	C	-1.44959300	1.92104700	-0.81130700
H	4.86799400	-2.54863800	-2.07265500	H	-1.19316900	1.76184900	-2.95602800
H	5.84619300	-3.83542900	-0.15367200	C	-0.38014600	3.78744500	0.24869800
C	-2.55938200	-1.51189400	-1.27414700	H	0.75767200	5.09041000	-1.04940500
C	-2.52582500	-1.13306500	-2.65115800	C	-1.17709000	2.64366600	0.38329200
C	-3.75339500	-2.16842900	-0.83877000	H	-2.19954200	1.13775600	-0.78621200
C	-3.57776900	-1.40681600	-3.51693400	H	-0.16415800	4.37188900	1.14001300
H	-1.62546000	-0.64507100	-3.01697900	B	-1.79442100	2.16975500	1.82932400
C	-4.79400200	-2.44770400	-1.72463900	O	-3.14793000	1.63370600	1.76909000
H	-3.87103200	-2.41746200	0.21138900	O	-0.80544000	1.01706000	2.31115400
C	-4.73096300	-2.07751300	-3.07472200	O	-1.72310100	3.27157300	2.76418800
H	-3.49546900	-1.10096300	-4.56046700	N	1.02714900	-1.59341900	0.19641400
H	-5.68618400	-2.94507800	-1.34224800	N	-1.48910900	-1.23949400	-0.47791700
H	-5.55425200	-2.28785300	-3.75476300				

4'TS$_{PO4}$_3 thermal Free Energies = -2059.114749 A.U.

C	-0.89648300	-2.33361200	-0.21191100	N	1.28277800	-1.42282800	-0.59724000
Pd	0.17508800	0.35789700	-0.43503200	N	-1.38267600	-1.29486100	-0.79144500
C	1.80248000	1.47100300	-0.14695000	H	0.92616200	-3.38798300	-0.00842500
C	0.56826700	-2.36779700	0.21014700	H	-1.46089400	-3.26547800	-0.14557200
C	2.24028300	2.40798100	-1.09887000	P	-0.44717900	-1.61497700	2.64770000
C	3.41157900	3.15121300	-0.90031900	O	0.03527400	-1.87669500	4.04534700
C	4.17063400	2.97618800	0.26242900	O	0.74197700	-2.23521000	1.63531600
C	3.74116700	2.04858800	1.21947100	O	-1.77835500	-2.19455600	2.13591300
C	2.57231900	1.30398100	1.01730400	H	-0.64301000	1.80449100	3.55557600
H	1.65418700	2.57651500	-2.00053800	H	-2.70081300	-0.58792200	1.87714900
H	3.72691700	3.87256800	-1.65547100	C	2.57875100	-1.69849700	-0.93424600
H	5.08299100	3.55116500	0.41870400	C	3.37087500	-2.70641600	-0.30507400
H	4.32180200	1.89609100	2.12922900	C	3.20055700	-0.98807800	-2.00236100
H	2.25182900	0.58714500	1.76843600	C	4.65455800	-3.01095300	-0.76204700
H	-2.18846800	5.36031400	-1.50367000	H	2.98593100	-3.21168900	0.57515200
C	-1.90931600	4.44286800	-0.98405900	C	4.48490200	-1.29242900	-2.43448400
C	-2.60682800	3.25592300	-1.21897600	H	2.63275700	-0.19280100	-2.47547200
C	-0.85143100	4.44497000	-0.06261100	C	5.23385300	-2.31985200	-1.83306600
C	-2.24282500	2.08798200	-0.53131700	H	5.22313000	-3.78635700	-0.24689000
H	-3.44149300	3.23917700	-1.92087400	H	4.91440500	-0.71871100	-3.25626700
C	-0.49919400	3.26576100	0.59371400	H	6.24232400	-2.55112400	-2.17189000
H	-0.30259500	5.36622100	0.13515900	C	-2.70005800	-1.35932300	-1.29936700
C	-1.17761300	2.03353200	0.39866200	C	-2.95990500	-0.80210600	-2.56211700
H	-2.84535900	1.19724100	-0.67307300	C	-3.74811100	-1.96136000	-0.58092700
H	0.31789000	3.30037500	1.30902600	C	-4.23906200	-0.87659900	-3.11510600
B	-1.49337300	0.93858900	2.03108400	H	-2.14577600	-0.31269000	-3.08939800
O	-2.77409000	0.38570400	1.77876800	C	-5.02770100	-2.02188000	-1.13818100
O	-0.40722000	-0.03367800	2.28079400	H	-3.54792600	-2.33701200	0.41884700
O	-1.44057800	1.97600800	3.03411000	C	-5.28109800	-1.48885500	-2.40708400
H	-5.83601400	-2.47385300	-0.56605500	H	-4.42582300	-0.44580500	-4.09742900
H	-6.28203300	-1.53357300	-2.83281600				

5'$_{PO4}$_3

C	-0.43517700	-1.98412200	-1.26514400	Pd	0.02088000	0.81859800	-0.40352000
O	-0.55680200	-0.20223700	3.32702000	C	1.18805700	2.06108600	0.67404000
N	1.55050000	-0.63078400	-0.97981800	C	1.06241100	-1.94853800	-1.11154800

N	-1.15928600	-0.92512500	-1.20840200	C	1.22033900	3.46789700	0.61563600
H	1.46835700	-2.42955300	-2.02301000	C	2.08239200	4.22157300	1.42049200
H	-0.87627500	-2.95923900	-1.47203700	C	2.93248100	3.59297400	2.33339300
P	0.64007600	-3.35288200	1.26589400	C	2.91629900	2.19838500	2.41634100
O	1.50775200	-4.28527500	2.04465500	C	2.06763800	1.44725600	1.59486700
O	1.47255000	-2.93010100	-0.09050500	H	0.55113000	3.99007900	-0.06340900
O	-0.79453600	-3.73666000	0.88622500	H	2.08064400	5.30971300	1.33973400
H	0.23882600	0.26662300	3.02843800	H	3.59759700	4.17905500	2.96714600
H	-1.64102000	-2.93463700	2.19942900	H	3.57865200	1.68594100	3.11382700
C	2.83450000	-0.42198900	-1.41564600	H	2.10865600	0.36149800	1.64359500
C	3.78851800	-1.46782600	-1.60536500	H	-4.65809600	4.43550000	0.42337200
C	3.28079500	0.89121700	-1.74376000	C	-3.79141300	3.78833200	0.28897200
C	5.05407500	-1.21284500	-2.13269700	C	-3.00271400	3.88545100	-0.85964500
H	3.54053000	-2.47234400	-1.27989000	C	-3.44612100	2.84817700	1.26456600
C	4.54909800	1.12731000	-2.25601900	C	-1.89097900	3.04942600	-1.02234600
H	2.58980900	1.71278600	-1.58755200	H	-3.25117700	4.61571600	-1.63178100
C	5.45729000	0.08010700	-2.47482900	C	-2.33392900	2.01598400	1.09447300
H	5.74618000	-2.04714000	-2.25671500	H	-4.04718600	2.76156400	2.17017900
H	4.83509700	2.15164300	-2.49752800	C	-1.52494200	2.08408200	-0.05935000
H	6.45073200	0.27240700	-2.87701900	H	-1.29028200	3.15468000	-1.92641200
C	-2.56522800	-1.07220600	-1.35600400	H	-2.08556900	1.30540300	1.87947400
C	-3.27197600	-0.13029600	-2.11536300	B	-0.60935700	-1.43936000	2.71627700
C	-3.25280800	-2.13143300	-0.74020700	O	-1.75588100	-2.17098800	2.82309800
C	-4.64689100	-0.27138800	-2.29628500	O	0.52039800	-1.88020700	2.03797600
H	-2.73419800	0.71002800	-2.53987200	H	-5.18672000	0.46440900	-2.88881500
C	-4.63089300	-2.25532400	-0.92079300	H	-5.15951200	-3.07200500	-0.43324600
H	-2.69661800	-2.82067200	-0.10894000	H	-6.40871300	-1.43549600	-1.83663100
C	-5.33282700	-1.33601300	-1.70451700				