Electronic Supplementary Materials

Computational Design of SCS Nickel Pincer Complexes for Asymmetric Transfer Hydrogenation of Naphthyl Ketone

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1. Evaluation of Density Functionals

In order to examine the reliability of density functionals for this Ni system, we also calculated the free energy gaps between **1**$_{tBu}$ and the corresponding key transition states using six functionals with different percentage of Hartree-Fock exchange, including ωB97X [1], M06 [2], M06-2X [2], M11 [3], B3LYP [4,5], and ωB97X-D [1]. All structures were optimized independently using above functionals with same basis set. The computed free energy gaps are listed in Table S1. We can see that the functionals without dispersion corrections, such as B3LYP and ωB97X, have much larger relative free energies than the functionals with dispersion corrections. Such a strong influence of the dispersion correction is not unexpected because this (SCS)Ni pincer system has many non-covalent interactions in the reaction. The ωB97X-D functional has very similar results in relative free energies and is therefore suitable for the study of this (SCS)Ni system.

Table S1. Relative free energies of **1**$_{t\text{Bu}}$ calculated by using different functionals. All other computational details are the same as described in the text.

Functionals	ΔG_1 (kcal/mol) (**1**$_{t\text{Bu}}$→**TS**$_{2,3\text{-}t\text{Bu}}$)	ΔG_2 (kcal/mol) (**1**$_{t\text{Bu}}$→**TS**$_{5,6\text{-}t\text{Bu}}$)	ΔG_3 (kcal/mol) (**1**$_{t\text{Bu}}$→**TS**$_{5',6'\text{-}t\text{Bu}}$)	$\Delta\Delta G = \Delta G_2 - \Delta G_3$
M11	29.8	30.7	33.4	−2.7
M06	25.9	28.1	29.1	−1.0
M06-2X	30.2	30.1	33.0	−3.0
B3LYP	42.0	44.6	45.8	−1.1
ωB97X	36.9	38.5	40.9	−2.4
ωB97X-D	27.9	28.5	32.2	−3.7

2. Evaluation of Solvent Effect

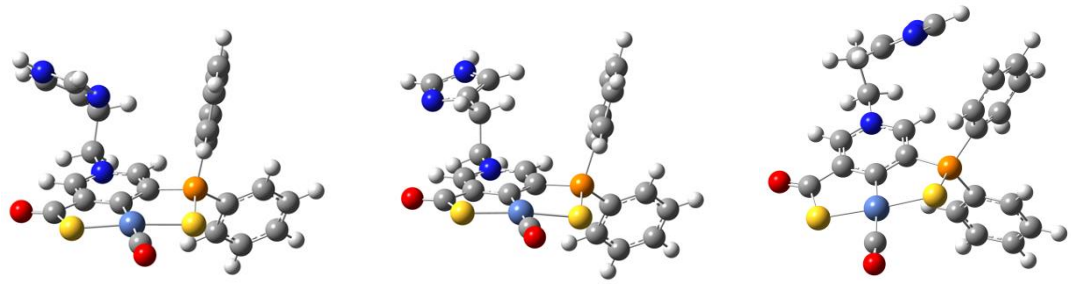
The calculated relative free energies of complexes **1**$_{tBu}$ in water, THF and acetonitrile are listed in Table S2. We can see differences of relative free energies and the enantioselectivity are less than 3 and 1 kcal/mol, respectively, in different solvents. THF has lowest free energy barriers and the highest enantioselectivity.

Table S2. Relative free energies (**1**$_{tBu}$) calculated by using different solvent. All other computational details are the same as described in the text.

Solvent	ΔG_1 (Kcal/mol) (**1**$_{tBu}$→**TS**$_{2,3\text{-}tBu}$)	ΔG_2 (Kcal/mol) (**1**$_{tBu}$→**TS**$_{5,6\text{-}tBu}$)	ΔG_3 (Kcal/mol) (**1**$_{tBu}$→**TS**$_{5',6'\text{-}tBu}$)	$\Delta\Delta G=\Delta G_2-\Delta G_3$
Acetonitrile	27.9	28.5	32.2	-3.7
Wate	27.0	27.0	30.7	-3.7
THF	25.4	25.9	30.2	-4.3

3. Isomers of **1**$_{Ph}$ their relative energies

Figure S3 shows optimized structure of **1**$_{Ph}$, the proposed catalyst with the imidazole group on top of the pyridinium ring, and two isomers with the imidazole group far away from the metal center (**1**$_{Ph}$′) and close to the PPh2 group in the pincer ligand (**1**$_{Ph}$″). Calculation results indicate that **1**$_{Ph}$ is 2.5 and 1.6 kcal/mol more stable than **1**$_{Ph}$′ and **1**$_{Ph}$″, respectively.



1$_{Ph}$ **1**$_{Ph}$′ **1**$_{Ph}$″

G_{solv} = −2548.622993 a.u. G_{solv} = −2548.618964 a.u. G_{solv} = −2548.620380 a.u.

Figure S3. Optimized structures and solvent corrected absolute free energies of **1**$_{Ph}$ and its isomers with the imidazole group far away from the metal center (**1**$_{Ph}$′) and on the other side of the pincer ligand close to the PPh_2 group (**1**$_{Ph}$″).

4. Absolute free energies (Hartree) and Cartesian coordinates (Ångström) of all structures optimized in acetonitrile.

1$_{Ph}$

G_{solv} = -2548.622993

Ni	0.11784964	-2.69903941	0.30404798
C	-1.33896087	1.26141827	0.15870062

C	-0.74986224	0.06352383	-0.19183665
C	-1.13566785	-1.86211116	2.98371467
C	-0.67680021	-1.01125504	0.70804612
C	-1.23325851	-0.77325476	1.96923052
C	-1.81519843	0.43486333	2.29338304
S	0.37572111	-2.18495544	-1.86869219
S	-0.26900317	-3.28150457	2.38882024
H	-1.39569255	2.11529172	-0.50899313
H	-2.23727201	0.63589961	3.27180299
C	-1.17141957	3.73407874	1.96886226
C	-2.35324818	2.77162743	1.77728429
H	-3.02381375	3.12283881	0.99165868
H	-2.91775402	2.64987699	2.70119725
N	-1.86664936	1.42828163	1.38600666
C	-0.09131071	3.17664481	2.84305370
N	0.89037207	2.35134010	2.32648892
C	0.08209427	3.30774124	4.19792672
C	1.63951294	1.99890120	3.35307213
N	1.18737503	2.55295227	4.50173808
H	-0.46634297	3.85708170	4.94810973
H	2.50824684	1.35757410	3.31835129
H	-0.75016475	3.98641424	0.99024485
H	-1.57959890	4.65345786	2.39752018
H	1.59774564	2.44032336	5.41929324
C	0.91182840	-4.33390027	0.01703583
O	1.41638181	-5.33700290	-0.14228314
O	-1.59136761	-1.78214333	4.10799265
P	0.10988010	-0.16815745	-1.76243521
C	1.66166256	0.75785263	-1.65926452
C	1.61215477	2.15893146	-1.67881870
C	2.87869342	0.09450371	-1.49185532
C	2.78599015	2.88910200	-1.53340688
H	0.66595381	2.67867800	-1.80333707
C	4.05075937	0.83553277	-1.34954958
H	2.91706445	-0.99002407	-1.47245891
C	4.00476809	2.22786412	-1.36964060
H	2.74883668	3.97364301	-1.54740584
H	4.99785541	0.32098736	-1.22273887
H	4.91962328	2.80165838	-1.25770519
C	-0.87821492	0.47516928	-3.12371212
C	-2.27219774	0.34530765	-3.07292090
C	-0.25582186	1.03135582	-4.24722159
C	-3.04161334	0.79288692	-4.14177100
H	-2.75745962	-0.10087576	-2.20940744

C	-1.03580962	1.47262872	-5.31302170
H	0.82485529	1.12368001	-4.29517043
C	-2.42438600	1.35756832	-5.25878541
H	-4.12215563	0.70067848	-4.10151673
H	-0.55693965	1.90746544	-6.18435557
H	-3.02842744	1.70744194	-6.09029419

2$_{Ph}$

G_{solv} = -2934.497939

Ni	0.80365400	-2.00877600	1.49153400
C	-2.33424400	-0.06982200	-0.55558800
C	-1.19194200	-0.79672100	-0.28693600
C	-1.14594000	-0.66373600	3.44724000
C	-0.77657300	-1.04554900	1.03198200
C	-1.58380900	-0.49261500	2.03220600
C	-2.72507100	0.22072600	1.73397700
S	1.03089900	-2.81703100	-0.58852800
S	0.39397900	-1.51407700	3.59356000
H	-2.68858200	0.13291800	-1.56085200
H	-3.36979000	0.64185000	2.49717400
C	-3.90492500	2.71709900	-0.04577300
C	-4.27676400	1.24116800	0.13258300
H	-4.70794400	0.83871400	-0.78409700
H	-4.98881000	1.10688800	0.94768500
N	-3.08711200	0.41681100	0.45063300
C	-3.38824800	3.36475900	1.19994400
N	-2.07800700	3.21956100	1.61506800
C	-4.07437600	4.11814500	2.11778500
C	-1.98085900	3.87816500	2.75529900
N	-3.16292100	4.43296100	3.09472700
H	-5.10093700	4.44934500	2.15603400
H	-1.08712600	3.97544000	3.35430300
H	-3.16947800	2.80820900	-0.85254100
H	-4.81490500	3.22783900	-0.37318900
H	-3.34044900	4.99241500	3.91860500
C	4.79750300	1.10254100	-0.03710900
C	5.11829800	2.27226900	-0.72897000
C	4.14222100	3.25053200	-0.91658400
C	2.85410100	3.06565600	-0.41147500
C	2.52824100	1.90063400	0.28432600
C	3.50957300	0.91938500	0.46096900
H	5.54764600	0.32937400	0.10423300
H	6.11941600	2.41501500	-1.12562500
H	4.38164600	4.15915300	-1.46230300

H	2.09062500	3.82205500	-0.56524300
H	3.25734800	-0.00038800	0.98751000
C	1.15616300	1.69302200	0.89164900
H	0.96124900	0.60999400	0.85967300
O	0.18111900	2.37284000	0.12999300
H	-0.59687400	2.58785400	0.68950500
C	1.13645600	2.12739500	2.35718300
H	1.91236000	1.60320400	2.92294800
H	1.31344600	3.20614600	2.43555400
H	0.16918400	1.89496900	2.81393200
C	2.41341700	-2.75657100	1.97286700
O	3.43253600	-3.16680200	2.25535100
O	-1.77465200	-0.25093500	4.40322300
P	-0.15289300	-1.49480100	-1.58983600
C	0.79972200	-0.21093700	-2.43365500
C	2.19155600	-0.29809900	-2.50550300
C	0.12181500	0.83934000	-3.06720000
C	2.90671100	0.66570600	-3.21299000
H	2.71895000	-1.10890100	-2.01395500
C	0.84449600	1.80261600	-3.76086200
H	-0.96162400	0.90810900	-3.02977800
C	2.23610900	1.71545200	-3.83461400
H	3.98840400	0.59874200	-3.26552100
H	0.32143900	2.62073100	-4.24546400
H	2.79693300	2.47078700	-4.37666900
C	-1.20518800	-2.30621200	-2.80989500
C	-2.33158300	-3.01683800	-2.37347300
C	-0.86670100	-2.27770000	-4.16708300
C	-3.12460300	-3.68323300	-3.30136800
H	-2.59193400	-3.05138800	-1.31922600
C	-1.66534000	-2.95226600	-5.08770900
H	0.00887400	-1.73475600	-4.50922600
C	-2.79221900	-3.65038700	-4.65680500
H	-4.00105600	-4.22868500	-2.96658300
H	-1.40549700	-2.92942700	-6.14112800
H	-3.41395000	-4.17166100	-5.37829000

$TS_{2,3\text{-Ph}}$

G_{solv} = -2934.462759

Ni	1.95419879	-1.75781307	-0.43356963
C	-1.96786512	-0.58999114	0.58454381
C	-0.78791116	-0.65701881	-0.08919385
C	1.32086472	-2.31224070	2.55133992
C	0.47544137	-1.01449680	0.57420736

C	0.21843327	-1.58490961	1.90036035
C	-0.98285023	-1.46787021	2.52749031
S	1.01896382	-1.30596791	-2.42341809
S	2.69009296	-2.59860304	1.46055658
H	-2.90131848	-0.30793718	0.10674041
H	-1.14608736	-1.84641778	3.53112612
C	-3.38456895	0.79867849	3.11188124
C	-3.31347931	-0.65450805	2.62541207
H	-4.14400075	-0.86275547	1.94773097
H	-3.37036866	-1.34795038	3.46668206
N	-2.06632243	-0.92475164	1.90234294
C	-2.35053205	1.13803640	4.13843702
N	-1.03996022	1.44444310	3.81575960
C	-2.48304818	1.16148871	5.50136061
C	-0.40637934	1.65041604	4.95853893
N	-1.24438493	1.48725256	5.99678032
H	-3.33232871	0.98136612	6.14222857
H	0.63593932	1.91205110	5.06435325
H	-3.29507579	1.47091893	2.25122615
H	-4.37871357	0.95035984	3.54241365
H	-1.00203324	1.59388473	6.97330763
C	3.80407143	2.02033239	-1.42019125
C	3.32879584	3.21659149	-1.96094246
C	2.17560975	3.80329332	-1.44222176
C	1.48768897	3.19186238	-0.39742310
C	1.96562136	1.99784491	0.15321516
C	3.13235013	1.41902488	-0.36203673
H	4.69915431	1.55586128	-1.82261785
H	3.85666529	3.68847535	-2.78430388
H	1.80381425	4.73488693	-1.85698187
H	0.58684498	3.64328324	0.00223798
H	3.50684245	0.48579038	0.04966826
C	1.25086285	1.38669579	1.30981055
H	1.09205453	0.03676863	0.73934847
O	0.02812380	1.82208495	1.49049133
H	-0.37779377	1.61649441	2.43249723
C	2.04730761	0.98747453	2.52049872
H	2.97502001	0.48691362	2.24366864
H	2.29509301	1.90522937	3.06706288
H	1.46612517	0.34215599	3.18261951
C	3.50498118	-2.24587256	-1.26739367
O	4.48825109	-2.50631811	-1.77585571
O	1.32384237	-2.69713100	3.71193787
P	-0.71994135	-0.40003298	-1.85630869

C	-0.76783573	1.35059627	-2.31630742
C	-0.07632247	1.79058354	-3.44887588
C	-1.58859173	2.23204543	-1.60465340
C	-0.21318622	3.11035671	-3.87142555
H	0.56770844	1.11316069	-4.00135807
C	-1.71768802	3.55031057	-2.03182597
H	-2.12298082	1.90346486	-0.71944930
C	-1.03425737	3.98851629	-3.16588745
H	0.32765002	3.45201197	-4.74822384
H	-2.34963140	4.23487357	-1.47477530
H	-1.13607670	5.01805124	-3.49535661
C	-2.16551187	-1.17817646	-2.62451762
C	-2.45725317	-2.50769467	-2.28909009
C	-2.96748818	-0.49096222	-3.54015772
C	-3.55171013	-3.14126166	-2.86631684
H	-1.83393339	-3.04549094	-1.57979995
C	-4.06261624	-1.13434240	-4.11570682
H	-2.74905119	0.53814441	-3.80653200
C	-4.35468523	-2.45447018	-3.77975769
H	-3.77850128	-4.16985729	-2.60429638
H	-4.68600260	-0.59954274	-4.82523787
H	-5.20892028	-2.95149021	-4.22940741

3$_{Ph}$

G_{solv} = -2934.496078

Ni	1.06174600	-2.08795900	1.40511000
C	-2.06079100	-0.10224600	-0.58264100
C	-0.83612200	-0.63329000	-0.37413300
C	-0.81532500	-0.58307100	3.40275800
C	-0.14847200	-0.61852600	0.96193200
C	-1.15221500	-0.26330100	2.01370800
C	-2.36538300	0.26184600	1.73161900
S	1.28796200	-2.72922500	-0.74167700
S	0.55636100	-1.70772500	3.51089000
H	-2.53848800	-0.09299700	-1.55785600
H	-3.07038600	0.52458900	2.51453700
C	-3.92460400	2.60918100	-0.05616400
C	-4.07755500	1.09419100	0.15281200
H	-4.49330600	0.65116500	-0.75457900
H	-4.76899600	0.89194800	0.97466200
N	-2.81140900	0.42994800	0.44045800
C	-3.62940300	3.35941000	1.20062800
N	-2.35619500	3.55796200	1.70566600
C	-4.48244500	3.92969000	2.10026700

C	-2.42527700	4.22199300	2.85532600
N	-3.70847100	4.45272400	3.11105900
H	-5.55784300	4.00649300	2.10152500
H	-1.58778600	4.51669800	3.46727900
H	-3.14376600	2.79892300	-0.79955100
H	-4.86631600	2.98805300	-0.46234300
H	-4.05542300	4.94825200	3.92435500
C	4.43531300	0.88633000	0.44384900
C	4.71080200	1.49377500	-0.78106800
C	3.82238500	2.42906000	-1.31345700
C	2.65151400	2.74276800	-0.63248300
C	2.37456300	2.14684100	0.60433900
C	3.27980900	1.22220700	1.14353700
H	5.12159700	0.15365500	0.85707000
H	5.61696100	1.23807200	-1.32236800
H	4.03850500	2.90530900	-2.26411900
H	1.94959700	3.45873600	-1.04753900
H	3.07931900	0.74217500	2.09588300
C	1.11354900	2.50680200	1.31399200
H	0.68658100	0.10053600	0.95083800
O	0.17737000	3.00210600	0.68390000
H	-1.45589400	3.27424400	1.27759100
C	1.03207300	2.28945500	2.79618000
H	1.24769800	1.24812500	3.05345700
H	1.79241200	2.90466700	3.29004000
H	0.04510600	2.55454100	3.17249700
C	2.41599100	-3.19846100	1.90982600
O	3.28347500	-3.85710500	2.24722000
O	-1.38509900	-0.15580200	4.40163700
P	0.07997000	-1.38728500	-1.69132300
C	1.02328900	-0.15626300	-2.63539700
C	2.26219400	-0.48709700	-3.19203500
C	0.43364900	1.08095700	-2.91990000
C	2.89761800	0.41004800	-4.04762100
H	2.72827300	-1.44206800	-2.96807400
C	1.07448800	1.97270900	-3.77548800
H	-0.52431500	1.34927200	-2.48381800
C	2.30089600	1.63408900	-4.34615600
H	3.85993000	0.15157800	-4.47817600
H	0.61585700	2.93235800	-3.99248900
H	2.79875300	2.33109200	-5.01343800
C	-1.03975200	-2.18154400	-2.87681800
C	-2.00740100	-3.06521900	-2.37917500
C	-0.94373500	-1.94866400	-4.25209600

C	-2.87787000	-3.70395700	-3.25571500
H	-2.08279500	-3.25246500	-1.31142300
C	-1.81859300	-2.59440200	-5.12486800
H	-0.19737700	-1.26752200	-4.64838100
C	-2.78372500	-3.46856400	-4.62889800
H	-3.62830700	-4.38566100	-2.86798200
H	-1.74406300	-2.41036000	-6.19202800
H	-3.46397400	-3.96847900	-5.31181200

4$_{Ph}$

G_{solv} = -2549.804932

Ni	-0.00950630	-2.75867602	0.03519859
C	-1.29743540	1.18671702	0.33480117
C	-0.54680852	0.15279912	-0.09871592
C	-0.65086070	-2.01302034	2.99999052
C	-0.03972271	-0.94677366	0.79367074
C	-0.72221337	-0.84138702	2.12164805
C	-1.45778130	0.22745137	2.49556012
S	-0.09645140	-2.02803989	-2.10287581
S	-0.19101077	-3.47959096	2.10817103
H	-1.62931643	1.99191387	-0.31436888
H	-1.93047751	0.28230782	3.47139092
C	-1.11759720	3.57619964	2.39288377
C	-2.23637273	2.54562505	2.15214427
H	-2.95326008	2.95023678	1.43323036
H	-2.76376764	2.33891013	3.08521394
N	-1.71260400	1.28330163	1.64548364
C	-0.02011383	3.02996718	3.24306910
N	1.04224754	2.31464518	2.71706166
C	0.15703923	3.00786532	4.59489562
C	1.83423910	1.87734285	3.69099904
N	1.30803004	2.29124429	4.83773894
H	-0.43310461	3.43315126	5.39060068
H	2.73754092	1.30133193	3.57122757
H	-0.70265909	3.90059567	1.43314049
H	-1.55002209	4.45355182	2.87999548
H	1.70647236	2.10797557	5.75187143
H	1.05682930	-0.87012216	0.91172658
H	1.20611003	2.14519632	1.72970557
C	0.23492976	-4.47072038	-0.54736756
O	0.39245598	-5.54875972	-0.88281739
O	-0.88125485	-2.02833356	4.20415201
P	-0.01555225	-0.01653249	-1.77835786
C	1.67794646	0.62772427	-1.90587598

C	2.64001909	-0.01476423	-2.68892183
C	1.99775048	1.81096551	-1.22865126
C	3.91923079	0.52833113	-2.79577878
H	2.39816918	-0.93598107	-3.21050228
C	3.27770179	2.34697881	-1.33726183
H	1.25126572	2.31593518	-0.62185251
C	4.23819182	1.70597341	-2.12089908
H	4.66643359	0.02764888	-3.40345070
H	3.52439433	3.26320434	-0.80980029
H	5.23667900	2.12443660	-2.20345734
C	-1.05254335	0.92892029	-2.91952329
C	-2.43618880	0.70359080	-2.90528782
C	-0.49901325	1.85427460	-3.81023857
C	-3.25976287	1.41061814	-3.77490960
H	-2.86959257	-0.01803751	-2.21836836
C	-1.33157370	2.55630052	-4.68036490
H	0.57163882	2.03165997	-3.83066114
C	-2.70772813	2.33643291	-4.66224873
H	-4.33112822	1.23730744	-3.76155219
H	-0.90194542	3.27432866	-5.37170709
H	-3.35272481	2.88539261	-5.34166849

5$_{Ph}$

G_{solv} = -3088.048781

Ni	2.66135587	-1.37586859	0.21737113
C	-1.30469439	-1.42709556	1.61817746
C	-0.27619435	-1.38743471	0.74430639
C	2.41263364	-0.07187237	3.05139469
C	1.02280239	-0.69322522	1.03527033
C	1.09536020	-0.39070331	2.49714552
C	0.02354577	-0.45628168	3.31807651
S	1.54601584	-2.60314865	-1.30886502
S	3.72605321	-0.51575280	1.94026292
H	-2.25615871	-1.89725356	1.38871023
H	0.09543243	-0.20951586	4.37315686
C	-3.17233072	0.48013616	3.54992156
C	-2.38552243	-0.82599979	3.74059025
H	-3.03437217	-1.67066113	3.49880806
H	-2.06663166	-0.92983406	4.78065821
N	-1.20586277	-0.89972516	2.88631251
C	-2.44852318	1.68873710	4.04423249
N	-1.54808140	2.41566134	3.28475253
C	-2.46555729	2.28149986	5.27334091
C	-1.04350496	3.40835119	4.01067529

N	-1.58687968	3.33983272	5.22073478
H	-3.02459935	2.04226788	6.16372145
H	-0.32248667	4.13579068	3.67283456
H	-3.42564991	0.60336224	2.49190624
H	-4.10968880	0.39349226	4.10605534
H	-1.38487311	3.98049304	5.97994510
C	0.45301507	2.56638817	0.26119106
H	1.09201122	0.23036281	0.44027271
O	-0.71641627	2.39763547	0.60821723
H	-1.28903281	2.26671359	2.29417174
C	4.23499343	-1.63170194	-0.66353908
O	5.22407566	-1.72750838	-1.22298353
O	2.63154610	0.43410914	4.14756347
P	-0.38115618	-2.09267650	-0.87847906
C	1.53132712	2.82253903	1.27321896
H	2.43712811	2.24633267	1.06996244
H	1.80544681	3.88278544	1.20870389
H	1.17878607	2.59811961	2.27962996
C	0.82658768	2.56904207	-1.18666913
C	-0.00299893	3.19649186	-2.17901245
C	1.98785111	1.92455271	-1.56916592
C	-1.19261947	3.91680504	-1.87589866
C	0.41159269	3.12943450	-3.54267509
C	2.36552035	1.83054987	-2.92538983
H	2.61694643	1.43991418	-0.82888093
C	-1.92572139	4.51904278	-2.87024963
H	-1.52878944	3.98832924	-0.84927395
C	-0.37125515	3.75933552	-4.54762654
C	1.59572071	2.42620017	-3.89023128
H	3.26721471	1.28803172	-3.19109925
C	-1.51799907	4.43861121	-4.22245732
H	-0.04126238	3.69079954	-5.58089034
H	1.87831770	2.36777241	-4.93793551
H	-2.83005313	5.06339193	-2.61459172
H	-2.11159859	4.91644965	-4.99595649
C	-1.05162500	-0.88212609	-2.05462955
C	-2.18441333	-0.14632404	-1.68618993
C	-0.52009498	-0.75496948	-3.34055037
C	-2.78922279	0.70134926	-2.60941793
H	-2.59967312	-0.23559823	-0.68644822
C	-1.13278847	0.09353063	-4.26045271
H	0.36532777	-1.31458625	-3.62640321
C	-2.26922244	0.81433634	-3.89873182
H	-3.66509065	1.27426111	-2.32160849

H	-0.71643884	0.19488173	-5.25778406
H	-2.74350965	1.47474558	-4.61786677
C	-1.50174293	-3.51607279	-0.91078712
C	-1.35891917	-4.50075302	0.07641533
C	-2.46719999	-3.66082119	-1.91223361
C	-2.18930190	-5.61663130	0.06539947
H	-0.60558315	-4.39597761	0.85228813
C	-3.29266118	-4.78399564	-1.91882374
H	-2.58209121	-2.90617201	-2.68392095
C	-3.15606959	-5.75839780	-0.93178769
H	-2.08108938	-6.37578493	0.83362978
H	-4.04201711	-4.89434183	-2.69630059
H	-3.80212704	-6.63111795	-0.93906351

$TS_{5,6\text{-Ph}}$

G_{solv} = -3088.014601

Ni	2.38510625	-1.75202038	-0.19619418
C	-1.62245934	-1.36076720	1.03709425
C	-0.50941227	-1.30336558	0.24985580
C	2.14282789	-1.63209724	2.88585513
C	0.82853007	-1.21803296	0.80167736
C	0.83294894	-1.43339358	2.23389723
C	-0.31008495	-1.47485148	2.97590544
S	1.23688802	-1.99622937	-2.11562456
S	3.46127307	-1.84145643	1.72235180
H	-2.62763705	-1.40949782	0.63104307
H	-0.29203930	-1.60588513	4.05277951
C	-3.27303018	0.07315572	3.36096882
C	-2.76439272	-1.36391414	3.19747674
H	-3.52178032	-1.96909552	2.69580249
H	-2.54621057	-1.81440128	4.16713797
N	-1.53737144	-1.41998807	2.39175896
C	-2.35187394	0.95448227	4.14051158
N	-1.20712467	1.51960050	3.60699074
C	-2.41521583	1.33525974	5.45105880
C	-0.60346903	2.22092220	4.55556771
N	-1.31362293	2.12522071	5.68189151
H	-3.14042238	1.11907880	6.21952803
H	0.31513470	2.77501497	4.44228566
H	-3.46138239	0.50652534	2.37276303
H	-4.23197357	0.02382328	3.88351874
H	-1.07609674	2.57025248	6.56016010
C	0.83806762	1.39270383	0.91859989
H	1.11834774	0.14166230	0.66339959

O	-0.43384093	1.42681451	1.22935876
H	-0.81815011	1.44269685	2.52119245
C	3.94563103	-2.12910530	-1.07546709
O	4.92413743	-2.34356199	-1.61196811
O	2.32528374	-1.66653782	4.09297021
P	-0.61801997	-1.37428881	-1.53614091
C	1.82801628	1.65520455	2.05073626
H	2.85634999	1.45024022	1.74510138
H	1.75414728	2.71138298	2.33648397
H	1.58740805	1.04696532	2.92753604
C	1.24708210	2.06087282	-0.39065056
C	0.60669958	3.25635654	-0.86850342
C	2.32027436	1.55488532	-1.09047142
C	-0.45724947	3.91516682	-0.18476337
C	1.08425851	3.84841322	-2.07934742
C	2.78393856	2.13917386	-2.28806815
H	2.82844503	0.67044187	-0.71740482
C	-1.01890598	5.06662340	-0.68100428
H	-0.83084745	3.48286967	0.73390838
C	0.46880251	5.03114580	-2.57494650
C	2.17024332	3.26148420	-2.78056135
H	3.62183603	1.68979757	-2.81277279
C	-0.56167694	5.62999482	-1.89574582
H	0.83800058	5.45477748	-3.50554150
H	2.50671185	3.72136827	-3.70614249
H	-1.82850212	5.54616286	-0.13804511
H	-1.02253362	6.53425433	-2.28241902
C	-1.07987292	0.21540730	-2.26847303
C	-2.14718286	0.93494571	-1.71886592
C	-0.45233963	0.66455018	-3.43332838
C	-2.58718496	2.09761089	-2.34292509
H	-2.63434207	0.59837841	-0.80960610
C	-0.90068200	1.82886087	-4.05244484
H	0.38228334	0.11486177	-3.85704546
C	-1.96823327	2.54228712	-3.51140582
H	-3.41024170	2.65938696	-1.91287234
H	-0.40771210	2.18113751	-4.95295564
H	-2.31351602	3.45081352	-3.99496762
C	-1.90278626	-2.56093756	-2.00421865
C	-1.94040515	-3.80045953	-1.35088719
C	-2.81735933	-2.27188072	-3.02137852
C	-2.89919986	-4.74069554	-1.71139186
H	-1.22769884	-4.03075032	-0.56372834
C	-3.77328484	-3.22159790	-3.37843846

H	-2.79176288	-1.31525615	-3.53359643
C	-3.81569988	-4.45137862	-2.72452436
H	-2.93137023	-5.69872590	-1.20235573
H	-4.48411271	-2.99642266	-4.16706984
H	-4.56330909	-5.18771093	-3.00393905

6$_{Ph}$

G_{solv} = -3088.050649

Ni	2.60859561	-1.23991022	0.71461852
C	-1.29473629	-0.45370206	2.11203110
C	-0.23592194	-0.97838043	1.39856574
C	2.57384770	1.11005306	2.69679648
C	1.07704249	-0.52510186	1.59964935
C	1.21477044	0.52480694	2.51528976
C	0.13659557	1.04033252	3.20250039
S	1.44943017	-2.98448086	-0.10000856
S	3.80149772	0.32810086	1.69760200
H	-2.31584749	-0.80431554	2.00878376
H	0.23056049	1.84388000	3.92378405
C	-2.97464108	2.17607669	2.91003567
C	-2.26402778	1.09304153	3.72722362
H	-2.93931230	0.26028824	3.92581902
H	-1.89818803	1.48530273	4.67662709
N	-1.09636257	0.53345637	3.00567527
C	-2.19338562	3.44270315	2.75609349
N	-1.13161822	3.56203358	1.87910125
C	-2.35798503	4.62374249	3.43310122
C	-0.67286140	4.79131196	2.02699941
N	-1.38406296	5.46438825	2.95498743
H	-3.06636182	4.92899802	4.18814502
H	0.15374916	5.22783319	1.48578869
H	-3.24279918	1.76829366	1.92884393
H	-3.90874288	2.39446034	3.43542897
H	-1.23055557	6.42287020	3.23969754
C	0.82774482	1.88653604	-0.72152022
H	1.49284632	1.22028515	-0.15625589
O	-0.48590781	1.76856609	-0.20659088
H	-0.61809863	2.39742770	0.53688180
C	4.11769533	-1.82218484	-0.16471756
O	5.04257112	-2.15654704	-0.72976511
O	2.81489579	2.03886202	3.44440431
P	-0.44478493	-2.27985057	0.16616493
C	1.39229822	3.30017750	-0.56721533
H	2.39713289	3.35031593	-0.99834796

H	0.76170517	4.04553166	-1.06226855
H	1.47296399	3.55386251	0.49494012
C	0.89489924	1.39669960	-2.15886292
C	0.01325237	1.85395507	-3.19378268
C	1.90970831	0.52386881	-2.48565657
C	-1.07197109	2.74650627	-2.95516675
C	0.22180272	1.39461107	-4.52984978
C	2.11943561	0.07568046	-3.81022748
H	2.57460388	0.17014887	-1.70053445
C	-1.89907992	3.14871000	-3.97591127
H	-1.25460146	3.08882838	-1.94436847
C	-0.65538875	1.82501866	-5.56336509
C	1.29306437	0.50549484	-4.81537022
H	2.93293761	-0.61269885	-4.02052074
C	-1.69426052	2.68137834	-5.29655678
H	-0.48766273	1.45778492	-6.57282928
H	1.43513880	0.16678491	-5.83845318
H	-2.72258977	3.82585721	-3.76755330
H	-2.35916967	3.00173312	-6.09342374
C	-1.17700623	-1.62398619	-1.35181835
C	-2.30785664	-0.80172426	-1.27789230
C	-0.67273590	-2.01848031	-2.59428916
C	-2.92997635	-0.38105810	-2.44832202
H	-2.71184345	-0.48615100	-0.32231097
C	-1.30772867	-1.59888110	-3.76048340
H	0.20992393	-2.64671697	-2.65839205
C	-2.43473217	-0.78340500	-3.68850252
H	-3.80062755	0.26428894	-2.39068009
H	-0.91211497	-1.90221967	-4.72425451
H	-2.92292973	-0.45196429	-4.59971028
C	-1.55655276	-3.54209322	0.82159660
C	-1.35873366	-4.00070735	2.13155465
C	-2.57749504	-4.07708995	0.02987693
C	-2.19240170	-4.98670881	2.64676458
H	-0.56270441	-3.59117176	2.74779813
C	-3.40489056	-5.06834309	0.55428127
H	-2.73270285	-3.72749296	-0.98593253
C	-3.21456586	-5.51997223	1.85869216
H	-2.04487839	-5.33941919	3.66245654
H	-4.19786397	-5.48440648	-0.05877934
H	-3.86321685	-6.29040705	2.26434684

5$_{Ph}$'

G_{solv} = -3088.049007

Ni	1.41323100	-1.66601800	1.69270000
C	-2.19985200	-0.77838900	-0.23783000
C	-0.89528200	-1.10439900	-0.10150300
C	-0.27617200	0.40861700	3.30551100
C	-0.00814400	-0.52985100	0.96852500
C	-0.86489700	0.15567100	1.98623500
C	-2.17025500	0.43867100	1.78739400
S	1.33158800	-3.12210400	-0.02730100
S	1.15290400	-0.59868100	3.59435800
H	-2.82533900	-1.18117600	-1.02862600
H	-2.76994800	0.93372700	2.54521300
C	-4.30518000	1.84428200	-0.28997900
C	-4.21757300	0.47590500	0.40347000
H	-4.69840900	-0.27574200	-0.22586700
H	-4.74646800	0.50489800	1.35976200
N	-2.84166700	0.05716500	0.64497900
C	-3.81430300	2.95882400	0.57272400
N	-2.49823000	3.38562600	0.60056000
C	-4.46598900	3.69312200	1.52010900
C	-2.35139000	4.34158300	1.51278600
N	-3.53537200	4.53717600	2.08178400
H	-5.49728300	3.68325800	1.83394100
H	-1.43694700	4.86158900	1.74757900
H	-3.74040600	1.81891900	-1.22697100
H	-5.35332000	2.03300600	-0.53720700
H	-3.71571500	5.21307800	2.81554700
C	0.59125000	2.80286300	-1.85129300
H	0.71983800	0.17529300	0.53341200
O	-0.54452400	2.94620500	-1.40471300
H	-1.73951700	3.05424100	-0.00845100
C	2.98134600	-2.37681800	2.27882100
O	3.99785000	-2.75302600	2.63487400
O	-0.70680600	1.19085100	4.14790700
P	-0.12435400	-2.28170200	-1.18048600
C	0.92180800	3.25214100	-3.24298500
H	1.46987900	4.19906400	-3.15313700
H	1.57817500	2.55284100	-3.76418000
H	0.00863700	3.41860000	-3.81618800
C	1.68352200	2.22164400	-1.01134300
C	1.88463700	2.63324700	0.34872800
C	2.46740300	1.22427100	-1.55309500
C	1.18554700	3.71577400	0.94906300
C	2.87381400	1.95710000	1.12072400
C	3.42267500	0.53834800	-0.77059300

H	2.32707500	0.92362500	-2.58572800
C	1.43519600	4.08196400	2.24957100
H	0.45796800	4.27092200	0.36785800
C	3.10508800	2.35590900	2.46430000
C	3.61442400	0.89168500	0.54030300
H	3.99192200	-0.27214300	-1.21474500
C	2.39946100	3.39208900	3.02166100
H	3.85397600	1.82158300	3.04204500
H	4.34149500	0.36712000	1.15507000
H	0.89158900	4.91339700	2.68886900
H	2.58018100	3.68813900	4.05052300
C	0.55983500	-1.47843400	-2.65813900
C	-0.19630400	-0.49643400	-3.30931400
C	1.78721400	-1.88440600	-3.18660700
C	0.27651100	0.07008900	-4.48908800
H	-1.15031000	-0.17227200	-2.90357300
C	2.25823700	-1.30881200	-4.36534100
H	2.37945400	-2.64055700	-2.68055200
C	1.50352600	-0.33426600	-5.01681400
H	-0.30860400	0.83404200	-4.99083300
H	3.21528800	-1.62164500	-4.77088500
H	1.87331400	0.11512000	-5.93347900
C	-1.33297000	-3.49651100	-1.77410600
C	-2.15242400	-4.13122900	-0.83052700
C	-1.43710300	-3.82721700	-3.12869300
C	-3.07766000	-5.08299700	-1.24569600
H	-2.07059600	-3.88180700	0.22388000
C	-2.36524900	-4.78407200	-3.53709400
H	-0.80387500	-3.34521100	-3.86683900
C	-3.18454700	-5.40930100	-2.59911400
H	-3.71388300	-5.57051700	-0.51368100
H	-2.44579100	-5.03821800	-4.58933700
H	-3.90687800	-6.15318100	-2.92133300

$TS_{5',6'\text{-Ph}}$

G_{solv} = -3088.008921

Ni	1.71599468	0.40318489	1.46725189
C	-1.74717041	-1.85919338	0.58675005
C	-0.45920724	-1.42458982	0.56942294
C	-0.86766614	1.81244515	2.44599252
C	-0.10242736	-0.05316023	0.95760484
C	-1.18503138	0.58270707	1.70060919
C	-2.45797426	0.10071446	1.67863991
S	2.55258263	-1.56732869	0.78442450

S	0.87467514	2.13760607	2.51944304
H	-2.04288060	-2.84834127	0.25058265
H	-3.27990019	0.61482969	2.16521100
C	-4.62383919	-0.95279403	-0.56742422
C	-4.14982438	-1.45869696	0.80315335
H	-4.20286235	-2.54860012	0.83442139
H	-4.76956318	-1.05757852	1.60752850
N	-2.75878338	-1.07537225	1.06366157
C	-4.91042836	0.51604547	-0.62960210
N	-3.93953676	1.50247102	-0.68679715
C	-6.14360607	1.11392432	-0.61574872
C	-4.58230415	2.65934500	-0.70413897
N	-5.91224055	2.46587658	-0.66323890
H	-7.13933814	0.69909569	-0.58134213
H	-4.12307043	3.63588789	-0.74806377
H	-3.88198839	-1.23366253	-1.32408090
H	-5.54686425	-1.48853966	-0.80855747
H	-6.61634495	3.19240929	-0.67228648
C	-0.45886058	1.46970619	-1.15872903
H	0.00099624	0.59840121	-0.09831808
O	-1.41992558	2.14776745	-0.56863904
H	-2.35332001	1.72496741	-0.64593074
C	3.39860434	1.04653926	1.77679977
O	4.43704278	1.47337307	1.95722629
O	-1.68772759	2.54169417	2.98304715
P	0.88744766	-2.47368630	0.03255315
C	-0.91321318	0.44272304	-2.16326128
H	-1.36106919	0.98124497	-3.00659615
H	-0.10055444	-0.17400272	-2.54090140
H	-1.67678519	-0.20687012	-1.72605485
C	0.85739988	2.15808700	-1.32395188
C	1.11513534	3.53272861	-0.97304938
C	1.91140697	1.35619725	-1.72684799
C	0.11778118	4.48557797	-0.61366158
C	2.47297523	3.98454863	-1.00088742
C	3.23924968	1.81687303	-1.76477150
H	1.72947248	0.31573623	-1.96684789
C	0.45058092	5.77748074	-0.28226590
H	-0.92028158	4.19111427	-0.59668189
C	2.78348450	5.32567428	-0.64318562
C	3.51781140	3.10498172	-1.38781853
H	4.03194533	1.14009120	-2.06745744
C	1.79699774	6.20780429	-0.28506195
H	3.82440030	5.63731953	-0.66739058

H	4.53956339	3.47509743	-1.38430823
H	-0.33572403	6.47726249	-0.01428884
H	2.04236704	7.23029580	-0.01455893
C	0.93430544	-2.59262722	-1.77769007
C	-0.20480326	-3.05099559	-2.45365870
C	2.07001284	-2.21304499	-2.49456401
C	-0.20725799	-3.10638214	-3.84253257
H	-1.09079218	-3.35789576	-1.90542041
C	2.06111525	-2.27198015	-3.88768969
H	2.95504215	-1.85975667	-1.97469749
C	0.92376795	-2.71174315	-4.56057622
H	-1.09266461	-3.45447023	-4.36492257
H	2.94334810	-1.96888448	-4.44245713
H	0.91624451	-2.75029811	-5.64560359
C	0.65748608	-4.14695350	0.67930670
C	0.20412061	-4.30339486	1.99589695
C	0.98361083	-5.26631053	-0.09300385
C	0.06351705	-5.58030969	2.52876611
H	-0.03914663	-3.43513820	2.60166556
C	0.84281057	-6.54184863	0.45022282
H	1.34275480	-5.15145094	-1.11100879
C	0.38134367	-6.69880676	1.75611303
H	-0.29297696	-5.70222107	3.54664175
H	1.09311084	-7.41099322	-0.14964584
H	0.27057880	-7.69450599	2.17474380

6$_{Ph}$'

G_{solv} = -3088.048650

Ni	0.78145500	-2.02536300	1.56970000
C	-2.72169100	-0.90021000	-0.49190600
C	-1.49724000	-1.46064500	-0.18980200
C	-0.99938300	-0.21220600	3.29398800
C	-0.90547100	-1.28996800	1.07325800
C	-1.62813600	-0.50175400	1.97390300
C	-2.85691700	0.03408400	1.65084000
S	0.85206900	-3.36134000	-0.24061600
S	0.58790300	-0.96199800	3.48124800
H	-3.21121000	-1.01937400	-1.45294700
H	-3.43730400	0.63466400	2.34152000
C	-4.45396600	1.78809200	-0.67337400
C	-4.67052800	0.45592300	0.05095900
H	-5.18895700	-0.25093800	-0.59768500
H	-5.24839900	0.58751300	0.96586300
N	-3.38521000	-0.17440900	0.42946300

C	-3.94121400	2.89162400	0.19774000
N	-2.63376300	2.95448800	0.64393600
C	-4.64302800	3.95913700	0.69699200
C	-2.55784000	4.04044700	1.39234200
N	-3.74692900	4.67437200	1.45117300
H	-5.67214300	4.26259900	0.57881300
H	-1.67380400	4.39621600	1.90143100
H	-3.78524500	1.62713500	-1.52660700
H	-5.42686000	2.08100500	-1.07823800
H	-3.93844500	5.53006400	1.95536500
C	0.74540500	1.48302200	0.01623900
H	0.53345000	0.41158900	-0.11412800
O	-0.02003500	1.97681500	1.10137700
H	-0.93595000	2.15227900	0.80255900
C	2.45226200	-2.59430000	2.07852800
O	3.49516300	-2.91902000	2.38495800
O	-1.52108100	0.46867800	4.15559800
P	-0.54459900	-2.42230700	-1.38638800
C	0.38487600	2.17106600	-1.30107200
H	0.54984900	3.25145500	-1.25555000
H	0.98785100	1.76103800	-2.11623800
H	-0.66996700	1.99270900	-1.53714500
C	2.22574300	1.57238900	0.34648300
C	2.87108500	2.79375000	0.73784000
C	2.98623600	0.43207900	0.20895400
C	2.17153700	4.02213600	0.92358100
C	4.28321900	2.78924000	0.95377600
C	4.38344800	0.42713900	0.42999500
H	2.50084700	-0.49513800	-0.08426300
C	2.83461200	5.17144200	1.28071700
H	1.09623900	4.03824500	0.79848700
C	4.93980900	3.99520900	1.32660900
C	5.02143200	1.58424500	0.79274700
H	4.94092900	-0.49730700	0.31012400
C	4.23577300	5.16279700	1.48334300
H	6.01488700	3.97258900	1.48655900
H	6.09456900	1.59951600	0.96475800
H	2.27854800	6.09475100	1.41620500
H	4.74761000	6.07787700	1.76662300
C	0.18167200	-1.31291300	-2.61832700
C	-0.66996400	-0.57421900	-3.45138900
C	1.56706500	-1.21385600	-2.75991900
C	-0.12806200	0.25607800	-4.42572700
H	-1.74899600	-0.64660500	-3.34690000

C	2.10192500	-0.37728700	-3.73787400
H	2.22791800	-1.78418400	-2.11561000
C	1.25712400	0.35260000	-4.57098300
H	-0.78719700	0.82852400	-5.07038200
H	3.17905800	-0.29914000	-3.84485600
H	1.67667000	1.00259000	-5.33266300
C	-1.64608500	-3.57547700	-2.22871200
C	-2.65687300	-4.20445500	-1.48923300
C	-1.45714000	-3.88563200	-3.57973900
C	-3.48640100	-5.13135100	-2.11101200
H	-2.79917400	-3.97377500	-0.43684800
C	-2.29124200	-4.81832800	-4.19173100
H	-0.67051200	-3.40739900	-4.15495600
C	-3.30410300	-5.43723500	-3.46074200
H	-4.27379600	-5.61505000	-1.54205900
H	-2.14801600	-5.05918500	-5.24015900
H	-3.95358400	-6.16145900	-3.94283100

1$_{Me}$

G_{solv} = -2165.369344

Ni	0.06272547	-2.23037297	0.84620968
C	-0.79900577	0.97420785	-1.77688251
C	-0.41895402	-0.26377476	-1.29331093
C	-0.97351849	0.23014049	2.37078012
C	-0.45997824	-0.56052310	0.08036321
C	-0.92039299	0.47602441	0.90096897
C	-1.29223305	1.70133646	0.39032300
S	0.53855603	-3.14099040	-1.14443904
S	-0.40572511	-1.37902558	2.82080030
H	-0.76852682	1.23921714	-2.82906030
H	-1.63688349	2.51672122	1.01608698
C	-0.19527169	4.08677834	-1.60067330
C	-1.50034555	3.29348938	-1.45314526
H	-2.00378238	3.18416681	-2.41436431
H	-2.17854464	3.77324065	-0.74717923
N	-1.22724546	1.93377854	-0.93424879
C	0.60547231	4.14475019	-0.33730083
N	1.49940607	3.14356581	-0.00676021
C	0.55530689	5.07100148	0.67424621
C	1.97978242	3.46825373	1.17826178
N	1.43538343	4.62276278	1.62694700
H	-0.01211101	5.98151779	0.79447177
H	2.71136087	2.91077089	1.74502003
H	0.40892345	3.63820959	-2.39602198

H	-0.47537623	5.09308925	-1.92476689
H	1.65095444	5.08350430	2.50136829
O	-1.36133488	1.05121677	3.17979155
C	0.55345292	-3.79692687	1.67581256
O	0.85651531	-4.75627671	2.19960751
P	0.17043090	-1.56660701	-2.39241452
C	1.65003205	-0.99853618	-3.24826575
H	2.03036695	-1.80971327	-3.87502973
H	1.38852155	-0.14166457	-3.87621687
H	2.40333510	-0.70922786	-2.51210601
C	-1.09308005	-1.94280550	-3.61922320
H	-1.25797529	-1.05748224	-4.24051191
H	-0.74120178	-2.76699761	-4.24573643
H	-2.01898413	-2.22631407	-3.11386984

2$_{Me}$

G_{solv} = -2551.244355

Ni	1.78069967	-1.61534367	0.76349499
C	-1.34016502	-1.11137038	-2.03453804
C	-0.08437104	-1.21645699	-1.47114197
C	-0.97962962	-1.92962904	2.08546248
C	0.08534334	-1.51521579	-0.10906097
C	-1.09786665	-1.68917626	0.61914439
C	-2.33849966	-1.59736552	0.02537944
S	2.92306615	-1.44332611	-1.16258470
S	0.69293648	-1.93482750	2.64943454
H	-1.50752920	-0.86683184	-3.07836332
H	-3.26362471	-1.74281485	0.57159818
C	-4.24527985	0.30603907	-1.85237249
C	-3.77942773	-1.15275964	-1.90535527
H	-3.70118379	-1.49314753	-2.93787409
H	-4.46573859	-1.80831311	-1.36834632
N	-2.44334733	-1.31892547	-1.28879529
C	-4.48320885	0.81708204	-0.46644041
N	-3.45561452	1.26438246	0.34294360
C	-5.66665745	0.88623650	0.22292060
C	-4.01490868	1.60124171	1.49078184
N	-5.34651535	1.38552136	1.46058334
H	-6.67877176	0.63430004	-0.05490045
H	-3.49880177	1.99623930	2.35364189
H	-3.51308274	0.93679695	-2.36811327
H	-5.17673022	0.35336013	-2.42374484
H	-5.99510233	1.57259858	2.21395846
C	3.70178243	3.13144922	0.55204537

C	3.51554776	4.39066905	-0.02104652
C	2.23416476	4.79249457	-0.39989069
C	1.14466229	3.94201038	-0.20707035
C	1.32414347	2.68056572	0.36524800
C	2.61171815	2.28349606	0.74058020
H	4.69663433	2.80665379	0.84366573
H	4.36369193	5.05153050	-0.17517769
H	2.08220884	5.77003735	-0.84920700
H	0.14900882	4.24971181	-0.51178933
H	2.76149483	1.29611491	1.17469267
C	0.15652244	1.74636673	0.60958139
H	0.56037206	0.72460318	0.55745193
O	-0.81085294	1.92574271	-0.40508691
H	-1.69635978	1.63568493	-0.09166201
C	-0.43207229	1.93017487	2.00748109
H	0.34887152	1.81502738	2.76551769
H	-0.87705499	2.92631634	2.11069745
H	-1.20086198	1.17398443	2.19945287
C	3.36251553	-1.62406836	1.69836677
O	4.33077274	-1.59645706	2.28888166
O	-1.93289446	-2.09530992	2.82296728
P	1.41196169	-0.91292053	-2.42804721
C	1.46551015	0.82454009	-2.89690845
H	1.44252213	1.44632158	-1.99928588
H	2.38685921	1.00862298	-3.45670691
H	0.59885516	1.04698185	-3.52626129
C	1.38753243	-1.90556794	-3.92970113
H	2.31990173	-1.74428384	-4.47797341
H	1.28531944	-2.96122395	-3.66895385
H	0.54204602	-1.58757334	-4.54707580

$TS_{2,3\text{-Me}}$

G_{solv} = -2551.207421

Ni	1.98446519	-0.53049635	1.24679745
C	-1.31062143	-1.91317575	-1.01653681
C	-0.06283609	-1.48550899	-0.68740743
C	-0.66635563	-0.49332785	2.88060307
C	0.19447767	-0.70822754	0.53371989
C	-0.92144522	-0.84238462	1.47503297
C	-2.15198176	-1.27318684	1.08333893
S	2.94648918	-1.10019351	-0.70872521
S	1.05649876	-0.21230941	3.21127778
H	-1.52467495	-2.45329327	-1.93418143
H	-2.99364090	-1.30836164	1.76750927

C	-4.34228473	-0.97432963	-1.49303693
C	-3.72262703	-2.08964801	-0.64226478
H	-3.64751060	-3.00632348	-1.23146370
H	-4.33798649	-2.29458510	0.23578533
N	-2.37544118	-1.74335509	-0.17677647
C	-4.61197319	0.28489811	-0.73239522
N	-3.62563613	1.20795607	-0.43328227
C	-5.79381263	0.71547580	-0.19026441
C	-4.20545500	2.16974215	0.26583626
N	-5.51244376	1.90612285	0.43384839
H	-6.78473543	0.28839601	-0.19910505
H	-3.71528270	3.04911139	0.65631310
H	-3.68640122	-0.76634964	-2.34583168
H	-5.28509954	-1.35731515	-1.89449285
H	-6.17355693	2.49175646	0.92753316
C	3.29560500	2.92376713	-0.69290801
C	3.46309289	2.91804840	-2.07935056
C	2.40688335	2.53408851	-2.90413065
C	1.18785745	2.15393445	-2.34766751
C	1.01399966	2.16011784	-0.95912739
C	2.07999369	2.54723290	-0.13504849
H	4.11656917	3.21627327	-0.04548293
H	4.41439069	3.21110531	-2.51330158
H	2.53026379	2.52940284	-3.98283955
H	0.36262857	1.86365669	-2.98851965
H	1.97499277	2.53467614	0.94498481
C	-0.28420980	1.72768629	-0.37834609
H	0.24211217	0.46806843	0.19577527
O	-1.18091940	1.34377996	-1.25445489
H	-2.15395240	1.26116891	-0.87451678
C	-0.77287452	2.32481455	0.91032132
H	0.02462614	2.42621758	1.64564038
H	-1.17433295	3.32036022	0.68824765
H	-1.57443704	1.71854361	1.33775373
C	3.60878923	-0.04870896	1.92385076
O	4.60394873	0.31716069	2.33600485
O	-1.51658824	-0.40862457	3.75556486
P	1.36126864	-1.95591290	-1.66435619
C	1.21281628	-1.42250007	-3.38069884
H	1.09698651	-0.33824785	-3.42311116
H	2.11235864	-1.72336301	-3.92522413
H	0.33951500	-1.90994392	-3.82490799
C	1.48593349	-3.75811240	-1.69367197
H	2.38649501	-4.04619115	-2.24354581

H	1.54125618	-4.13118219	-0.66847844
H	0.60284325	-4.16871090	-2.19290168

3$_{Me}$

G_{solv} = -2551.237754

Ni	2.13056987	-1.46487225	0.38554233
C	-0.91338159	-0.29971250	-2.29339154
C	0.27686170	-0.32257910	-1.65657394
C	-0.69931539	-2.41810075	1.32346297
C	0.42019015	-0.75214375	-0.22135455
C	-0.80112736	-1.52709996	0.16811955
C	-1.95861943	-1.47235376	-0.52924787
S	3.26626760	-0.36290756	-1.22102624
S	0.98956072	-2.68711046	1.80930665
H	-1.02971684	0.05339580	-3.31375588
H	-2.84196222	-2.02169258	-0.21692576
C	-4.17919877	0.54478282	-1.96907802
C	-3.34637431	-0.66994471	-2.40827763
H	-3.13906820	-0.58709902	-3.47711460
H	-3.91093536	-1.59202673	-2.24523627
N	-2.07033251	-0.77568912	-1.70932161
C	-4.73886591	0.41792626	-0.59071430
N	-4.06749444	0.81467859	0.55173628
C	-5.91582278	-0.12639986	-0.16521369
C	-4.79787324	0.53213770	1.62544173
N	-5.92184628	-0.04155206	1.20849621
H	-6.73527965	-0.55633934	-0.71843160
H	-4.52561741	0.73394258	2.64892069
H	-3.57290067	1.45288326	-2.04494574
H	-5.01488173	0.64598535	-2.66691303
H	-6.67024306	-0.35402388	1.81674633
C	2.91838479	2.73063106	2.05516549
C	3.06546097	3.75906099	1.12422304
C	1.97180195	4.17675832	0.36368887
C	0.73651574	3.55890237	0.52583701
C	0.58058740	2.52699813	1.46047800
C	1.67969718	2.12007075	2.22930429
H	3.76869118	2.40252706	2.64487048
H	4.03221244	4.23548037	0.99086979
H	2.08584000	4.97688072	-0.36117974
H	-0.11537027	3.86870721	-0.07079891
H	1.58124403	1.31828359	2.95367782
C	-0.74799271	1.86353914	1.59135667
H	0.54234757	0.13316010	0.42275390

O	-1.63691533	2.11684672	0.77592373
H	-3.14029315	1.27908017	0.60089808
C	-0.97953999	0.90326467	2.72168118
H	-0.25801376	0.08032103	2.68222515
H	-0.83423255	1.41602601	3.67838792
H	-1.98863960	0.49468215	2.67587060
C	3.69161870	-1.95033939	1.19184757
O	4.66089010	-2.24964765	1.71262632
O	-1.63558951	-2.94292673	1.91895996
P	1.76652611	0.17179237	-2.49968946
C	1.77803748	1.94779619	-2.83143093
H	1.66555005	2.49210215	-1.89116354
H	2.72282861	2.22387877	-3.30821616
H	0.94672419	2.18843909	-3.50090611
C	1.90734064	-0.64463259	-4.10613657
H	2.84529011	-0.34286312	-4.58135409
H	1.89335710	-1.72771305	-3.96440098
H	1.06628716	-0.34180474	-4.73778807

4$_{Me}$

G_{solv} = -2166.549022

Ni	0.06330519	-2.40021405	0.74708020
C	-0.88646479	0.91480942	-1.54509219
C	-0.17923241	-0.18312372	-1.20798251
C	-0.42462552	0.08975838	2.56336064
C	0.22848222	-0.51736428	0.20214807
C	-0.43329544	0.44258101	1.14055497
C	-1.12669553	1.52732215	0.73175177
S	-0.03578051	-3.16440644	-1.37688820
S	-0.10181585	-1.64066694	2.81064630
H	-1.17199950	1.14436144	-2.56720417
H	-1.60267806	2.19870664	1.43977344
C	-0.87464430	4.11646015	-1.44360603
C	-1.92817172	3.08053470	-1.01489214
H	-2.60708333	2.89265916	-1.85060201
H	-2.51596900	3.46386417	-0.17834090
N	-1.32758003	1.81915556	-0.59976806
C	0.14534855	4.36811525	-0.38508926
N	1.22929358	3.53065170	-0.18248012
C	0.22972637	5.31911075	0.58841328
C	1.94594064	3.94374197	0.85811144
N	1.34977702	5.02955485	1.33636976
H	-0.40435906	6.16305219	0.80720312
H	2.84343744	3.48448240	1.23971071

H	-0.37470956	3.77388556	-2.35546092
H	-1.38444618	5.05422616	-1.67773341
H	1.68312108	5.56515763	2.12998302
O	-0.62497468	0.85662471	3.49933554
C	0.11349121	-4.11490065	1.36800207
O	0.14361854	-5.17843721	1.77808529
P	0.28956260	-1.41872911	-2.38987286
C	2.03969493	-1.22788771	-2.80509030
H	2.35099346	-2.04975452	-3.45567042
H	2.18166195	-0.27324508	-3.32038424
H	2.63207603	-1.24552395	-1.88679708
C	-0.64339911	-1.30454415	-3.92912281
H	-0.41773062	-0.35322115	-4.42003803
H	-0.33964634	-2.12494577	-4.58544815
H	-1.71297359	-1.37592545	-3.72103199
H	1.45240156	2.71417604	-0.74282343
H	1.32694593	-0.47256572	0.30756256

5$_{Me}$

G_{solv} = -2704.790795

Ni	0.24774659	-2.36763745	-1.93270201
C	-2.19328566	-0.76054857	1.02671890
C	-1.55127351	-0.80417553	-0.15812749
C	1.51918084	-2.75144965	0.89726987
C	-0.14962189	-1.31479601	-0.32679778
C	0.30555140	-1.93342604	0.95433153
C	-0.39446217	-1.85649352	2.10793137
S	-1.63387262	-1.71546809	-3.00310584
S	1.90795154	-3.23633086	-0.76853417
H	-3.20513759	-0.38381126	1.13637210
H	-0.04321167	-2.33171431	3.01878867
C	-2.07672217	0.14717309	4.22850726
C	-2.34802837	-1.14995807	3.45158331
H	-3.41606701	-1.21185152	3.23034886
H	-2.08075450	-2.01748575	4.06036053
N	-1.61778737	-1.22951305	2.19052787
C	-0.68916713	0.23689294	4.76947301
N	0.40334087	0.61633228	4.01052148
C	-0.20129334	-0.06100960	6.00853060
C	1.50691122	0.55879909	4.74823628
N	1.15886619	0.14804471	5.96329928
H	-0.70184907	-0.39698221	6.90245405
H	2.50394991	0.79992403	4.41606958
H	-2.28524272	1.00906640	3.58609483

H	-2.77217260	0.18757001	5.07107646
H	1.80339062	0.01742684	6.73460587
C	1.46249231	1.48414427	0.70019239
H	0.52227393	-0.49523592	-0.62941483
O	0.48508746	1.60219223	1.44204732
H	0.39374857	0.93044484	3.01975168
C	0.85958608	-3.17272011	-3.44878462
O	1.27572170	-3.66632294	-4.38907065
O	2.20467883	-3.09697810	1.85438897
P	-2.31393579	-0.31092515	-1.67965170
C	-1.74213870	1.33686561	-2.15482291
H	-2.18293953	1.61034349	-3.11753701
H	-2.04058874	2.05729695	-1.38790363
H	-0.65448023	1.31472014	-2.24635956
C	-4.11314023	-0.24249422	-1.57062480
H	-4.50694489	-1.21516374	-1.26865842
H	-4.40160120	0.52313551	-0.84438970
H	-4.51182767	0.02961215	-2.55217520
C	2.65396881	0.68544934	1.14619545
H	3.14100575	0.13876338	0.33822606
H	3.39024338	1.39583207	1.54323914
H	2.36819593	-0.01185692	1.93433357
C	1.48459266	2.16998225	-0.62491687
C	0.81990143	3.42992405	-0.83679862
C	2.08821081	1.52655504	-1.69009942
C	0.22035860	4.19854415	0.20064658
C	0.78283889	3.95648805	-2.16301591
C	2.03705319	2.05376325	-2.99785618
H	2.57293827	0.56683968	-1.54800353
C	-0.39491455	5.39724737	-0.07250449
H	0.24506795	3.83521009	1.21945494
C	0.13156243	5.19487711	-2.41388681
C	1.39265500	3.24120399	-3.22850005
H	2.50022093	1.50642841	-3.81231660
C	-0.45177511	5.90133349	-1.39277992
H	0.11114209	5.57230529	-3.43277610
H	1.33818266	3.65525792	-4.23179209
H	-0.84250564	5.96535645	0.73776322
H	-0.94725401	6.84686946	-1.59091076

$TS_{5,6\text{-Me}}$

G_{solv} = -2704.75536

Ni	-2.17769284	0.33934135	1.73329963
C	-0.83518181	-2.09939218	-1.42768292

C	-0.95733132	-1.56133902	-0.18072458
C	-2.81219573	1.58982808	-1.02881322
C	-1.46421193	-0.22154791	0.03674936
C	-2.03558369	0.34217165	-1.16832871
C	-1.88554654	-0.23790538	-2.39373263
S	-1.48688900	-1.52284720	2.79474044
S	-3.11677958	2.01977747	0.66265280
H	-0.42785926	-3.08959553	-1.60439224
H	-2.28908876	0.20984206	-3.29591753
C	0.40225830	-1.78661167	-4.34350051
C	-1.03288597	-2.02825566	-3.86221060
H	-1.22260180	-3.10114327	-3.79393115
H	-1.75554380	-1.59198348	-4.55361953
N	-1.27233105	-1.44332576	-2.53631578
C	0.72241463	-0.34787615	-4.58565619
N	1.00801533	0.55047432	-3.57288277
C	0.76766734	0.34760124	-5.76031093
C	1.22403562	1.74239350	-4.11177694
N	1.08360269	1.64588412	-5.43482752
H	0.61014957	0.03097688	-6.77914275
H	1.46677049	2.64411848	-3.57216463
H	1.10574833	-2.21154463	-3.61960969
H	0.53017046	-2.33273444	-5.28173403
H	1.19660912	2.41069039	-6.08927292
C	0.88046335	0.93126083	-0.20268312
H	-0.28263865	0.51462496	0.21775336
O	1.27123497	0.06997127	-1.10797979
H	1.08245604	0.34286257	-2.46232854
C	-2.78999290	1.01703044	3.31801730
O	-3.15962303	1.45511338	4.29951678
O	-3.22347353	2.26669016	-1.95885107
P	-0.51768910	-2.49660464	1.28224049
C	1.26780059	-2.54615148	1.53506727
H	1.47627236	-3.17113629	2.40826557
H	1.74244433	-2.97540324	0.64792033
H	1.64111977	-1.53561060	1.70498362
C	-1.06914782	-4.20635673	1.11686553
H	-2.14382235	-4.22841433	0.92321457
H	-0.52905027	-4.67701221	0.28930115
H	-0.84520611	-4.74053510	2.04439805
C	0.49794686	2.32353100	-0.70115098
H	0.03202518	2.92446476	0.08292414
H	1.40956295	2.83380103	-1.03450244
H	-0.18719223	2.25593688	-1.55119699

C	1.65983743	0.96253206	1.11017607
C	3.05680681	0.62973911	1.19152746
C	1.00300227	1.36051347	2.25468211
C	3.85984424	0.28378134	0.06398168
C	3.69297930	0.66430948	2.47287255
C	1.63563534	1.39878860	3.51496086
H	-0.04647414	1.63685249	2.19316086
C	5.19220447	-0.02113030	0.20458822
H	3.39723572	0.25669556	-0.91349435
C	5.07214961	0.33076124	2.58446417
C	2.95469518	1.04219063	3.62578974
H	1.06777560	1.70028883	4.39013008
C	5.80919043	-0.00805596	1.47860952
H	5.53185642	0.35697562	3.56920403
H	3.45646819	1.05241395	4.58985721
H	5.77933125	-0.27690732	-0.67299137
H	6.86167453	-0.25818528	1.57490852

6Me

G_{solv} = -2704.796788

Ni	0.79253468	-2.66615873	0.71518826
C	-1.93756726	0.13737379	2.29340298
C	-1.40664195	-0.94194675	1.61606564
C	2.20828438	-0.60221134	2.50104122
C	-0.03532683	-1.23998865	1.67586199
C	0.73644594	-0.36866903	2.45400350
C	0.17649669	0.69531196	3.12911871
S	-1.17420368	-3.53900972	0.07418652
S	2.72258386	-1.96086303	1.49879899
H	-2.98795847	0.40655968	2.26064340
H	0.75882097	1.37536561	3.74083573
C	-1.81056168	3.31277350	2.77838075
C	-1.74339892	2.10521380	3.71907019
H	-2.74240648	1.81471299	4.04502940
H	-1.13334929	2.31919514	4.59721400
N	-1.14823160	0.92719643	3.04750716
C	-0.47095305	3.84166247	2.37349287
N	0.28366620	3.25491747	1.37491913
C	0.22215628	4.89943880	2.90400979
C	1.40319649	3.95171940	1.30596941
N	1.40694542	4.95048314	2.21290567
H	-0.02053300	5.60031689	3.68812825
H	2.22097765	3.76782952	0.62481263
H	-2.39602999	3.04558327	1.89180633

H	-2.36316096	4.09097298	3.31245779
H	2.14837829	5.62511805	2.34827762
C	0.54908979	0.58625725	-1.09441998
H	0.53950795	-0.38167882	-0.57281958
O	-0.50927196	1.38092137	-0.58720366
H	-0.18435050	1.97279930	0.12768914
C	1.66513683	-3.92564501	-0.29532160
O	2.19998697	-4.67933868	-0.95342595
O	2.98009345	0.07524174	3.15350254
P	-2.41768986	-1.99381064	0.55694122
C	-2.94725671	-1.04097704	-0.87596202
H	-3.52466832	-1.69325256	-1.53702805
H	-3.57269229	-0.21042057	-0.53581067
H	-2.07098932	-0.65419587	-1.39985320
C	-3.88274741	-2.55163901	1.44275750
H	-3.58299615	-3.06485747	2.35921411
H	-4.50384647	-1.68347585	1.68246439
H	-4.44576105	-3.23294448	0.79876659
C	1.92565615	1.20161881	-0.84449429
H	2.70455883	0.54260367	-1.23962025
H	2.02693517	2.18190042	-1.32000598
H	2.09464639	1.31514329	0.23125299
C	0.31923689	0.25752179	-2.56084144
C	0.08768924	1.25738758	-3.56433125
C	0.39686176	-1.06512560	-2.93948928
C	-0.01227963	2.64923037	-3.27189311
C	-0.04200020	0.84876872	-4.92690441
C	0.26282678	-1.46824174	-4.28899158
H	0.57062687	-1.82382250	-2.17897301
C	-0.21581523	3.57240444	-4.26920009
H	0.05631874	2.97788276	-2.24245906
C	-0.25606334	1.82908815	-5.93576312
C	0.04828892	-0.52981466	-5.26461940
H	0.33027576	-2.52219262	-4.54252673
C	-0.33861937	3.16177533	-5.61861350
H	-0.35246620	1.49956406	-6.96725278
H	-0.05544733	-0.82241871	-6.30637835
H	-0.28888490	4.62723517	-4.02030811
H	-0.50114728	3.90154604	-6.39699836

5Me'

G_{solv} = -2704.78837

Ni	1.99772103	-0.48071552	1.09698262
C	-1.54089771	-2.54011190	0.04777748

C	-0.24805117	-2.16325173	0.11561135
C	-0.53190831	0.66872407	2.53541649
C	0.14949114	-0.78972631	0.58100783
C	-0.92128704	-0.27616374	1.48990371
C	-2.20113024	-0.70208354	1.38483173
S	2.71709329	-2.02844046	-0.41228094
S	1.23266428	0.73915450	2.74382137
H	-1.86352933	-3.49954057	-0.34570750
H	-3.00047309	-0.29589923	1.99859254
C	-4.66889801	-1.31800978	-0.71275967
C	-3.95017814	-2.12320197	0.38030794
H	-3.97966136	-3.18261696	0.11802199
H	-4.46609217	-1.99721763	1.33673173
N	-2.55269952	-1.73599197	0.54373215
C	-4.82912764	0.12413360	-0.36015823
N	-3.96521223	1.11492915	-0.78709120
C	-5.73037618	0.74187384	0.45769603
C	-4.31885863	2.28503103	-0.26403610
N	-5.38754690	2.07433187	0.49687546
H	-6.57028756	0.34849315	1.00743447
H	-3.82626420	3.22967539	-0.42928292
H	-4.12566679	-1.41084980	-1.65805811
H	-5.66080794	-1.75564436	-0.85546628
H	-5.87590812	2.79395685	1.01773740
C	-0.66038178	0.79900116	-2.50724681
H	0.26551597	-0.12075856	-0.28695391
O	-1.64679391	1.49104930	-2.25160933
H	-3.16620924	1.00773484	-1.42845551
C	3.69481509	0.12165431	1.37117395
O	4.75358556	0.52046201	1.51496474
O	-1.29339925	1.34556331	3.22098969
P	1.09765340	-3.25705818	-0.28472503
C	0.80659920	-4.16508832	-1.81727704
H	1.65762660	-4.82511457	-2.00741063
H	-0.09844911	-4.76981035	-1.70631571
H	0.68691854	-3.46683156	-2.64833255
C	1.29103543	-4.49394186	1.02080967
H	1.43719141	-3.98237395	1.97569844
H	0.38576958	-5.10715592	1.06537521
H	2.15791449	-5.12417474	0.80227789
C	-0.85142780	-0.59000156	-3.05477782
H	-0.67809056	-0.58151069	-4.13736727
H	-0.15529410	-1.30192512	-2.60692270
H	-1.88075299	-0.90586005	-2.87373311

C	0.72292291	1.30627666	-2.28270632
C	1.03005937	2.29983623	-1.28337949
C	1.74157020	0.75710817	-3.03900730
C	0.06892073	2.89183263	-0.41603771
C	2.39766368	2.66894729	-1.10690432
C	3.08407956	1.15662077	-2.87817995
H	1.51559141	0.00013654	-3.78228697
C	0.44382103	3.80642378	0.53907283
H	-0.97251905	2.61894956	-0.50974866
C	2.75263654	3.61767583	-0.10989755
C	3.40445514	2.08540367	-1.92297961
H	3.85422188	0.71165661	-3.49968278
C	1.79646833	4.18383589	0.69457386
H	3.80084076	3.88186360	0.00320382
H	4.43670357	2.38987132	-1.77111680
H	-0.31130557	4.23659129	1.19056882
H	2.07488288	4.90656796	1.45552906

TS$_{5',6'\text{-Me}}$

G_{solv} = -2704.752471

Ni	1.77267607	-1.08278383	0.84675625
C	-2.26427528	-2.17759315	0.25444997
C	-0.90340245	-2.17159671	0.21296511
C	-0.16528268	0.73361431	2.44436633
C	-0.13973497	-1.04972058	0.71480614
C	-0.91135741	-0.18523635	1.56060419
C	-2.27904518	-0.21446440	1.55507976
S	1.92695807	-2.75586723	-0.67347066
S	1.57508337	0.39444410	2.46056165
H	-2.87036248	-2.97719169	-0.15902081
H	-2.88052722	0.48844303	2.12220287
C	-4.83275184	-0.42859041	-0.59802843
C	-4.41316198	-1.11098560	0.71081443
H	-4.77839543	-2.13926215	0.72100799
H	-4.82164175	-0.58912062	1.57767175
N	-2.95204197	-1.16220490	0.85594379
C	-4.73072090	1.06225591	-0.58362302
N	-3.54944175	1.77577930	-0.68159497
C	-5.73939545	1.97521348	-0.45373368
C	-3.83242933	3.06950459	-0.61147756
N	-5.15141580	3.21724718	-0.47443820
H	-6.80513187	1.84308904	-0.35376417
H	-3.11547300	3.87402331	-0.65978024
H	-4.25244343	-0.84499360	-1.42842304

H	-5.88024250	-0.68554950	-0.77724440
H	-5.63389672	4.10459924	-0.40104686
C	-0.24639313	0.65095687	-1.33821016
H	0.03793486	-0.20070059	-0.44342643
O	-1.09452254	1.50568497	-0.80685529
H	-2.45646095	1.45766614	-0.79107194
C	3.59006558	-0.88931668	0.87813780
O	4.71697320	-0.74188095	0.88574122
O	-0.66965436	1.60580477	3.13340112
P	0.06299796	-3.54274479	-0.41774399
C	-0.63602444	-4.19921002	-1.94303785
H	-0.00388841	-5.01744470	-2.29909582
H	-1.63812111	-4.58409649	-1.73126030
H	-0.68983317	-3.41395115	-2.69953672
C	0.03764561	-4.87247465	0.80290484
H	0.40556486	-4.48918091	1.75762509
H	-0.99021372	-5.22997010	0.91625474
H	0.67815316	-5.68884887	0.45776776
C	-0.85289282	-0.25556372	-2.40687063
H	-0.95111253	0.29581995	-3.34865957
H	-0.26914813	-1.15946418	-2.59301731
H	-1.85028825	-0.56222816	-2.08019986
C	1.17425071	1.15028430	-1.60074058
C	1.77839362	2.23479904	-0.86408964
C	1.95408464	0.45884671	-2.50871981
C	1.08375383	3.04774532	0.08061936
C	3.16647728	2.51566555	-1.07076114
C	3.31994609	0.75158254	-2.71504896
H	1.52858615	-0.35901287	-3.07659917
C	1.71649453	4.06156654	0.75863758
H	0.03706674	2.84355642	0.25450844
C	3.79536829	3.56527523	-0.34412414
C	3.92180280	1.75211299	-1.99998732
H	3.88566396	0.16893036	-3.43618054
C	3.08980982	4.32752655	0.55182074
H	4.85203071	3.75217379	-0.51933583
H	4.97576397	1.98139963	-2.13517729
H	1.15537744	4.65944399	1.47170171
H	3.57905307	5.12795238	1.09943846

6$_{Me}$'

G_{solv} = -2704.797919

Ni	2.16301484	0.42328935	1.25861838
C	-1.03531492	-2.32001117	0.91328325

C	0.23796316	-1.77839957	0.91046380
C	-0.45638952	1.62969203	2.28747536
C	0.47240994	-0.45447805	1.32058216
C	-0.65669900	0.24802784	1.75902252
C	-1.91091208	-0.31962851	1.76224997
S	3.20854069	-1.37078688	0.42158612
S	1.23645089	2.11180236	2.32475028
H	-1.25379399	-3.33518011	0.59970513
H	-2.78957179	0.20428945	2.12066693
C	-4.25630415	-1.68719580	0.07764590
C	-3.45696213	-2.15335107	1.29890703
H	-3.35344285	-3.23814609	1.29313556
H	-3.94360797	-1.85224982	2.22790027
N	-2.08817870	-1.58446612	1.32663552
C	-4.56030203	-0.21957709	0.05325816
N	-3.92570711	0.64722612	-0.81450171
C	-5.41940762	0.49124117	0.85353759
C	-4.39616360	1.85155716	-0.54251706
N	-5.29658103	1.80005198	0.46040403
H	-6.08339729	0.18766679	1.64856645
H	-4.11410071	2.76883235	-1.03816794
H	-3.71666141	-1.95718679	-0.83317222
H	-5.18548076	-2.26535094	0.08924449
H	-5.80265228	2.58800101	0.84387740
C	-1.28499722	-0.73663027	-2.31485362
H	-1.48746307	-0.67102463	-1.23662272
O	-2.25516620	0.05523681	-2.99379394
H	-2.93334534	0.28877967	-2.32296081
C	3.68633281	1.42602182	1.05557335
O	4.60456877	2.07331725	0.89567926
O	-1.36648190	2.33489124	2.68198022
P	1.71337271	-2.75389680	0.54876874
C	1.56120020	-3.72735026	-0.95504434
H	2.46931569	-4.32878518	-1.05841760
H	0.69646845	-4.39185308	-0.87150917
H	1.45801676	-3.06712482	-1.81780562
C	1.95059968	-3.89747776	1.92186803
H	2.00617556	-3.33225029	2.85516826
H	1.10767031	-4.59418031	1.95555266
H	2.88056334	-4.45080210	1.76518222
C	-1.44263778	-2.19440554	-2.72760382
H	-1.27351782	-2.32571324	-3.80127092
H	-0.75913466	-2.84910636	-2.18020755
H	-2.46540844	-2.51686032	-2.51413550

C	0.10369835	-0.15122251	-2.54332417
C	0.42374919	1.14273160	-2.00564099
C	1.06401652	-0.82114960	-3.26766436
C	-0.50955058	1.91964734	-1.26138141
C	1.72050851	1.69224344	-2.23109381
C	2.35327487	-0.27598163	-3.48709458
H	0.84431641	-1.79560951	-3.69089924
C	-0.18353466	3.16960237	-0.79616797
H	-1.49665305	1.52190767	-1.05903490
C	2.03433557	2.98358645	-1.72215645
C	2.67844500	0.95268196	-2.97716438
H	3.08000608	-0.84348487	-4.06099807
C	1.10150526	3.71334306	-1.02980712
H	3.02854726	3.38484786	-1.90258413
H	3.66449158	1.38116496	-3.13758993
H	-0.91419916	3.74121470	-0.23136338
H	1.34870762	4.69995579	-0.64929534

1$_{Et}$

G_{solv} = -2243.926773

Ni	0.11632407	-1.77763116	1.54209113
C	-0.79498023	0.83206444	-1.65163769
C	-0.43538303	-0.29603503	-0.93904411
C	-1.10465778	0.85261335	2.55577122
C	-0.48390346	-0.31914041	0.46661759
C	-0.97719267	0.84224063	1.06998585
C	-1.32782777	1.95341583	0.33222389
S	0.99866751	-2.86173888	-0.21393554
S	-0.59422350	-0.66440837	3.30159110
H	-0.74443779	0.89703473	-2.73345083
H	-1.68336240	2.87060128	0.78804957
C	-0.11354374	3.87886386	-2.07563724
C	-1.44810229	3.18186246	-1.77922486
H	-1.96554380	2.91059291	-2.70023643
H	-2.09988218	3.81416560	-1.17683488
N	-1.22098409	1.93790492	-1.00947366
C	0.71516991	4.10525278	-0.84953195
N	1.59496601	3.14329126	-0.38982605
C	0.70855792	5.17376092	0.01190885
C	2.11216721	3.63166306	0.72141515
N	1.60369476	4.85377072	1.00152857
H	0.16425612	6.10603281	0.00483343
H	2.84761770	3.14879177	1.34828062
H	0.45407413	3.27656985	-2.79225245

H	-0.35470144	4.82946208	-2.55960499
H	1.84754666	5.43386490	1.79337632
O	-1.52375415	1.80133376	3.19081730
C	0.63989242	-3.15309933	2.64238633
O	0.94934594	-4.00634646	3.32287573
P	0.10744771	-1.82309117	-1.73228128
C	1.24465828	-1.43594290	-3.09109373
H	0.70134561	-0.75738734	-3.75972233
H	2.07056417	-0.87068831	-2.64714974
C	-1.34308364	-2.72000586	-2.36261666
H	-0.97257247	-3.70376456	-2.67140840
H	-1.99643239	-2.87241918	-1.49712410
C	1.74014756	-2.67000364	-3.84526397
H	2.42034701	-2.34976709	-4.63866583
H	2.28793799	-3.35260501	-3.18884049
H	0.91413969	-3.21837189	-4.30714326
C	-2.07551841	-2.01886312	-3.50577219
H	-2.91512806	-2.64429602	-3.82109064
H	-2.47739117	-1.05011177	-3.19409273
H	-1.42514379	-1.86585765	-4.37180941

2$_{Et}$

G_{solv} = -2629.803537

Ni	1.22399444	-1.10142919	1.80861552
C	-1.32445264	-1.60872087	-1.52099717
C	-0.19184948	-1.58080209	-0.73018458
C	-1.73409557	-0.98679697	2.62693907
C	-0.27782510	-1.36897784	0.65833177
C	-1.57685581	-1.25694234	1.16933466
C	-2.68916026	-1.32491879	0.35792996
S	2.70419109	-1.46853088	0.17389149
S	-0.19364876	-0.81686269	3.46763031
H	-1.29669958	-1.71002712	-2.60033123
H	-3.70084934	-1.23498454	0.73702833
C	-4.00164062	0.02136110	-2.30289488
C	-3.73674921	-1.41945410	-1.85046057
H	-3.54393757	-2.06391168	-2.70817364
H	-4.58002062	-1.82014337	-1.28713472
N	-2.54876606	-1.48907191	-0.97096471
C	-4.32194545	0.95810754	-1.18043228
N	-3.33957003	1.59205923	-0.44188189
C	-5.55372082	1.29395372	-0.67960667
C	-3.97273899	2.29942012	0.47629649
N	-5.30877468	2.14412077	0.36914522

H	-6.55310915	1.01238818	-0.97446533
H	-3.51053269	2.92631483	1.22468625
H	-3.13416163	0.38781478	-2.86189480
H	-4.84511921	-0.02264113	-2.99779665
H	-6.00568710	2.59085316	0.95048141
C	3.93795172	2.95784388	0.18418419
C	4.08767427	3.63268794	-1.02964656
C	2.98972594	3.77346961	-1.87696233
C	1.74783968	3.24690727	-1.51479700
C	1.59122865	2.57127642	-0.30315413
C	2.69935192	2.42996974	0.53993915
H	4.78870779	2.83583697	0.84875040
H	5.05404129	4.03938958	-1.31344634
H	3.09771681	4.29220772	-2.82558937
H	0.89613110	3.34712862	-2.17981002
H	2.59082883	1.88976572	1.47823160
C	0.25853699	1.98838233	0.12482999
H	0.47382878	0.99860371	0.55904737
O	-0.57043517	1.83825749	-1.00907365
H	-1.50627945	1.70925190	-0.73736644
C	-0.40600980	2.82536627	1.21671753
H	0.27593311	2.96037366	2.06210969
H	-0.68764082	3.81116250	0.83028924
H	-1.30131581	2.31743436	1.58974176
C	2.61236962	-0.74218718	2.95733789
O	3.46680814	-0.50366042	3.66456681
O	-2.81227554	-0.88055300	3.18092594
P	1.46546760	-1.67009478	-1.43952109
C	1.60204919	-0.32056875	-2.64422368
H	1.18216724	0.56380856	-2.15521916
H	0.92321445	-0.58520101	-3.46410670
C	1.79005573	-3.27098261	-2.23994920
H	2.87300470	-3.28871151	-2.40762608
H	1.56664254	-4.03084777	-1.48397520
C	3.02254632	-0.07713029	-3.14813751
H	3.00422270	0.72054624	-3.89547616
H	3.68316978	0.23831272	-2.33505956
H	3.44718536	-0.97055640	-3.61630375
C	1.03614654	-3.53481672	-3.54249356
H	1.33843135	-4.51326936	-3.92574312
H	-0.04633766	-3.55565591	-3.39013323
H	1.27032824	-2.78830093	-4.30632836

$TS_{2,3\text{-Et}}$

G_{solv} = -2629.764996

Ni	1.77003584	-1.20937844	1.09233542
C	-1.19087434	-0.75562579	-1.90045209
C	-0.00363697	-0.68688872	-1.23969678
C	-1.02210847	-2.21647827	2.03228388
C	0.07834267	-0.87918327	0.21652392
C	-1.11482066	-1.56953894	0.71505222
C	-2.27322197	-1.61729216	0.00137865
S	2.95044365	-0.36065618	-0.62618298
S	0.63666173	-2.23419779	2.66891246
H	-1.28515638	-0.55249290	-2.96267077
H	-3.17565527	-2.07072171	0.39838035
C	-4.22039191	0.31693368	-2.00109201
C	-3.61216987	-1.09058092	-2.00860993
H	-3.41941160	-1.40512835	-3.03671021
H	-4.29424584	-1.80997793	-1.55157375
N	-2.34214084	-1.14811112	-1.27676236
C	-4.64660581	0.78090487	-0.64474287
N	-3.75552738	1.26711968	0.29501226
C	-5.90176626	0.77592385	-0.09667618
C	-4.46155978	1.55171443	1.37680177
N	-5.75981492	1.26648004	1.17839114
H	-6.85805171	0.47610519	-0.49667757
H	-4.06937606	1.95397816	2.29891545
H	-3.50038805	1.02197242	-2.43167618
H	-5.09186572	0.29855927	-2.66208719
H	-6.50292389	1.40118902	1.85174331
C	3.03770286	2.68748575	1.93305420
C	3.33005189	3.55653644	0.87985051
C	2.38016768	3.78584714	-0.11445511
C	1.14313006	3.14834049	-0.05917890
C	0.84458146	2.27738061	0.99472382
C	1.80411835	2.05035663	1.99091257
H	3.77588765	2.50085135	2.70701207
H	4.29568231	4.05129203	0.83525028
H	2.60060718	4.46163322	-0.93523769
H	0.39925138	3.33323174	-0.82616499
H	1.60371553	1.35890078	2.80304928
C	-0.46945086	1.58349498	1.02383060
H	0.07792321	0.24351736	0.71182425
O	-1.26152743	1.86071141	0.01640067
H	-2.25912736	1.56816537	0.15307062
C	-1.10512582	1.21878410	2.33499380
H	-0.38303240	0.81724496	3.04494965

H	-1.54643534	2.12807061	2.75924587
H	-1.90206037	0.48664918	2.18745192
C	3.28224198	-1.27822193	2.11020164
O	4.20655420	-1.26191534	2.77320769
O	-1.95755917	-2.70946136	2.64696266
P	1.54550815	-0.44932247	-2.10531756
C	1.48869752	1.05180405	-3.12614562
H	1.25752175	1.87690983	-2.44698691
H	0.63126770	0.92724057	-3.79864339
C	1.89996559	-1.86990700	-3.19260542
H	2.94697891	-1.75242994	-3.49456472
H	1.84508341	-2.75414864	-2.54895295
C	2.77458820	1.31276529	-3.90900410
H	2.66561050	2.23903453	-4.47952285
H	3.63386222	1.42998355	-3.24139849
H	2.99064165	0.50503496	-4.61447964
C	0.99364776	-2.00944658	-4.41498235
H	1.32682216	-2.86823794	-5.00454472
H	-0.04809006	-2.18570879	-4.13268682
H	1.03727384	-1.12437116	-5.05646696

3_{Et}

G_{solv} = -2629.79521

Ni	1.82354077	1.25544411	1.29900868
C	-0.72149646	-2.03497704	0.57677366
C	0.36088837	-1.22782221	0.56250791
C	-1.14009204	1.83566244	2.13836180
C	0.24982206	0.26262220	0.73058197
C	-1.04280189	0.56811921	1.41739584
C	-2.08196828	-0.29774879	1.42469291
S	3.18944107	-0.21491874	0.22973089
S	0.45759772	2.58018928	2.38762254
H	-0.66267731	-3.10446954	0.39878011
H	-3.02714945	-0.05543139	1.90170843
C	-4.02621907	-2.35477631	-0.32737950
C	-3.12423919	-2.47493988	0.91019272
H	-2.73824366	-3.49470376	0.96544574
H	-3.70702730	-2.28706619	1.81640434
N	-1.98313950	-1.56305081	0.89119479
C	-4.77530394	-1.06521805	-0.39219869
N	-4.24903470	0.09274387	-0.93417775
C	-6.00909432	-0.73043554	0.08532220
C	-5.11619016	1.08987230	-0.79915835
N	-6.18983254	0.60830744	-0.18043492

H	-6.75914393	-1.32420190	0.58261899
H	-4.97107773	2.10546060	-1.13090037
H	-3.42696524	-2.48644280	-1.23368034
H	-4.75367570	-3.17016890	-0.28986643
H	-7.01470904	1.15012919	0.05009143
C	2.46795418	1.96993205	-3.42232816
C	2.82732050	0.72827047	-3.94674634
C	1.92836330	-0.33884554	-3.89929496
C	0.67143257	-0.16254369	-3.33165427
C	0.30177461	1.08321540	-2.80675728
C	1.21090935	2.14854000	-2.85112355
H	3.16825012	2.79871633	-3.45461088
H	3.80980397	0.59055835	-4.38851800
H	2.21022436	-1.30716625	-4.30147739
H	-0.03235142	-0.98724111	-3.28497379
H	0.94653530	3.11814101	-2.44220981
C	-1.04702959	1.23322305	-2.19179694
H	0.28833091	0.74925254	-0.25678601
O	-1.83417673	0.28533205	-2.22137739
H	-3.32366227	0.18828871	-1.39878065
C	-1.42867223	2.53477917	-1.54788335
H	-0.69362547	2.82343465	-0.78933270
H	-1.44814746	3.32788346	-2.30330102
H	-2.41295225	2.45430922	-1.08641798
C	3.23037967	2.36919485	1.62374573
O	4.10574000	3.07463428	1.81411634
O	-2.17068034	2.36456552	2.54402986
P	2.01548009	-1.87207908	0.42511339
C	2.14504343	-3.00564117	-0.98872928
H	1.83574704	-2.43166117	-1.86751136
H	1.39037698	-3.78397529	-0.82337421
C	2.49018822	-2.77885031	1.93572996
H	3.56416029	-2.97773860	1.84482814
H	2.35978713	-2.06571270	2.75697476
C	3.53333928	-3.61489687	-1.17685940
H	3.52491114	-4.26923337	-2.05293568
H	4.29128611	-2.84297280	-1.34233348
H	3.83284258	-4.21451434	-0.31211786
C	1.71107842	-4.06782996	2.19003114
H	2.07602899	-4.52969027	3.11193646
H	0.64135721	-3.87571740	2.31502536
H	1.84246543	-4.78933684	1.37793550

4$_{Et}$

G_{solv} = -2245.104456

Ni	0.29662681	1.49471375	1.80444140
C	-0.72742411	-1.62667826	-0.82762319
C	-0.19181192	-0.94642500	0.20693495
C	-1.22993354	2.52946930	-0.72304840
C	0.09303179	0.53439618	0.12027505
C	-0.85420828	1.12620267	-0.88025713
C	-1.36644837	0.39075231	-1.89345885
S	1.26713158	-0.32622024	2.77205438
S	-0.72613260	3.18163304	0.85606127
H	-0.88381830	-2.70209580	-0.82375335
H	-1.98807487	0.82604214	-2.67049567
C	-0.19088067	-2.04578215	-3.95788272
C	-1.47448321	-1.71894481	-3.17441139
H	-1.98463904	-2.64994125	-2.91297782
H	-2.14863191	-1.11775718	-3.78830906
N	-1.18449120	-0.97167764	-1.95840112
C	0.62590185	-0.83035153	-4.24186507
N	1.50072981	-0.28779024	-3.31563245
C	0.66677953	0.00579698	-5.31818487
C	2.05695477	0.81927685	-3.79720171
N	1.55769251	1.01107122	-5.01251063
H	0.14491366	-0.03228397	-6.26075704
H	2.77825381	1.44264749	-3.29449177
H	0.41211811	-2.76045991	-3.38832500
H	-0.46644890	-2.52167030	-4.90219019
H	1.81007206	1.78125004	-5.62134561
H	1.13783674	0.69451867	-0.20432878
H	1.69275577	-0.66954348	-2.39507020
C	0.63476490	2.49511047	3.29182829
O	0.83859040	3.11485075	4.22658085
O	-1.82022773	3.22150405	-1.54639934
P	0.14105118	-1.70845526	1.78166345
C	1.00479310	-3.29449099	1.57140495
H	1.93646270	-3.06978528	1.04253652
H	0.38262719	-3.89579180	0.89807617
C	-1.41675206	-2.01568879	2.67963424
H	-1.13685158	-2.29418489	3.70166037
H	-1.92291327	-1.04560906	2.73153829
C	1.26635443	-4.03395518	2.88341020
H	1.81043014	-4.95914126	2.67470457
H	1.87369074	-3.43533565	3.56916171
H	0.33357090	-4.29910943	3.38960769
C	-2.31002313	-3.07620931	2.03833656

H	-3.23101401	-3.17073631	2.62061306
H	-2.58824692	-2.80361575	1.01572830
H	-1.82350467	-4.05609193	2.01626812

5$_{Et}$

G_{solv} = -2783.349122

Ni	0.22691244	-1.31354930	2.46822992
C	-2.05636871	0.71314751	-0.44833923
C	-1.39781607	-0.26858686	0.20453253
C	0.28047778	1.79169724	2.86424763
C	-0.24884126	0.02156948	1.13393670
C	-0.36629637	1.43783695	1.60232090
C	-1.07680057	2.36779160	0.92572695
S	-0.42090950	-2.98978899	1.08375438
S	0.75575864	0.35098086	3.79364719
H	-2.83942282	0.51792251	-1.17444125
H	-1.13816752	3.39823990	1.26314961
C	-1.72126621	3.84604089	-1.93698516
C	-2.56477739	3.08656998	-0.90195027
H	-3.39928023	2.60604888	-1.41592766
H	-2.97928561	3.78856245	-0.17196837
N	-1.82095114	2.05139125	-0.18882998
C	-0.66668969	4.71294034	-1.33064456
N	0.60905218	4.26929101	-1.03340939
C	-0.72277247	6.00798000	-0.90382107
C	1.30486712	5.24354356	-0.45774442
N	0.51013533	6.30566845	-0.36856738
H	-1.52350851	6.72907671	-0.93809085
H	2.32770446	5.18130323	-0.12285347
H	-1.26792204	3.13692179	-2.63612769
H	-2.39889246	4.48565890	-2.50914949
H	0.78112795	7.19801860	0.02835977
C	2.24513008	1.00051525	-0.97216103
H	0.70220558	-0.13309374	0.60083386
O	1.56101698	1.77355491	-1.64775363
H	0.99209065	3.32422723	-1.23207998
C	0.90453864	-2.51337450	3.66267239
O	1.32954756	-3.25523536	4.41706824
O	0.49080036	2.92760926	3.27882014
P	-1.85244672	-1.98299214	0.03421870
C	-1.88159599	-2.45182306	-1.71913677
H	-2.57225080	-1.75700258	-2.21112716
H	-0.87837778	-2.23278774	-2.09255821
C	-3.49525191	-2.32139902	0.75002264

H	-3.43872354	-1.99253502	1.79315404
H	-3.59964140	-3.41234062	0.75742145
C	2.94875500	1.53255428	0.25179010
H	2.70152108	0.95369391	1.14634361
H	4.03408002	1.48777854	0.11341643
H	2.65604573	2.57110040	0.40712590
C	2.38909266	-0.43505190	-1.34479341
C	1.69492497	-1.04333093	-2.45864132
C	3.21907169	-1.21703539	-0.55775155
C	0.81885898	-0.35669476	-3.34849427
C	1.89743932	-2.44035805	-2.68947571
C	3.41233904	-2.59060999	-0.80064210
H	3.74323136	-0.77742200	0.28235200
C	0.20360456	-1.01194570	-4.39086718
H	0.63604239	0.69687742	-3.20164684
C	1.23992820	-3.08877376	-3.77005851
C	2.75908314	-3.18997857	-1.84478119
H	4.07145537	-3.16136978	-0.15494281
C	0.41103092	-2.39125096	-4.61202050
H	1.41100317	-4.15215685	-3.91487533
H	2.88962348	-4.25004894	-2.04549149
H	-0.45800917	-0.45708452	-5.04984638
H	-0.08708655	-2.89292480	-5.43594109
C	-2.26869976	-3.90426780	-1.98536220
H	-3.27959160	-4.12641299	-1.63066820
H	-2.23946083	-4.09247375	-3.06234954
H	-1.57234553	-4.59892053	-1.50542384
C	-4.66492902	-1.66206784	0.02187989
H	-5.59907419	-1.94857988	0.51362059
H	-4.59500612	-0.57091216	0.05093608
H	-4.72531233	-1.97988570	-1.02353346

$TS_{5,6\text{-Et}}$

G_{solv} = -2783.314067

Ni	2.33442505	0.09298178	-1.12804530
C	-0.29593127	-2.04682169	1.40227632
C	0.26459706	-1.50551681	0.28631838
C	2.94227440	0.58469918	1.88390688
C	1.19066816	-0.36766853	0.36303977
C	1.72395711	-0.22297202	1.71860349
C	1.13104382	-0.80405576	2.79792661
S	1.01381074	-0.97807610	-2.60518853
S	3.69669012	1.00831778	0.33305623
H	-1.03980353	-2.83596016	1.36637164

H	1.49203290	-0.64577523	3.80883631
C	-1.91830249	-1.42700065	4.11845648
C	-0.62734844	-2.19918091	3.82292969
H	-0.85937971	-3.24704846	3.61987478
H	0.05334493	-2.15553375	4.67521090
N	0.08329079	-1.66332384	2.65720826
C	-1.68897915	-0.00839437	4.53291923
N	-1.40859903	1.00049631	3.62873715
C	-1.67498337	0.51923441	5.79686854
C	-1.23808167	2.10628296	4.33418429
N	-1.38734128	1.85394542	5.64618653
H	-1.84411800	0.07044058	6.76353638
H	-1.00707196	3.08210943	3.93404244
H	-2.56799429	-1.46157456	3.23676566
H	-2.43590580	-1.95507257	4.92460003
H	-1.31214121	2.53575962	6.39003551
C	-0.56945532	1.60339197	0.38482257
H	0.50366310	0.64416158	0.14170985
O	-1.46445040	0.90148760	1.04530139
H	-1.37378334	0.94290423	2.08529976
C	3.34050963	0.74884949	-2.50631419
O	3.94399921	1.18104465	-3.36798489
O	3.41929627	0.93467535	2.95410780
P	-0.03659832	-2.18828046	-1.34135267
C	-1.81633820	-2.21276028	-1.69508989
H	-2.27326657	-2.82755965	-0.91036070
H	-2.16936604	-1.18764857	-1.55328955
C	0.60743948	-3.88950348	-1.46515565
H	1.66514091	-3.82544230	-1.18923030
H	0.56373733	-4.13881368	-2.53151946
C	0.22325222	2.59431402	1.19889819
H	1.07327370	3.00642318	0.65893913
H	-0.44890219	3.41693102	1.46902455
H	0.58209692	2.12821410	2.11947754
C	-0.85661358	1.89808427	-1.05298353
C	-2.09563229	1.58062585	-1.72167653
C	0.17327349	2.46619303	-1.78401924
C	-3.26768568	1.07668622	-1.08269813
C	-2.17203832	1.81222515	-3.13298467
C	0.07400070	2.71608037	-3.16348260
H	1.11911574	2.68697731	-1.30072227
C	-4.40491602	0.78611222	-1.79811481
H	-3.26265281	0.91062408	-0.01654446
C	-3.35984517	1.48607640	-3.84473161

C	-1.07414790	2.37829019	-3.83106490
H	0.91813280	3.15029770	-3.68947349
C	-4.45526947	0.97575072	-3.19771809
H	-3.38091767	1.66073999	-4.91723185
H	-1.16405280	2.54019383	-4.90184646
H	-5.27709042	0.40259696	-1.27659472
H	-5.35802447	0.73073672	-3.74885855
C	-2.17027597	-2.73528525	-3.08610477
H	-1.84508696	-3.77033633	-3.22660237
H	-3.25554989	-2.70048920	-3.21489952
H	-1.72004509	-2.11929291	-3.87070428
C	-0.12708560	-4.93587744	-0.62874290
H	0.31457125	-5.91733427	-0.82275572
H	-0.03407745	-4.73728320	0.44255869
H	-1.18955055	-4.98973716	-0.88390585

6$_{Et}$

G_{solv} = -2783.355527

Ni	1.17535476	-2.62673414	-0.05311469
C	-2.04996291	-0.60077062	1.77177454
C	-1.32133278	-1.39258739	0.90462061
C	2.00226294	-1.37464783	2.62439575
C	0.03090809	-1.68717485	1.15347086
C	0.55507856	-1.15705176	2.33885539
C	-0.21054226	-0.40597064	3.20411763
S	-0.50385053	-3.14035231	-1.43647277
S	2.82934390	-2.27689547	1.35474897
H	-3.07544962	-0.30015296	1.59136991
H	0.17761349	-0.00123112	4.13177613
C	-2.15530425	2.22012871	3.37492791
C	-2.28902478	0.75098024	3.79044696
H	-3.32751409	0.42658555	3.72351193
H	-1.93494288	0.59312482	4.80976232
N	-1.49684461	-0.13756085	2.90942513
C	-0.77917236	2.78170486	3.55099203
N	0.22211080	2.58703767	2.61816677
C	-0.27971392	3.50082620	4.60657787
C	1.29636728	3.18281569	3.10184371
N	1.03634710	3.74367180	4.30109657
H	-0.73544338	3.85312558	5.51941356
H	2.26329601	3.22867927	2.62252524
H	-2.47789835	2.32889892	2.33379188
H	-2.85975650	2.78103479	3.99580537
H	1.69320608	4.26606824	4.86598296

C	1.03550155	1.04215494	-0.58421723
H	1.13058308	-0.04614604	-0.45059485
O	-0.14163863	1.47525761	0.07424331
H	0.06395428	1.82154515	0.97242366
C	2.35715303	-3.41352135	-1.21289616
O	3.09500682	-3.87199940	-1.94291796
O	2.56213233	-0.96281679	3.62328949
P	-1.99314835	-1.96817920	-0.67063782
C	-2.34168280	-0.49538615	-1.67171667
H	-3.11920496	0.05989572	-1.13372311
H	-1.43268967	0.11136379	-1.63898189
C	-3.49829958	-2.97349027	-0.48928136
H	-3.24160533	-3.77779217	0.20761300
H	-3.64347591	-3.43150043	-1.47488740
C	2.30438119	1.65917675	0.00320223
H	3.18158371	1.28884510	-0.53645153
H	2.29659798	2.75189618	-0.05427139
H	2.40757580	1.36274641	1.05270371
C	0.89721133	1.25471826	-2.08431167
C	0.52357153	2.51112907	-2.66912456
C	1.14796780	0.18108855	-2.91058889
C	0.25309365	3.68171950	-1.90125265
C	0.41622892	2.60483098	-4.09059333
C	1.04693110	0.27750475	-4.31823788
H	1.41804000	-0.77504933	-2.46777635
C	-0.09622069	4.86465637	-2.50677769
H	0.30808534	3.62960730	-0.82146770
C	0.04579024	3.84260229	-4.68679390
C	0.68275541	1.46484764	-4.89782920
H	1.24945722	-0.59619284	-4.93083920
C	-0.20373671	4.95019819	-3.91592323
H	-0.03310956	3.89399898	-5.76983954
H	0.59313808	1.55434345	-5.97745507
H	-0.29704733	5.74214539	-1.89877170
H	-0.48478086	5.89045049	-4.38117109
C	-2.76440234	-0.80846143	-3.10477778
H	-3.68863927	-1.39311590	-3.13746545
H	-2.93714898	0.13101721	-3.63681392
H	-1.98481413	-1.35840843	-3.64050077
C	-4.75893084	-2.22788050	-0.05247561
H	-5.59983495	-2.92636320	-0.07502556
H	-4.67162711	-1.84597022	0.96802320
H	-4.99530548	-1.39665405	-0.72261142

5$_{Et}$'

G_{solv} = -2783.346014

Ni	1.91081680	0.47242214	1.03837979
C	-0.66819815	-2.74922886	0.14374588
C	0.40555080	-1.93340173	0.17251975
C	-0.83069878	0.67187958	2.54267853
C	0.28542611	-0.49355035	0.59253845
C	-0.87814018	-0.37472871	1.52431672
C	-1.92285750	-1.23288415	1.45995559
S	3.09800616	-0.74763769	-0.48484098
S	0.79306344	1.38840901	2.68206579
H	-0.63118895	-3.77386931	-0.21444173
H	-2.80527389	-1.12295933	2.08399201
C	-3.96101356	-2.80843878	-0.66426813
C	-3.06099712	-3.20846819	0.51421841
H	-2.71460028	-4.23371057	0.36683203
H	-3.63017625	-3.17495385	1.44718498
N	-1.89269622	-2.34551928	0.64858415
C	-4.60224627	-1.47403010	-0.47319609
N	-4.06968617	-0.29599859	-0.96301754
C	-5.71412919	-1.11491843	0.23224614
C	-4.81845437	0.73555466	-0.58473713
N	-5.81931107	0.25482372	0.14412943
H	-6.42519198	-1.71104482	0.78122087
H	-4.64086703	1.77129487	-0.82716972
H	-3.37854465	-2.81047398	-1.59082533
H	-4.74522308	-3.56392151	-0.76247002
H	-6.55159993	0.81963285	0.55914792
C	-0.75072673	0.72695133	-2.54430714
H	0.12748395	0.14252861	-0.29401005
O	-1.97188660	0.82496191	-2.41658388
H	-3.23886544	-0.19328267	-1.55730469
C	3.29906685	1.63168592	1.26582549
O	4.15503055	2.37391817	1.39544110
O	-1.76300634	1.03994446	3.25136907
P	2.05696637	-2.47860525	-0.20183303
C	2.07181988	-3.56673236	-1.65831225
H	1.35787774	-4.37124128	-1.44537015
H	1.66548045	-2.98157710	-2.48926392
C	2.74522727	-3.40757390	1.20840422
H	2.66319646	-2.73899789	2.07237934
H	3.81230483	-3.54349379	0.99984863
C	-0.16700673	-0.54576100	-3.09872439
H	0.10526203	-0.39719944	-4.15020826

H	0.73367632	-0.84272872	-2.55764564
H	-0.91929301	-1.33436028	-3.04430668
C	0.16948036	1.83608099	-2.16016479
C	-0.18940390	2.85082640	-1.19926316
C	1.43346735	1.84615492	-2.72159647
C	-1.43331339	2.90197234	-0.50962690
C	0.78860081	3.83769900	-0.86932763
C	2.38435966	2.83564453	-2.39966277
H	1.71587115	1.07901824	-3.43389771
C	-1.69364909	3.88356319	0.41773617
H	-2.18674983	2.15812684	-0.72082673
C	0.48765121	4.84255174	0.08957408
C	2.06771109	3.80822670	-1.48775631
H	3.36275368	2.81154090	-2.86832686
C	-0.73107193	4.87306485	0.71936045
H	1.24975520	5.58258474	0.31915879
H	2.79364231	4.57072675	-1.21769256
H	-2.65124723	3.89220728	0.93042413
H	-0.95277071	5.64172045	1.45335790
C	3.44994777	-4.13640025	-1.99407051
H	3.37467427	-4.75545275	-2.89228460
H	4.17681581	-3.34299653	-2.19301590
H	3.83511656	-4.76313629	-1.18439771
C	2.05542848	-4.74514100	1.47056138
H	2.50701596	-5.21728647	2.34769248
H	0.98796895	-4.61548598	1.67333369
H	2.16798585	-5.42961847	0.62446168

$TS_{5',6'\text{-Et}}$

G_{solv} = -2783.311865

Ni	1.68416803	-0.61239855	1.07421855
C	-2.25789441	-1.85895324	0.20681471
C	-0.90132736	-1.79244009	0.23701882
C	-0.44482689	1.19445764	2.43554699
C	-0.20860137	-0.57280229	0.67505903
C	-1.08110351	0.26023758	1.49515290
C	-2.43742276	0.15207515	1.42383923
S	2.01304642	-2.31964748	-0.37691938
S	1.28774248	0.86980592	2.64145231
H	-2.80404253	-2.71504085	-0.17604541
H	-3.10249584	0.81810177	1.96366873
C	-4.84924495	-0.08989115	-0.81892007
C	-4.47528435	-0.84390474	0.46423297
H	-4.79173768	-1.88550762	0.38385181

H	-4.96630371	-0.40147132	1.33410227
N	-3.02868800	-0.84171570	0.70455870
C	-4.72245659	1.39922307	-0.72580295
N	-3.51830788	2.08190037	-0.76581565
C	-5.73623576	2.30617570	-0.55716699
C	-3.80995823	3.36478449	-0.62430050
N	-5.13704799	3.53944049	-0.49569497
H	-6.80527535	2.17889005	-0.48208552
H	-3.09807714	4.17689430	-0.61333252
H	-4.24907681	-0.47871014	-1.64887244
H	-5.89405626	-0.32967265	-1.03875386
H	-5.60789505	4.42765723	-0.38272005
C	-0.23385411	1.00366239	-1.45550620
H	0.03253571	0.08875998	-0.35060529
O	-0.91965755	1.97397974	-0.88678102
H	-1.93810763	1.83717356	-0.87456294
C	3.48462827	-0.43181805	1.33003913
O	4.60623606	-0.30575990	1.47028777
O	-1.01979015	2.08018434	3.05274573
P	0.16378592	-3.16360097	-0.19179872
C	-0.39010608	-3.97195207	-1.72097107
H	-1.44507593	-4.22862977	-1.56894867
H	-0.34787665	-3.21379442	-2.50871467
C	0.15181901	-4.38865355	1.15672831
H	0.43411583	-3.83618883	2.05944174
H	0.96289240	-5.09142348	0.93660859
C	-1.02428168	0.07932097	-2.34394773
H	-1.08691968	0.51709182	-3.34614885
H	-0.57838154	-0.91221910	-2.42228161
H	-2.03615960	-0.03209555	-1.95168028
C	1.20528686	1.26782934	-1.73924121
C	2.00140255	2.24042614	-1.02502786
C	1.81655817	0.45465546	-2.67732748
C	1.49718296	3.15240523	-0.05485368
C	3.40460367	2.28678683	-1.29770311
C	3.19633097	0.52970007	-2.95229395
H	1.23691377	-0.28074747	-3.22030420
C	2.32422051	4.04360628	0.58748378
H	0.44659429	3.14342226	0.19153251
C	4.23467310	3.21146656	-0.60839255
C	3.97904886	1.41538076	-2.26181547
H	3.62784401	-0.13040053	-3.69778785
C	3.70934590	4.07801324	0.31666766
H	5.29754734	3.21916805	-0.83540461

H	5.04871579	1.47296090	-2.44503209
H	1.90350833	4.72186235	1.32419682
H	4.34969212	4.78394896	0.83689472
C	0.42933057	-5.20910063	-2.08953338
H	0.05067094	-5.62266567	-3.02796664
H	1.48635351	-4.96479286	-2.23262781
H	0.35383601	-5.98599328	-1.32322852
C	-1.18036306	-5.11464287	1.33985931
H	-1.09172783	-5.81508988	2.17495454
H	-1.99100442	-4.41799368	1.57388772
H	-1.45794425	-5.68575440	0.44911075

6$_{Et}$'

G_{solv} = -2783.358355

Ni	1.82888085	-1.96063235	-0.15205197
C	-0.98269778	0.47821281	-2.14503509
C	0.21355908	-0.02932301	-1.67366566
C	-0.92528135	-3.30130093	-0.26463603
C	0.27122129	-1.26253645	-0.99997217
C	-0.94222710	-1.95329502	-0.90454783
C	-2.11766702	-1.43012384	-1.39895237
S	3.03914805	-0.12196610	-0.58760569
S	0.69011064	-3.81267931	0.22290714
H	-1.06731803	1.43627743	-2.64781861
H	-3.06430570	-1.95491898	-1.33450554
C	-4.12114933	1.13642496	-1.37074996
C	-3.40801606	0.35065349	-2.47470283
H	-3.17987683	0.99520695	-3.32413150
H	-4.01883479	-0.48353100	-2.82202373
N	-2.12667377	-0.22194991	-1.99803978
C	-4.50092992	0.29667526	-0.18933859
N	-3.84341176	0.40054976	1.01992681
C	-5.44362820	-0.69693807	-0.10714996
C	-4.38376767	-0.50694849	1.81406809
N	-5.34978848	-1.19253443	1.16894403
H	-6.14668471	-1.08763667	-0.82691077
H	-4.11065216	-0.69495064	2.84191192
H	-3.48209245	1.96003646	-1.03864631
H	-5.00964024	1.57765129	-1.83256896
H	-5.91381541	-1.93544956	1.56132248
C	-1.32599228	2.74223313	0.91647169
H	-1.39993395	1.90293325	0.20894843
O	-2.39067828	2.64101735	1.85708965
H	-2.93571946	1.86204777	1.60859070

C	3.23797109	-2.65385531	0.80228231
O	4.09181386	-3.07223340	1.42151856
O	-1.92073368	-3.98485382	-0.11214810
P	1.79915319	0.79197109	-1.92652556
C	1.62441322	2.56973553	-1.63812100
H	0.86276048	2.92211139	-2.34372313
H	1.21761663	2.67222762	-0.62839754
C	2.35477566	0.49185581	-3.63250994
H	2.36896274	-0.59625417	-3.75391242
H	3.39340329	0.83883618	-3.67026324
C	-1.48763141	4.02345362	0.10887151
H	-1.50482687	4.90480602	0.75815537
H	-0.68507861	4.14292650	-0.62614794
H	-2.44081348	3.98436897	-0.42715951
C	0.00835190	2.60486143	1.64120323
C	0.39548945	1.32712066	2.17210284
C	0.86404256	3.67258893	1.79478951
C	-0.42236687	0.16751188	2.05696644
C	1.65346916	1.19495868	2.83119427
C	2.11210788	3.54093945	2.45205932
H	0.59762601	4.64466084	1.39315017
C	-0.01785223	-1.04124421	2.56787781
H	-1.38242021	0.22787974	1.55745351
C	2.05080930	-0.07236896	3.33957992
C	2.50188858	2.32861673	2.95780279
H	2.75779172	4.40917013	2.54650036
C	1.23500302	-1.16913530	3.21412860
H	3.01832911	-0.15652415	3.82834666
H	3.46006316	2.21468066	3.45830505
H	-0.66009929	-1.91048082	2.46440317
H	1.54833474	-2.13541186	3.59913971
C	2.92792124	3.35239672	-1.79106886
H	2.73043892	4.40874945	-1.59048328
H	3.68531342	3.01225219	-1.07853339
H	3.33593288	3.26899003	-2.80260559
C	1.50506196	1.16765109	-4.70831711
H	1.92908532	0.93540579	-5.68894075
H	0.47310507	0.80424281	-4.69563824
H	1.49388184	2.25533997	-4.59458553

1$_{tBu}$

G_{solv} = -2401.042341

Ni	-0.03159201	2.10685041	1.28883815
C	-1.07320962	-1.39781464	-0.82072997

C	-0.64403450	-0.55037090	0.18232426
C	-0.99927443	2.75128064	-1.54803060
C	-0.63122490	0.84397287	-0.00990961
C	-1.07064512	1.28846474	-1.26237734
C	-1.50592758	0.41365777	-2.23502072
S	0.01796702	0.56617593	2.90153794
S	-0.28499140	3.67939324	-0.22807014
H	-1.07669948	-2.47745105	-0.73084756
H	-1.84186393	0.74063161	-3.21270170
C	-0.54672965	-2.43685242	-3.69490733
C	-1.83280243	-1.85814647	-3.08785771
H	-2.45897081	-2.64606944	-2.66720746
H	-2.40830492	-1.30596213	-3.83079577
N	-1.50911199	-0.91043626	-1.99803636
C	0.44578621	-1.38709211	-4.08749735
N	1.30675228	-0.83411525	-3.15761102
C	0.63570204	-0.78593776	-5.30653636
C	2.00266918	0.07635929	-3.80991874
N	1.62998428	0.13973088	-5.10912875
H	0.16800778	-0.93550613	-6.26798856
H	2.77662017	0.70498655	-3.39403504
H	-0.08605373	-3.12040348	-2.97390744
H	-0.84546493	-3.02887597	-4.56443968
H	2.02420058	0.75144510	-5.81150306
C	0.62187174	3.35216606	2.46647685
O	1.05036711	4.11567422	3.18845317
O	-1.37506857	3.25346785	-2.59054683
P	0.04099004	-1.13797366	1.75611110
C	1.80022600	-1.67857318	1.39410556
C	-1.08071533	-2.40481621	2.56690845
C	2.59092931	-0.44326584	0.93005056
H	2.67192517	0.31597826	1.71197414
H	3.60222642	-0.77766975	0.67509980
H	2.15798174	0.01428612	0.03445034
C	1.82878974	-2.72293320	0.26575782
H	1.49050726	-2.30276174	-0.68595294
H	2.87185446	-3.02961358	0.13118018
H	1.24802924	-3.61812667	0.48984735
C	2.42751397	-2.24650978	2.67493763
H	1.96680035	-3.19169122	2.97273875
H	3.48735268	-2.43877203	2.47672887
H	2.36749222	-1.54222015	3.51098239
C	-0.80186687	-2.42256878	4.08070822
H	-1.45361624	-3.18217243	4.52508127

H	0.23104305	-2.68919465	4.31622763
H	-1.03568371	-1.46505792	4.55328609
C	-2.52986520	-1.94664827	2.32430284
H	-3.18707022	-2.58695433	2.92189647
H	-2.69566859	-0.91093740	2.63640081
H	-2.82583543	-2.05063548	1.27695073
C	-0.87929058	-3.81781342	2.00056132
H	0.10186271	-4.22434619	2.25622888
H	-1.63629714	-4.46406894	2.45797006
H	-1.01543134	-3.86889284	0.91781174

2$_{t\mathbf{Bu}}$

G_{solv} = -2786.908579

Ni	1.34143711	0.60454717	1.92523859
C	-0.68222219	-2.31884559	-0.36529074
C	0.31770572	-1.49114580	0.11246102
C	-1.53600612	0.20488066	2.89750450
C	0.07536800	-0.62747928	1.20039570
C	-1.21431772	-0.68683267	1.74599487
C	-2.18612017	-1.52213380	1.24022771
S	2.92868848	-0.00545350	0.49848719
S	-0.17849542	1.20910917	3.39822310
H	-0.54984607	-3.00922711	-1.18892135
H	-3.18693077	-1.57884578	1.65239828
C	-3.73203674	-2.41585724	-1.49989965
C	-2.97114387	-3.16313087	-0.39917143
H	-2.48523230	-4.05040088	-0.80532006
H	-3.63652860	-3.46316358	0.41099219
N	-1.90868368	-2.32048826	0.19359820
C	-4.55655493	-1.26954343	-1.00434255
N	-4.01846577	-0.02246388	-0.74649773
C	-5.89288631	-1.25921330	-0.69540633
C	-5.01512981	0.72050335	-0.30010888
N	-6.16163537	0.01111459	-0.25078978
H	-6.65277513	-2.02342503	-0.75595555
H	-4.94807812	1.75846199	-0.00837371
H	-3.01997846	-2.07260019	-2.25828197
H	-4.38563865	-3.15224641	-1.97619040
H	-7.06360628	0.36120783	0.04427265
C	1.79356535	4.56246827	-1.14131984
C	1.59444244	4.97624384	-2.46019710
C	0.52762225	4.45335125	-3.19050340
C	-0.33582056	3.52245067	-2.60925152
C	-0.14187002	3.10443852	-1.29176887

C	0.93090596	3.63274931	-0.56561277
H	2.62563753	4.95728849	-0.56491744
H	2.26897759	5.69594942	-2.91508519
H	0.36840606	4.76664770	-4.21872509
H	-1.15622021	3.10353659	-3.18332333
H	1.09737982	3.30073822	0.45751790
C	-1.05952243	2.09844389	-0.62619793
H	-0.41948757	1.46654606	0.00676616
O	-1.67974808	1.30224636	-1.61601905
H	-2.43440102	0.80631988	-1.22886969
C	-2.08374637	2.78139433	0.27962411
H	-1.58220711	3.41743868	1.01528370
H	-2.76449347	3.40128404	-0.31460415
H	-2.66892755	2.03280095	0.82401691
C	2.47785818	1.85787330	2.63687426
O	3.16039662	2.65553194	3.06767826
O	-2.62558861	0.23380376	3.43952041
P	2.00945690	-1.51678633	-0.54812944
C	2.00969880	-1.10064217	-2.37553677
C	2.79476981	-3.15359239	-0.06102131
C	1.54088619	0.35564253	-2.51801096
H	2.24088285	1.06573529	-2.07210757
H	1.46774915	0.57649575	-3.58872752
H	0.54919975	0.50656323	-2.08233176
C	1.04089713	-1.99297377	-3.16868205
H	-0.00168815	-1.75003119	-2.94681983
H	1.20116908	-1.78161441	-4.23132557
H	1.20322782	-3.06091981	-3.01604286
C	3.43798723	-1.25336478	-2.91937211
H	3.74459699	-2.30096433	-2.97463630
H	3.45393287	-0.84545709	-3.93568241
H	4.17274643	-0.69734654	-2.32810871
C	4.32648953	-3.01570143	-0.06490148
H	4.74489458	-3.98706468	0.21980404
H	4.72539329	-2.75669614	-1.04796696
H	4.67181044	-2.27611575	0.66175063
C	2.32173826	-3.47136091	1.36871976
H	2.88048255	-4.34513976	1.71985438
H	2.51670675	-2.64810040	2.06356413
H	1.25669774	-3.71663055	1.40464947
C	2.37935250	-4.28857762	-1.00652429
H	2.79048084	-5.22063603	-0.60358052
H	1.29472453	-4.41115108	-1.07111410
H	2.78531474	-4.15331692	-2.01166548

$TS_{2,3\text{-}tBu}$

G_{solv} = -2786.874359

Ni	1.66457521	1.10478360	1.26461947
C	-1.11210895	-1.93856309	0.36511049
C	-0.01522071	-1.14137196	0.28665976
C	-0.97587572	1.41126122	2.86984899
C	-0.01082840	0.21022366	0.88233890
C	-1.09334445	0.34676251	1.86309076
C	-2.17971172	-0.47444554	1.86180221
S	2.73219026	-0.06158217	-0.33089325
S	0.63838683	2.15076694	2.89982078
H	-1.15298171	-2.93621316	-0.05410355
H	-3.01919211	-0.32429304	2.53289242
C	-4.15377451	-2.22682377	-0.37701958
C	-3.42968135	-2.41247987	0.96128268
H	-3.11840219	-3.45432186	1.07232541
H	-4.08582902	-2.15747801	1.79520170
N	-2.23355561	-1.56979492	1.05681060
C	-4.78209964	-0.88012897	-0.54269412
N	-4.07110421	0.25200381	-0.89977903
C	-6.09302885	-0.53225043	-0.35048966
C	-4.93866418	1.25095914	-0.92421987
N	-6.16722164	0.81670321	-0.59609459
H	-6.95578567	-1.11655045	-0.06985070
H	-4.71001709	2.27841892	-1.16528594
H	-3.45290924	-2.41962648	-1.19705835
H	-4.93417602	-2.99129157	-0.43365293
H	-7.00186521	1.38646544	-0.54725167
C	2.05753674	3.73242401	-1.88161972
C	2.27107822	3.38867597	-3.21819552
C	1.39934815	2.50667350	-3.85485027
C	0.32676688	1.95601268	-3.15723645
C	0.11480747	2.28774733	-1.81503342
C	0.98327370	3.19104472	-1.18652418
H	2.73201945	4.41887521	-1.37896507
H	3.11198582	3.81018185	-3.76084103
H	1.55402860	2.24296527	-4.89669559
H	-0.35247008	1.27386276	-3.65581413
H	0.84203479	3.45163498	-0.14175030
C	-1.03696467	1.69699871	-1.07743770
H	-0.23947284	1.00447004	-0.02353149
O	-1.65435252	0.71945265	-1.69783012
H	-2.60318637	0.49988944	-1.31709042

C	-1.84197204	2.58473053	-0.17238497
H	-1.20516863	3.20666067	0.45685574
H	-2.44220076	3.24391359	-0.81027798
H	-2.51720388	2.00554835	0.45899361
C	3.16196784	2.10942465	1.53371844
O	4.09303206	2.74742815	1.67745167
O	-1.86478931	1.76499476	3.63264498
P	1.57361948	-1.75367467	-0.30176930
C	1.45783484	-2.46528389	-2.03571744
C	2.23708939	-2.93493381	1.01175853
C	1.15508855	-1.29718779	-2.98573859
H	1.98332805	-0.58840282	-3.05079209
H	0.97891349	-1.71195310	-3.98456038
H	0.25451414	-0.75884913	-2.67847070
C	0.31799158	-3.48979095	-2.17703086
H	-0.66041722	-3.00352806	-2.15089531
H	0.42091547	-3.95546104	-3.16336588
H	0.34405624	-4.28678270	-1.43262399
C	2.79580206	-3.11583097	-2.41635933
H	2.96272669	-4.05105851	-1.87615871
H	2.76281086	-3.34991912	-3.48605869
H	3.64852908	-2.45006892	-2.24877949
C	3.76132317	-3.08020257	0.88300743
H	4.10182292	-3.74316422	1.68602346
H	4.06680956	-3.52527759	-0.06587634
H	4.27102871	-2.12025471	0.99945772
C	1.91431717	-2.32048242	2.38522434
H	2.36852598	-2.95682565	3.15225190
H	2.33125217	-1.31379681	2.49807747
H	0.83863909	-2.27588262	2.57586432
C	1.57384692	-4.31571316	0.90802991
H	1.90424056	-4.91121996	1.76642910
H	0.48141607	-4.26204684	0.94805098
H	1.87331215	-4.84648288	0.00106528

3$_{t\mathbf{Bu}}$

G_{solv} = -2786.913722

Ni	1.36867292	1.00904896	1.79161763
C	-0.54452891	-2.21745738	-0.17284300
C	0.38010198	-1.28153915	0.12943356
C	-1.56435084	0.58542042	2.76787140
C	0.00398678	-0.01360701	0.85779615
C	-1.27357779	-0.25176384	1.60582853
C	-2.14602583	-1.22378626	1.25385839

S	2.98611157	0.20077174	0.47788004
S	-0.15552655	1.54222489	3.27608727
H	-0.32064488	-3.11737385	-0.73436032
H	-3.09611722	-1.35810981	1.76318377
C	-3.72672219	-2.51807182	-1.32739317
C	-2.84908525	-3.08797776	-0.20083803
H	-2.32436615	-3.96976032	-0.57402914
H	-3.47254878	-3.39659935	0.64299598
N	-1.85037450	-2.13895707	0.27489908
C	-4.68441378	-1.47097694	-0.86059827
N	-4.40889134	-0.11521980	-0.85068508
C	-5.92944558	-1.60367342	-0.31691190
C	-5.43566609	0.55105304	-0.33226563
N	-6.36580599	-0.33754592	-0.00002287
H	-6.52924912	-2.48095034	-0.13486310
H	-5.49649084	1.61981537	-0.20382874
H	-3.08985432	-2.11795708	-2.12261559
H	-4.30587619	-3.34336651	-1.75059541
H	-7.26213352	-0.10668535	0.41314728
C	1.71391768	3.95215492	-1.55540426
C	1.92238960	3.85445741	-2.93100837
C	0.96018648	3.25251333	-3.74408903
C	-0.20034823	2.73531721	-3.17955103
C	-0.42100535	2.83968770	-1.80028955
C	0.54003422	3.45984737	-0.99092635
H	2.46559727	4.41094533	-0.92043722
H	2.83581494	4.24478654	-3.36995076
H	1.12117961	3.17740658	-4.81511960
H	-0.94490384	2.24934168	-3.80204752
H	0.39575162	3.53609368	0.08250789
C	-1.66377575	2.25303003	-1.22284778
H	-0.12415576	0.79944100	0.12170339
O	-2.25008538	1.35510691	-1.83035786
H	-3.55583750	0.35622927	-1.20251548
C	-2.18565334	2.79426184	0.07447376
H	-1.43308105	2.70182700	0.86410349
H	-2.39986460	3.86246211	-0.03908113
H	-3.08918458	2.26724328	0.37935919
C	2.48239518	2.28914814	2.44606794
O	3.14221547	3.14406963	2.81359868
O	-2.64019161	0.65812234	3.35600901
P	2.10253979	-1.47149039	-0.32595512
C	2.26586654	-1.41254841	-2.19494665
C	2.84671096	-2.99198512	0.49960697

C	1.80593677	-0.01269326	-2.63465620
H	2.47816412	0.77472707	-2.28670064
H	1.78780473	0.01065167	-3.72975632
H	0.79548782	0.21114268	-2.27840904
C	1.35920904	-2.44356643	-2.88763679
H	0.30118139	-2.20746681	-2.74720073
H	1.56537805	-2.39405608	-3.96266903
H	1.53880969	-3.46985245	-2.56424805
C	3.72733281	-1.64048718	-2.60458365
H	4.03601175	-2.67686616	-2.44260908
H	3.82101107	-1.42643933	-3.67512755
H	4.41693308	-0.97781725	-2.07168371
C	4.37689452	-2.86286050	0.56969761
H	4.76417997	-3.75107488	1.08121117
H	4.84158227	-2.81947852	-0.41778980
H	4.68628096	-1.98369399	1.14060168
C	2.28161014	-3.03504943	1.93033522
H	2.78570131	-3.84310117	2.47175754
H	2.46365520	-2.10169021	2.47304346
H	1.20743703	-3.23828037	1.93974379
C	2.48118883	-4.28776931	-0.23549920
H	2.84137288	-5.12919130	0.36725462
H	1.40182849	-4.41347988	-0.35971272
H	2.96386549	-4.35058389	-1.21412696

4$_{tBu}$

G_{solv} = -2402.217005

Ni	0.39457560	-1.42161111	2.00880135
C	-1.10889034	0.88235671	-1.16473650
C	-0.38077287	-0.04510914	-0.50971668
C	-0.90231613	1.23778568	2.99929614
C	0.08200781	0.16484224	0.91474255
C	-0.77671054	1.22553349	1.54242989
C	-1.46415528	2.13257518	0.81296032
S	1.04625759	-2.59784203	0.21238318
S	-0.32875100	-0.27570483	3.73274030
H	-1.42304817	0.77422075	-2.19730437
H	-2.02717753	2.93823537	1.27516891
C	-0.82271558	3.85797559	-2.07808795
C	-2.00093186	3.16201282	-1.37137152
H	-2.70839471	2.80234262	-2.12374860
H	-2.51963566	3.86604089	-0.71772002
N	-1.55128374	2.04260322	-0.55494076
C	0.26352739	4.25095210	-1.13403648

N	1.21988980	3.35607023	-0.68170365
C	0.52941197	5.42517402	-0.49431658
C	2.03420393	3.94856184	0.18611358
N	1.62603377	5.20581357	0.31013788
H	0.03729188	6.38299462	-0.54575821
H	2.87034870	3.49233462	0.69062537
H	-0.40948407	3.19076734	-2.84195372
H	-1.19546029	4.75037423	-2.58651069
H	2.06741583	5.89600722	0.90743594
H	1.14094722	0.48368706	0.92005515
H	1.30248264	2.38486772	-0.96793382
C	0.84711919	-2.81011349	3.10188073
O	1.11262902	-3.68445927	3.78381856
O	-1.35236682	2.15493966	3.68011959
P	0.08993485	-1.58603649	-1.29616864
C	1.31380570	-1.22022462	-2.67227590
C	-1.43210791	-2.57159088	-1.81053798
C	2.56415704	-0.61015233	-2.01458612
H	3.09242156	-1.32837283	-1.38355049
H	3.24348911	-0.29009862	-2.81230265
H	2.31824190	0.27029381	-1.40938906
C	0.76255585	-0.19379832	-3.67734645
H	0.65466396	0.79549273	-3.22448574
H	1.49275548	-0.10425949	-4.48926845
H	-0.19044356	-0.48497932	-4.12064723
C	1.68400371	-2.52028879	-3.40052426
H	0.84984794	-2.90191047	-3.99531350
H	2.51296847	-2.30731706	-4.08447630
H	2.01455520	-3.30321219	-2.71025705
C	-1.07555363	-4.06164351	-1.93713205
H	-1.98329913	-4.59825112	-2.23499968
H	-0.31384955	-4.25061094	-2.69715241
H	-0.73376079	-4.48044033	-0.98750921
C	-2.46763964	-2.39997334	-0.68511287
H	-3.31064183	-3.06756495	-0.89473544
H	-2.06090089	-2.67082921	0.29499695
H	-2.84940851	-1.37697213	-0.63291240
C	-2.03013299	-2.08104704	-3.13650893
H	-2.96829148	-2.62275897	-3.30075776
H	-2.26653947	-1.01351993	-3.12510998
H	-1.37211059	-2.29237473	-3.98312638

5*t*Bu

G_{solv} = -2940.460001

Ni	-2.08363720	-1.26684446	-1.08338824
C	1.43379946	0.93180252	-1.91741669
C	0.63211449	-0.08727509	-1.54397722
C	-2.65698274	1.76504234	-1.56015100
C	-0.76300569	0.15844067	-1.02251274
C	-1.22011558	1.50856097	-1.48741935
C	-0.35412640	2.47824896	-1.86200651
S	-0.50386033	-2.84659211	-1.12690614
S	-3.61413102	0.27721537	-1.38818848
H	2.46001175	0.79399028	-2.23970564
H	-0.68842582	3.47276505	-2.14341870
C	2.47974681	3.94268822	-0.91457846
C	1.94215484	3.31944741	-2.21342023
H	2.78018091	2.91066007	-2.78207859
H	1.45659349	4.08288781	-2.82740259
N	0.99266316	2.24091575	-1.97136046
C	1.47899625	4.78973215	-0.19988476
N	0.54783610	4.30654458	0.70345174
C	1.23334090	6.12776521	-0.31019750
C	-0.22551409	5.30026187	1.12870092
N	0.17440182	6.41180473	0.52167900
H	1.71912041	6.88671824	-0.90225288
H	-1.03160385	5.21476917	1.83975875
H	2.84639736	3.15136405	-0.25303819
H	3.33144961	4.57768204	-1.17356301
H	-0.23996394	7.32569609	0.66381620
C	-0.89745025	1.29585853	2.27615608
H	-0.74664435	0.11666263	0.07956185
O	0.17221843	1.84116576	1.99917972
H	0.44950068	3.33963799	1.05641283
C	-2.20689981	1.96713736	1.97343716
H	-2.04286655	3.00355274	1.67887006
H	-2.71122114	1.44901414	1.14979369
C	-3.36635627	-2.51276506	-0.75541066
O	-4.17266970	-3.27781174	-0.49830392
O	-3.18909594	2.86122096	-1.71569586
P	1.20499432	-1.78481126	-1.55065848
C	2.44010329	-1.99688453	-0.15320925
C	1.82300092	-2.31715407	-3.24845722
C	1.68679619	-1.67297606	1.14650189
H	0.86885777	-2.37114680	1.33876108
H	2.39596280	-1.73973172	1.97932571
H	1.28254002	-0.65616085	1.13346055
C	3.61680984	-1.01409653	-0.27042225

H	3.28645863	0.02463069	-0.18739989
H	4.29313269	-1.20982675	0.56932487
H	4.19122334	-1.13079064	-1.18990933
C	2.96002189	-3.44001183	-0.12002195
H	3.61688305	-3.65367405	-0.96760642
H	3.54353591	-3.57413474	0.79770391
H	2.14724973	-4.17343851	-0.10793840
C	1.75340748	-3.84899631	-3.37124112
H	2.11372440	-4.12105251	-4.36966744
H	2.38424213	-4.35926377	-2.63974990
H	0.73061213	-4.22034589	-3.27043216
C	0.87303021	-1.68689460	-4.28165754
H	-0.17540622	-1.92723834	-4.07729359
H	0.97897925	-0.59965820	-4.32326006
H	1.12537435	-2.09188820	-5.26777868
C	3.26092457	-1.85716166	-3.52332347
H	3.98296547	-2.38355426	-2.89422887
H	3.49451195	-2.09458192	-4.56740917
H	3.39346326	-0.77943470	-3.39494956
H	-2.87198903	1.92231157	2.84039590
C	-0.91875600	-0.06544244	2.88877276
C	0.12189558	-0.52944403	3.76599110
C	-1.93272703	-0.92604916	2.51146256
C	1.17729135	0.29346019	4.24907987
C	0.08610319	-1.89082614	4.19146625
C	-1.94887689	-2.27461743	2.92549777
H	-2.71857534	-0.58752392	1.84453317
C	2.14793502	-0.21665182	5.07831511
H	1.22260420	1.33379029	3.95442013
C	1.10752242	-2.38952113	5.04450600
C	-0.95693334	-2.74668611	3.74527574
H	-2.74333195	-2.92891771	2.58081730
C	2.12310630	-1.57387984	5.47619166
H	1.06505220	-3.43184714	5.34921127
H	-0.95124453	-3.78508352	4.06580777
H	2.94416604	0.43129139	5.43303862
H	2.90119605	-1.96241892	6.12621830

$TS_{5,6\text{-}tBu}$

G_{solv} = -2940.423288

Ni	-0.80473605	-1.82054273	1.74810051
C	-1.84711115	0.81640819	-1.37780664
C	-1.27352272	-0.22685213	-0.70999230
C	-2.21293229	0.72756815	2.79699384

C	-1.14728569	-0.21863050	0.73928913
C	-1.96137522	0.81540288	1.34551326
C	-2.49651097	1.84387717	0.62668314
S	0.00632999	-2.88468574	-0.04730189
S	-1.68622476	-0.81325030	3.49335124
H	-1.95758754	0.84250534	-2.45483962
H	-3.05731631	2.64544733	1.09554821
C	-1.79848896	3.91982482	-2.01637467
C	-2.91968521	3.00446415	-1.51228045
H	-3.46828092	2.59703387	-2.36394517
H	-3.61912723	3.55631659	-0.88249592
N	-2.40340248	1.87529868	-0.72766231
C	-1.08052492	4.65588765	-0.93296489
N	-0.10521087	4.08305117	-0.13685741
C	-1.23134480	5.94686338	-0.51283042
C	0.32386434	4.99208917	0.72787566
N	-0.34476223	6.12801018	0.52267419
H	-1.87916529	6.73527191	-0.86193910
H	1.08352982	4.83834599	1.47815741
H	-1.08555506	3.33550903	-2.60815852
H	-2.25375656	4.65256743	-2.68785704
H	-0.21159954	6.98429362	1.04723818
C	1.12401933	1.11977974	0.88119181
H	0.16460357	0.23066313	0.95101002
O	0.91717404	1.77969503	-0.23169335
H	0.30845377	3.02830232	-0.17606308
C	0.88701014	1.88762845	2.18174751
H	-0.06062877	2.43075921	2.15026185
H	0.88862324	1.23033376	3.05403451
C	-0.41214496	-3.27368540	2.78317773
O	-0.15808424	-4.17464367	3.42846112
O	-2.74400267	1.59983214	3.46837042
P	-0.84737643	-1.77036804	-1.54370945
C	0.40152281	-1.49545259	-2.91621659
C	-2.45968196	-2.59896031	-2.06593921
C	1.70161355	-1.02308466	-2.24893424
H	2.14654917	-1.79116172	-1.61216557
H	2.41823558	-0.77803261	-3.04106531
H	1.53207439	-0.12168680	-1.65391875
C	-0.04369769	-0.39769947	-3.89834036
H	-0.01827758	0.59065271	-3.43213561
H	0.68040079	-0.38455590	-4.72036648
H	-1.03038646	-0.56591410	-4.33168303
C	0.63493962	-2.81198866	-3.67089121

H	-0.23064418	-3.09403972	-4.27613485
H	1.48378033	-2.66589841	-4.34776065
H	0.88505561	-3.64030641	-3.00007253
C	-2.24163611	-4.11033736	-2.24486326
H	-3.19764348	-4.55060425	-2.54869318
H	-1.50756617	-4.34321857	-3.01901316
H	-1.93126704	-4.58929644	-1.31300877
C	-3.47638477	-2.37392644	-0.93263601
H	-3.09838365	-2.71166263	0.03819678
H	-3.77049555	-1.32437681	-0.84618441
H	-4.37318466	-2.95866008	-1.16395831
C	-3.00925553	-2.00383244	-3.36987808
H	-2.37824450	-2.24970466	-4.22761415
H	-3.99752316	-2.44259816	-3.54702576
H	-3.13807367	-0.91893710	-3.31863970
H	1.69567316	2.61838068	2.29996096
C	2.35750520	0.21847554	0.96076748
C	3.53909259	0.41976638	0.16668595
C	2.34592633	-0.80691127	1.88180527
C	3.70547338	1.49345920	-0.75826876
C	4.62720173	-0.49790528	0.31665561
C	3.42382348	-1.70233253	2.03539447
H	1.46466433	-0.94856415	2.50156653
C	4.85724225	1.63002217	-1.49443385
H	2.89353176	2.19725375	-0.88252528
C	5.80182160	-0.33436296	-0.47072696
C	4.54161102	-1.56060947	1.25432425
H	3.35357736	-2.50483235	2.76378882
C	5.91849172	0.70259805	-1.36044826
H	6.61088450	-1.04962041	-0.34535202
H	5.37791493	-2.24870619	1.34612293
H	4.95415489	2.45877267	-2.19028234
H	6.82004755	0.81881201	-1.95481046

6*t*Bu

G_{solv} = -2940.467528

Ni	0.67930392	-1.77467193	1.98889384
C	-2.09872080	-1.15190669	-1.13359537
C	-0.97509244	-1.57020284	-0.44532444
C	-1.80875617	-0.28169075	2.97515274
C	-0.83503754	-1.30017898	0.92974603
C	-1.89572680	-0.59941865	1.51995493
C	-2.99789353	-0.19318964	0.80001668
S	1.69115600	-2.79557635	0.29494965

S	-0.33114023	-0.87585973	3.72845635
H	-2.26388117	-1.34686457	-2.18610846
H	-3.82571336	0.34592234	1.24557857
C	-3.99268275	1.34910489	-1.95479246
C	-4.24780560	-0.01477842	-1.30547681
H	-4.42510140	-0.77174980	-2.06961494
H	-5.10720039	0.01604585	-0.63450182
N	-3.08462208	-0.47576568	-0.51243394
C	-3.98129019	2.49742792	-0.99561133
N	-2.90893534	2.76636212	-0.16634292
C	-4.97764126	3.40931215	-0.75766163
C	-3.25540165	3.82013802	0.54967580
N	-4.49585318	4.23841896	0.22447442
H	-5.95653206	3.53739695	-1.19407435
H	-2.64505541	4.30258799	1.29907814
H	-3.05246940	1.30747734	-2.51601146
H	-4.79624714	1.50044437	-2.68111572
H	-4.98028360	5.02856015	0.62984144
C	0.49342052	1.85211321	0.80877856
H	0.47743899	0.85580262	1.27008104
O	-0.28140466	1.80908468	-0.37762307
H	-1.20312594	2.10804359	-0.20926785
C	-0.06336070	2.82583182	1.84724594
H	-1.08509208	2.53967670	2.11845563
H	0.54760579	2.78695495	2.75449635
C	2.13669374	-2.12401980	3.04708803
O	3.04779854	-2.31002319	3.69759199
O	-2.67450803	0.31961285	3.58415039
P	0.33623489	-2.54917160	-1.23245339
C	1.12248876	-1.57313546	-2.62724206
C	-0.37165135	-4.23184444	-1.68286552
C	1.83201218	-0.36496299	-1.99639480
H	2.67371477	-0.66049499	-1.36642854
H	2.21919573	0.25657654	-2.81160648
H	1.14155157	0.24724792	-1.40950100
C	0.07490669	-1.04673288	-3.62322135
H	-0.53757570	-0.25546914	-3.18287269
H	0.62138368	-0.60219319	-4.46178772
H	-0.57589440	-1.82342435	-4.02744298
C	2.14127179	-2.46655175	-3.35030749
H	1.65592404	-3.25408851	-3.93221128
H	2.70556539	-1.83484730	-4.04463722
H	2.85890225	-2.92338683	-2.66093906
C	0.76882182	-5.25877289	-1.78572956

H	0.32111276	-6.22329046	-2.04811367
H	1.49448642	-5.00676815	-2.56184363
H	1.29585382	-5.38070712	-0.83620960
C	-1.31751262	-4.64122348	-0.54007668
H	-0.82857749	-4.60302716	0.43859979
H	-2.21727200	-4.02063762	-0.50881912
H	-1.62905261	-5.67567453	-0.71893849
C	-1.14729180	-4.19466710	-3.00706158
H	-0.49039152	-4.01333472	-3.86120576
H	-1.61001346	-5.17797105	-3.14498523
H	-1.94971732	-3.45191662	-3.00838063
H	-0.07257933	3.85660309	1.48004713
C	1.95392913	2.11759611	0.47799330
C	2.39076069	3.20719385	-0.34679893
C	2.89544449	1.27226148	1.02239171
C	1.49563195	4.14219379	-0.94532398
C	3.78961003	3.37377494	-0.58478870
C	4.28021128	1.44183399	0.79105619
H	2.56349312	0.43974606	1.63976172
C	1.96146249	5.17490802	-1.72284275
H	0.43026381	4.02218524	-0.79509546
C	4.23939093	4.45029491	-1.39956766
C	4.71990907	2.46983595	-0.00194258
H	4.98690682	0.74806492	1.23721237
C	3.34905249	5.33385879	-1.95626118
H	5.30734620	4.56057286	-1.57056303
H	5.78018776	2.61087501	-0.19557652
H	1.25900680	5.87430320	-2.16721452
H	3.70342105	6.15320255	-2.57492312

5$_{t\mathrm{Bu}}$'

G_{solv} = -2940.456296

Ni	-1.18603814	-1.44975669	-1.33420247
C	-0.13309039	2.46382190	-0.11673377
C	-0.17371209	1.32385533	-0.83996757
C	-2.38527404	-0.69207778	1.43740397
C	-0.57229004	0.01185000	-0.20595160
C	-1.39550517	0.29902477	1.01243007
C	-1.30421033	1.47081931	1.67876701
S	0.04287626	-0.70895756	-3.06157363
S	-2.68554970	-1.91618288	0.19035666
H	0.16851938	3.41966142	-0.52738952
H	-1.87965791	1.66759101	2.57910637
C	0.55446643	3.71145565	3.11579558

C	-0.45443095	3.76285525	1.95852265
H	-0.14875545	4.54937018	1.26677696
H	-1.44721754	4.01906552	2.34219540
N	-0.54127350	2.51463162	1.20536051
C	0.12087670	2.84466769	4.25360321
N	0.54425978	1.54131912	4.43841200
C	-0.77387031	3.09149828	5.25466207
C	-0.05541533	1.01466733	5.50134174
N	-0.86108473	1.94218234	6.00663812
H	-1.34649915	3.97511837	5.48681648
H	0.08947532	0.01694997	5.88349115
H	1.52742601	3.38054130	2.74240050
H	0.67498958	4.73169645	3.49099541
H	-1.44249735	1.81418079	6.82695144
C	2.43294264	-0.36141387	1.96300343
H	0.33119945	-0.55723656	0.06759422
O	2.08065024	-0.37768084	3.14389831
H	1.22863842	1.01915549	3.86965673
C	2.90019889	0.93343606	1.35590355
H	2.22501616	1.22113505	0.54310893
H	2.90557142	1.70786421	2.12392796
C	-1.45761206	-3.05386100	-2.14281108
O	-1.57563327	-4.08636663	-2.61403506
O	-2.97691976	-0.70237821	2.51456090
P	0.10715949	1.29161692	-2.61163412
C	1.80523455	1.96386345	-3.06041657
C	-1.33778240	2.16281857	-3.45349040
C	2.84833929	0.93906609	-2.58549348
H	2.81862965	0.01710039	-3.17022838
H	3.84108235	1.38839795	-2.70105685
H	2.71382122	0.68582007	-1.53120637
C	2.09629085	3.29807029	-2.35217590
H	2.24384894	3.15592611	-1.27830426
H	3.03264194	3.69289370	-2.76181238
H	1.32308978	4.05330506	-2.50856114
C	1.92241529	2.14118924	-4.58129688
H	1.32370627	2.98036940	-4.94375922
H	2.97131189	2.35325497	-4.81685656
H	1.63590433	1.23753551	-5.12874099
C	-1.43759535	1.76119747	-4.93271847
H	-2.33762917	2.22829758	-5.34812776
H	-0.58527872	2.10411809	-5.52187754
H	-1.53448983	0.67881897	-5.05379375
C	-2.61579868	1.70096761	-2.72990537

H	-2.73671176	0.61335186	-2.76186606
H	-2.63585175	2.02268210	-1.68497340
H	-3.47511815	2.15036255	-3.23958880
C	-1.21353503	3.68822303	-3.33345782
H	-0.37409844	4.07975412	-3.91332686
H	-2.13114088	4.13516902	-3.73245490
H	-1.11436961	4.01738987	-2.29486040
H	3.90644261	0.84771926	0.93695087
C	2.35240720	-1.58130730	1.10910515
C	1.42270708	-2.65338008	1.37676706
C	3.16107278	-1.64592860	-0.01165195
C	0.52567847	-2.68700440	2.48167661
C	1.36017433	-3.73264165	0.44301247
C	3.10614611	-2.72949570	-0.91127139
H	3.86707849	-0.85033030	-0.21853352
C	-0.34791349	-3.73453331	2.65470281
H	0.53377518	-1.87898474	3.19894468
C	0.44322441	-4.79857387	0.64903563
C	2.21169336	-3.74435294	-0.69430333
H	3.76167627	-2.74148306	-1.77585087
C	-0.39142931	-4.80753711	1.73738444
H	0.41757871	-5.60598161	-0.07799626
H	2.14162616	-4.57878955	-1.38719653
H	-1.02311934	-3.72931363	3.50541436
H	-1.09067276	-5.62426093	1.88858411

TS$_{5',6'\text{-}t\mathbf{Bu}}$

G_{solv} = -2940.417379

Ni	-1.03251036	-1.68721864	-0.24196624
C	-0.10035287	2.23049732	-1.56542361
C	-0.11207221	0.87257175	-1.48147705
C	-2.35475653	0.48953344	1.51937155
C	-0.59648587	0.20441885	-0.25668676
C	-1.43712879	1.09210397	0.53997938
C	-1.37559172	2.44458441	0.40390616
S	0.24147979	-2.07657093	-2.03989359
S	-2.48926954	-1.26738801	1.34333195
H	0.27185215	2.77488033	-2.42385052
H	-1.93534946	3.11893567	1.04324301
C	0.82038360	4.86046942	0.25999418
C	-0.39670746	4.46464817	-0.58689676
H	-0.23927968	4.76752581	-1.62379716
H	-1.30101020	4.95482574	-0.21889595
N	-0.62858579	3.01737287	-0.57692007

C	0.61765785	4.74546117	1.74020484
N	0.63742111	3.55154915	2.44241622
C	0.35780308	5.76653072	2.61697901
C	0.39539102	3.85734314	3.70672287
N	0.22023020	5.18283686	3.85144084
H	0.26575471	6.83144499	2.46764787
H	0.34051641	3.15573791	4.52613385
H	1.68529305	4.27013449	-0.06066528
H	1.04373820	5.90654899	0.02918217
H	0.02868094	5.66214891	4.72162946
C	1.40977065	0.25801559	1.45483924
H	0.40448786	-0.01715766	0.45041207
O	0.74273316	0.93476240	2.36842820
H	0.74681250	1.94926516	2.23052092
C	2.37302941	1.06714199	0.62414001
H	2.45970357	0.69467047	-0.39488981
H	2.03149732	2.10154933	0.56961845
C	-1.28955371	-3.47691739	-0.01196864
O	-1.43005917	-4.59464258	0.14718174
O	-2.98995171	1.11009581	2.36130375
P	0.16660414	-0.21549503	-2.89485602
C	1.78207904	0.10426152	-3.81279136
C	-1.38712173	-0.05549013	-3.95811864
C	2.94124498	-0.50765109	-3.01028382
H	2.88727671	-1.59784975	-2.97066793
H	3.87389915	-0.22916248	-3.51301457
H	2.98877464	-0.12482652	-1.98973918
C	2.04133096	1.61185896	-3.96933772
H	2.27618873	2.07809844	-3.00842241
H	2.91750760	1.73267517	-4.61548237
H	1.21122467	2.14766585	-4.43601161
C	1.74588580	-0.57110131	-5.19316529
H	1.05334476	-0.08070027	-5.88017558
H	2.74970252	-0.49477036	-5.62496195
H	1.49321276	-1.63399406	-5.12773312
C	-1.52288473	-1.24541346	-4.92024055
H	-2.48609654	-1.15126322	-5.43357418
H	-0.74390616	-1.26864528	-5.68289381
H	-1.52059345	-2.19934023	-4.38520124
C	-2.59980162	-0.06049772	-3.00958373
H	-2.64548689	-0.96694879	-2.39712467
H	-2.61468864	0.81037543	-2.34901855
H	-3.50429622	-0.02921239	-3.62634018
C	-1.37503786	1.26741065	-4.73841094

H	-0.58926315	1.29884917	-5.49639981
H	-2.33745756	1.36318057	-5.25300495
H	-1.26827746	2.13618099	-4.08129536
H	3.36237215	1.04485579	1.09287188
C	1.68257878	-1.18252574	1.72984480
C	1.03932830	-1.95426492	2.76912825
C	2.51904050	-1.82575499	0.83322020
C	0.19825635	-1.41829748	3.78706888
C	1.25985039	-3.36773429	2.78387928
C	2.74275473	-3.21489519	0.87492937
H	3.00246922	-1.26347584	0.04424866
C	-0.37800002	-2.22600677	4.73891118
H	0.00072463	-0.35829810	3.81274727
C	0.63658854	-4.17707068	3.77262689
C	2.10735119	-3.97562097	1.81962289
H	3.40096615	-3.67126716	0.14263961
C	-0.16783701	-3.62264095	4.73516469
H	0.81969480	-5.24819746	3.75124276
H	2.24845847	-5.05262268	1.85415311
H	-1.01280140	-1.78065904	5.49953063
H	-0.63697801	-4.24711291	5.48945832

6*t*Bu'

G_{solv} = -2940.46375

Ni	-1.97541592	-1.52272896	-0.12045799
C	0.59109999	1.15677229	-2.15100342
C	0.07723164	-0.01068821	-1.61295190
C	-3.02664547	1.34814474	-0.00232194
C	-1.12100832	0.00932198	-0.86924649
C	-1.71875722	1.26734443	-0.71617958
C	-1.17670863	2.40778756	-1.26609240
S	-0.32041836	-2.87722608	-0.73076331
S	-3.67708745	-0.22934612	0.42661417
H	1.48172897	1.18909965	-2.76525784
H	-1.65260103	3.37818930	-1.18870429
C	1.34434457	4.40678183	-1.60280071
C	0.52112395	3.56941073	-2.58545040
H	1.14267843	3.25363560	-3.42307597
H	-0.32668309	4.13638278	-2.97289455
N	-0.03254983	2.33904992	-1.97146431
C	0.55084969	5.04425434	-0.50428818
N	0.21931010	4.39316844	0.67049939
C	-0.00386864	6.29897575	-0.49830062
C	-0.51415397	5.24567293	1.36408794

N	-0.67356092	6.40546572	0.69415067
H	0.02438466	7.10185244	-1.21926181
H	-0.93858169	5.06601320	2.34108437
H	2.15014898	3.79109404	-1.19379236
H	1.81387387	5.19208086	-2.20261239
H	-1.18686579	7.21381202	1.02072634
C	1.62278637	1.23945006	1.76457908
H	1.00952657	0.82861144	0.94562756
O	0.87496683	2.24973579	2.43150456
H	0.66940379	2.94233624	1.76737599
C	2.87898783	1.83446783	1.13848622
H	3.46775499	1.07825776	0.60998069
H	2.58517676	2.59952946	0.41594280
C	-2.83687280	-2.94331310	0.66253197
O	-3.36807613	-3.81744502	1.15382717
O	-3.59715836	2.39731610	0.23394965
P	0.73949246	-1.66040998	-2.00164667
C	2.56706583	-1.80097788	-1.60806080
C	0.24911006	-2.02555348	-3.78238897
C	2.71315223	-1.78886908	-0.07908760
H	2.33129123	-2.70150988	0.38362041
H	3.77927808	-1.70403827	0.15641979
H	2.20113648	-0.93515063	0.36594261
C	3.36432480	-0.61608128	-2.17794568
H	3.15395619	0.30859078	-1.63393590
H	4.42671552	-0.83924523	-2.03282559
H	3.20468900	-0.45243965	-3.24521036
C	3.10892533	-3.12481596	-2.16701470
H	3.16895598	-3.11777040	-3.25786568
H	4.12308506	-3.25815270	-1.77539242
H	2.51489588	-3.98678429	-1.84687724
C	0.26279891	-3.54342475	-4.02647116
H	-0.05467410	-3.71360387	-5.06076701
H	1.25495886	-3.98229223	-3.90738531
H	-0.43590625	-4.06828442	-3.36995652
C	-1.18437324	-1.50128446	-3.98146824
H	-1.88443724	-1.91143947	-3.24629807
H	-1.23527082	-0.40951411	-3.94395670
H	-1.51982547	-1.81911863	-4.97417594
C	1.19256895	-1.33141146	-4.77580887
H	2.20298172	-1.74530863	-4.73950136
H	0.79801332	-1.50279530	-5.78325378
H	1.24505815	-0.24904444	-4.62416550
H	3.51096533	2.31426607	1.89261653

C	1.88012105	0.10527624	2.74550212
C	0.78337577	-0.69424090	3.21636665
C	3.15394394	-0.20321082	3.16574990
C	-0.56956759	-0.44503265	2.84698222
C	1.04653950	-1.79068621	4.09156579
C	3.41232957	-1.28725648	4.03955794
H	3.99845586	0.38024919	2.81584299
C	-1.59048219	-1.23181737	3.32637971
H	-0.80101178	0.39108075	2.19564045
C	-0.03005260	-2.59419105	4.55801330
C	2.38248074	-2.06931824	4.49014157
H	4.43450327	-1.49440989	4.34253215
C	-1.32285123	-2.32197255	4.18708475
H	0.19259678	-3.42699872	5.22038863
H	2.56795328	-2.90823718	5.15589819
H	-2.61503724	-1.01297675	3.04220550
H	-2.14108753	-2.93598329	4.55179558

(R)-1-phenyl-ethanol

G_{solv} = -385.876538

C	-1.25429963	0.31389046	-1.77886407
C	-0.15973756	0.12535646	-2.62419270
C	1.08205577	-0.20477197	-2.08064853
C	1.22534739	-0.34632522	-0.70023368
C	0.13482401	-0.15452111	0.15308890
C	-1.10675112	0.17735594	-0.39882064
H	-2.22491077	0.56921330	-2.19485515
H	-0.27513381	0.23130696	-3.69900500
H	1.93842534	-0.35832891	-2.73120592
H	2.19396047	-0.61013387	-0.28120419
H	-1.96105559	0.32407908	0.25626637
C	0.32030140	-0.25792941	1.65806281
H	1.19363339	-0.89589917	1.85251118
O	-0.82342685	-0.81012332	2.30534172
H	-0.98029335	-1.69253851	1.94966212
C	0.56316213	1.10816214	2.28537180
H	1.45133259	1.57344999	1.84773177
H	-0.29563343	1.76542610	2.11069186
H	0.71767568	1.00710775	3.36408983

Acetophenone

G_{solv} = -384.692272

C	-1.81299123	-1.27769957	0.00182901
C	-0.42212736	-1.18925090	0.00233712

C	0.20560608	0.06299824	0.00111802
C	-0.58009194	1.22333554	-0.00151545
C	-1.96810008	1.13445023	-0.00202916
C	-2.58682284	-0.11765320	-0.00054784
H	-2.29144713	-2.25233078	0.00252908
H	0.16597933	-2.10123528	0.00321687
H	-0.09048104	2.19202299	-0.00266722
H	-2.56915397	2.03880134	-0.00384374
H	-3.67063721	-0.18794358	-0.00189622
C	1.69889195	0.19943832	0.00070335
O	2.21729767	1.30860748	0.00367497
C	2.54355078	-1.04750969	-0.00401763
H	2.32968506	-1.65789013	0.87979320
H	2.32158323	-1.65824632	-0.88535429
H	3.59859816	-0.77069192	-0.00844196

1-Acetonaphthone

G_{solv} = -538.242043

C	0.06423052	-1.58142521	-1.30717445
C	0.04218536	-0.23053273	-1.01958716
C	0.09690320	-2.55556232	-0.28522268
C	0.00748994	0.20512267	0.35163578
C	0.02180158	-0.78905436	1.37687195
C	0.07988044	-2.16594261	1.02886762
C	-0.03137014	-0.39497201	2.74216888
H	-0.01470882	-1.16783379	3.50610710
C	-0.11179946	0.93005259	3.08912079
C	-0.14810260	1.91793658	2.07701143
C	-0.08915259	1.56966040	0.74842125
H	0.13625059	-3.60751955	-0.54951975
H	0.10249722	-2.90476087	1.82567136
H	-0.15482690	1.22279323	4.13386941
H	-0.22576515	2.96558829	2.35283866
H	-0.11299457	2.34274059	-0.00849894
H	0.08165641	-1.91582234	-2.33934522
C	0.09883735	0.73543313	-2.16604083
C	-0.54625378	0.33586260	-3.47060166
H	0.08541195	-0.39408786	-3.98951434
H	-1.52477826	-0.12500549	-3.31234862
H	-0.64220923	1.21869056	-4.10496955
O	0.67019599	1.81321811	-2.06338945

(R)-(+)-1-(2-Naphthyl)ethanol

G_{solv} = -539.426163

C	-0.12292830	-2.32171815	-0.09460630
H	0.64498321	-3.08020958	-0.29528379
O	-1.08552185	-2.36047626	-1.15163845
H	-1.50476325	-3.22867622	-1.13628200
C	-0.75368998	-2.64965174	1.25986059
H	-1.22023255	-3.64073414	1.22463088
H	0.01854878	-2.66956465	2.03550949
H	-1.51374927	-1.91743466	1.54586865
C	0.57687940	-0.97401977	-0.10678036
C	-0.12712240	0.27753321	-0.05405330
C	1.95467881	-0.96659512	-0.10660311
C	-1.54945134	0.37824521	-0.06677667
C	0.62678001	1.48908034	0.01462572
C	2.69824796	0.23583182	-0.04078344
H	2.49076040	-1.91132026	-0.15161018
C	-2.17728672	1.59891834	-0.00124271
H	-2.14133342	-0.52454374	-0.15053585
C	-0.05319836	2.73726153	0.07864726
C	2.04796599	1.44015809	0.02066242
H	3.78340763	0.19420361	-0.04010578
C	-1.42428528	2.79515964	0.07454303
H	0.53828426	3.64785256	0.13129324
H	2.60440311	2.37239214	0.07359642
H	-3.26236949	1.64739143	-0.01367520
H	-1.93330339	3.75323323	0.12474290

(S)-(-)-1-(2-Naphthyl)ethanol

G_{solv} = -539.426163

C	0.22007431	2.07771126	-0.75452718
H	1.04795394	1.82380996	-1.43224504
O	-1.00370691	2.08542403	-1.50291167
H	-0.91360098	2.73452248	-2.21078164
C	0.50216029	3.46054692	-0.18303806
H	1.43245266	3.46833157	0.39347674
H	0.61457259	4.17232502	-1.00774500
H	-0.31641745	3.80775579	0.45507727
C	0.09936667	0.95884821	0.26670738
C	0.08450374	-0.40700572	-0.18105733
C	0.00220973	1.21919438	1.61460929
C	0.18883651	-0.77111823	-1.55449354
C	-0.03303675	-1.45359349	0.78160052
C	-0.11528464	0.17801043	2.56823861
H	0.01772239	2.24235759	1.97450694
C	0.18173494	-2.08950647	-1.94316145

H	0.26359276	0.00293890	-2.30980191
C	-0.04179780	-2.80836786	0.34853323
C	-0.13405680	-1.13020606	2.16275572
H	-0.18994920	0.42849053	3.62231618
C	0.06341917	-3.12327777	-0.98341024
H	-0.13273166	-3.59192457	1.09662686
H	-0.22294326	-1.93682812	2.88588848
H	0.26392463	-2.34176559	-2.99646424
H	0.05630254	-4.16081936	-1.30410298

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