Supporting Information

Bio-inspired computational design of iron catalysts for hydrogenation of carbon dioxide

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1. Computational details

All DFT calculations were performed using the Gaussian 09 suite of *ab initio* programs for a hybride meta-GGA density functional M06 in conjunction with all-electron 6-31++G(d,p) basis set for all atoms. All structures studied in this paper were fully optimized in solvent using the integral equation formalism polarizable continuum model (IEFPCM)[1] with radii and cavity-dispersion-solvent-structure terms in Truhlar and co-workers' SMD solvation model[2] for the solvent effect correction of THF (ε = 7.4257). An ultrafine integration grid (99,590) was used for numerical integrations. The ground states of intermediates and transition states were confirmed as singlets through comparison with the optimized high-spin analogs. Thermal corrections were calculated within the harmonic potential approximation on optimized structures under T = 298.15 K and 1 atm pressure. Unless otherwise noted, the energies reported in the text are solvent corrected free energies. Calculating the harmonic vibrational frequencies for optimized structures and noting the number of imaginary frequencies (IFs) confirmed the nature of all intermediates (no IF) and transition state structures (only one IF). The latter were also confirmed to connect reactants and products by intrinsic reaction coordinate (IRC) calculations. The 3D molecular structure figures displayed in this paper were drawn by using the *JIMP2* molecular visualizing and manipulating program.[3]

2. Evaluation of density functionals

In order to evaluate the dependency of our iron complexes to density functionals, we also calculated the total free energy barriers of the hydrogenation of CO_2 catalyzed by **1** (R1 = R2 = H) using other nine widely-used and/or recently developed density functionals, including ωB97X-D,[4] B3LYP,[5] B3PW91,[6] HSE06,[7] PBEh1PBE,[8] TPSSh,[9] M06L,[10] and TPSS.[9] All structures are optimized using these functionals, respectively, with the same basis set. The total free energy barriers of the catalytic reaction are the relative energies between $\mathbf{TS_{3,4}}$ and **4′**. As shown in Table S1, the ωB97X-D functional has the highest relative energy of 29.98 kcal/mol, while the TPSS functional has the lowest relative energy of 20.28 kcal/mol. Pure functionals without Hartree-Fock exchange (M06L and TPSS) have obviously lower relative energies. The difference between them is less than 10 kcal/mol, which indicates that the CO_2 hydrogenation reaction catalyzed by the newly designed iron complexes has a moderate dependence of density functionals. The M06 result of 25.24 kcal/mol is in the middle of them, and very close to the results of B3LYP, B3PW91, HSE06, PBEh1PBE and TPSSh functionals. Therefore, we believe the M06 functional is suitable for the study of this iron based catalytic system.

Table S1. Relative free energies and total free energy barriers of different density functionals.

Density functionals	Abosute free energies (Hartree)		Total barriers (kcal/mol)
	4′	$\mathbf{TS_{3,4}}$	(**4′** → $\mathbf{TS_{3,4}}$)
M06	−3296.369764	−3296.329534	25.24
ωB97X-D	−3296.974456	−3297.022235	29.98
B3LYP	−3297.382722	−3297.426175	27.27
B3PW91	−3296.742351	−3296.783331	25.71
HSE06	−3295.431011	−3295.471911	25.66
PBEh1PBE	−3295.464790	−3295.507000	26.49
TPSSh	−3297.495848	−3297.533201	23.44
M06L	−3297.168078	−3297.201476	20.96
TPSS	−3297.697377	−3297.729701	20.28

3. Absolute free energies (Hartree) and Cartesian coordinates (Ångström) of all structures optimized in the THF solvent

H_2

G_{solv} = -1.170583

H	0.00000000	0.00000000	0.37162100
H	0.00000000	0.00000000	-0.37162100

CO_2

G_{solv} = -188.516479

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16459200
O	0.00000000	0.00000000	-1.16459200

HCOOH

G_{solv} = -189.676889

H	-0.09934300	1.50291700	0.00002400
C	-0.12770000	0.40223100	0.00001000
O	1.11011900	-0.09199700	-0.00001000
O	-1.13355300	-0.26430900	0.00000300
H	1.05301200	-1.06585000	-0.00002700

1

G_{solv} = -3106.671339

Fe	-0.00001400	-0.38311000	-0.08062400
P	-2.28136100	-0.64348800	-0.03661700
P	2.28131900	-0.64371200	-0.03665400
N	-0.00006600	-2.43477300	-0.52703700
C	-2.44670100	-2.41261600	-0.57746600
H	-3.36068800	-2.88032900	-0.18860600
H	-2.52021200	-2.41152700	-1.67513800
C	-1.21172000	-3.18168800	-0.15124000
H	-1.18584100	-3.32292100	0.93834000
H	-1.19889900	-4.18490500	-0.60799600
C	1.21138300	-3.18176000	-0.15073600
H	1.19848800	-4.18514600	-0.60712300
H	1.18528000	-3.32257100	0.93889800
C	2.44656200	-2.41302400	-0.57697700
H	2.52035700	-2.41236100	-1.67462900
H	3.36041400	-2.88069100	-0.18774800
C	3.23819300	-0.61160400	1.57007600
H	4.25997800	-0.93965700	1.31880800
C	3.28121700	0.78363300	2.18263900
H	3.86877100	0.76072800	3.11098500
H	2.26610600	1.12045100	2.43479700
H	3.74072600	1.52837100	1.52406000
C	2.64481600	-1.59640000	2.57296400
H	3.17038300	-1.50599500	3.53342100
H	2.73679900	-2.64072600	2.25241900
H	1.58320800	-1.38018300	2.76237200
C	3.36919300	0.21615600	-1.29041600
H	2.82898300	-0.00580000	-2.22592600
C	3.43698300	1.73404200	-1.12841500
H	3.72757500	2.19756900	-2.08096900
H	4.19865200	2.01840200	-0.39191600
H	2.48747400	2.18312200	-0.81238600
C	4.77431300	-0.36433500	-1.39878700
H	5.31198300	0.11790100	-2.22694500
H	4.77926100	-1.44417000	-1.58961400
H	5.35567100	-0.17548700	-0.48608200
C	-3.36930700	0.21680000	-1.29003100
H	-2.82917000	-0.00488700	-2.22564900
C	-4.77446000	-0.36364600	-1.39840800
H	-5.31226000	0.11894700	-2.22627400
H	-5.35565000	-0.17515800	-0.48552200
H	-4.77948000	-1.44339800	-1.58968100
C	-3.43708900	1.73464200	-1.12761900
H	-3.72779500	2.19838600	-2.08003400
H	-2.48754500	2.18366400	-0.81158900
H	-4.19870100	2.01880200	-0.39098300
C	-3.23806200	-0.61174700	1.57020100
H	-4.26007600	-0.93899700	1.31884400
C	-2.64526200	-1.59755200	2.57247300
H	-3.17052600	-1.50720800	3.53310200
H	-1.58343400	-1.38228600	2.76170500
H	-2.73815400	-2.64164000	2.25144000
C	-3.28022300	0.78315300	2.18362800
H	-3.86791600	0.76002400	3.11187700
H	-3.73912600	1.52865700	1.52548700
H	-2.26491800	1.11910800	2.43614500
H	0.00012300	-2.32833100	-1.55108300
C	-0.00025400	3.68526300	-0.92314600
C	0.00003600	4.28721000	0.34639000
C	0.00036900	3.51694200	1.49276100
C	0.00036200	2.08815800	1.40612800
C	-0.00021700	2.29912700	-0.97256100
H	-0.00047200	4.27136100	-1.83951000
H	0.00004500	5.37415400	0.42803500
H	0.00066400	3.96879000	2.48302500
C	-0.00037600	1.48148800	-2.22681500
H	-0.87758800	1.70625200	-2.85483800
H	0.87666000	1.70633400	-2.85506100
C	-0.00020000	-0.02414600	-1.90408700
O	-0.00019900	-0.81203100	-2.86458000
N	0.00003100	1.54741600	0.14130200
O	0.00079400	1.30017000	2.39128800

1′

G_{solv} = -3106.667586

Fe	-0.00207600	-0.42031600	-0.08237900
P	2.27333200	-0.69341700	0.08360400
P	-2.27578000	-0.67429300	0.12889400
N	-0.00401200	-2.51627500	-0.07044500
C	2.45819900	-2.53449800	-0.13533700
H	3.31499900	-2.77639000	-0.77581600
H	2.66274100	-2.98289600	0.84674500
C	1.18626900	-3.09809900	-0.73029400

H	1.10181100	-2.83415700	-1.79113000
H	1.16463400	-4.19681500	-0.64735600
C	-1.23119700	-3.10165800	-0.65418100
H	-1.20874400	-4.19924700	-0.55815000
H	-1.20823700	-2.85230900	-1.72193700
C	-2.46119500	-2.52282600	0.00867700
H	-2.57908000	-2.92479700	1.02472600
H	-3.36376700	-2.80326800	-0.54766000
C	-3.48865600	-0.06542300	-1.15566500
C	-3.43301700	1.44567900	-1.37908200
H	-3.85138400	1.69463300	-2.36354500
H	-2.41785000	1.85437500	-1.33252900
H	-4.03033800	1.98086300	-0.63109300
C	-3.05970300	-0.35875700	1.79520300
C	-3.40484300	1.10763700	2.02405100
H	-3.74096600	1.25169900	3.06036600
H	-4.20793100	1.46107400	1.36844600
H	-2.52242000	1.74568900	1.87696900
C	3.04478200	-0.47853200	1.77331700
C	3.41669800	0.96408600	2.09231900
H	3.74288800	1.03772100	3.13933000
H	2.54980700	1.62813700	1.97390700
H	4.23674900	1.33682200	1.46926900
C	3.49878600	-0.01815100	-1.15459200
C	3.44294600	1.50066500	-1.30585800
H	3.95290600	1.80081800	-2.23132200
H	3.95521700	2.00616800	-0.47834200
H	2.42201100	1.89544400	-1.34299800
H	0.02626600	-2.79836400	0.91524200
C	0.01202300	3.52005200	-1.43488500
C	0.03341300	4.28030200	-0.25367000
C	0.04695300	3.66103300	0.98007100
C	0.03665300	2.23240100	1.07538000
C	0.00397200	2.13883000	-1.30614100
H	0.00438800	3.98342700	-2.41915200
H	0.04072700	5.36889500	-0.31092400
H	0.06504300	4.23244300	1.90639100
C	-0.00848600	1.17127200	-2.44459200
H	-0.87828500	1.32862600	-3.10238700
H	0.87697000	1.29857000	-3.08843300
C	-0.03145000	-0.29118300	-1.94557200
O	-0.06883600	-1.15985700	-2.82607600
N	0.01205800	1.53079300	-0.10822500
O	0.05096700	1.58092600	2.15411100
C	-2.11076700	-0.84207000	2.88871000
H	-2.59625700	-0.76050200	3.87089000
H	-1.80394700	-1.89004300	2.76722000
H	-1.21241900	-0.20847000	2.89945900
C	2.07227100	-1.00809200	2.82416200
H	1.17823300	-0.36857200	2.85351700
H	1.76142500	-2.04631500	2.64384100
H	2.53938800	-0.98001900	3.81818600
C	4.93609300	-0.47048100	-0.92232900
H	5.56788300	-0.15067700	-1.76240000
H	5.35323600	-0.01671400	-0.01353800
H	5.04007300	-1.55842600	-0.83307500
C	-4.92885200	-0.50831900	-0.92475900
H	-5.35352600	-0.03046600	-0.03186600
H	-5.55135800	-0.20823100	-1.77908700
H	-5.03668800	-1.59343300	-0.81045700
H	-3.10702600	-0.56249700	-2.06477200
H	3.13179500	-0.47097200	-2.09287500
H	-3.98317200	-0.96165000	1.81588800
H	3.95615800	-1.09968900	1.77166500

$\mathbf{1}_{Cl}$

G_{solv} = -3567.490618

Fe	-0.00006400	-0.34878200	-0.10455800
P	-2.30680600	-0.57540000	-0.23599600
P	2.30646000	-0.57625300	-0.23577400
N	-0.00039900	-2.31071000	-0.80261000
C	-2.41738800	-2.26946500	-0.98412700
H	-3.36701100	-2.77110000	-0.76312000
H	-2.36398000	-2.13879400	-2.07513500
C	-1.22285500	-3.08084000	-0.52156700
H	-1.25977400	-3.27764300	0.55806400
H	-1.18559700	-4.05294100	-1.04003000
C	1.22172200	-3.08132400	-0.52140600
H	1.18416400	-4.05340300	-1.03988600
H	1.25842900	-3.27813200	0.55823000
C	2.41662900	-2.27039300	-0.98378000
H	2.36346700	-2.13972700	-2.07480400
H	3.36601900	-2.77237900	-0.76261100
C	3.49733500	-0.61426700	1.21995400
H	4.49085700	-0.45838600	0.77007200
C	3.21869000	0.52650400	2.19400400
H	4.03119600	0.59477700	2.93074000
H	2.28691300	0.34323200	2.74186800
H	3.13381100	1.50479500	1.70522500
C	3.53076300	-1.94070500	1.97152400
H	4.27293700	-1.87912000	2.78005200
H	3.81862100	-2.78657100	1.33616800
H	2.55760900	-2.16144500	2.42633500
C	3.26130300	0.44296000	-1.48620400
H	2.57900500	0.47036600	-2.35003500
C	3.49637300	1.87244700	-1.00562300
H	3.84024400	2.49807800	-1.84075600
H	4.27790900	1.90676900	-0.23452500
H	2.59492400	2.34147800	-0.58934200
C	4.57409100	-0.17780800	-1.95084000
H	5.03807700	0.46824800	-2.70923500
H	4.44105700	-1.16601900	-2.40545100
H	5.29760500	-0.27627800	-1.13035700
C	-3.26147000	0.44404500	-1.48638800
H	-2.57944400	0.47101200	-2.35042700
C	-4.57463600	-0.17629900	-1.95046000
H	-5.03871900	0.46984300	-2.70872400
H	-5.29782200	-0.27446400	-1.12964500
H	-4.44210900	-1.16459900	-2.40502500
C	-3.49598900	1.87369000	-1.00598400
H	-3.83994600	2.49927800	-1.84111700
H	-2.59430200	2.34255400	-0.59007800
H	-4.27729300	1.90834000	-0.23466100
C	-3.49786300	-0.61374200	1.21954200

H	-4.49136700	-0.45797600	0.76954700
C	-3.53095100	-1.94040100	1.97074500
H	-4.27344000	-1.87936600	2.77902400
H	-2.55783500	-2.16074700	2.42585600
H	-3.81814100	-2.78625100	1.33506400
C	-3.21952300	0.52675700	2.19400200
H	-4.03197900	0.59441300	2.93085300
H	-3.13508000	1.50528600	1.70563300
H	-2.28763800	0.34364700	2.74173600
H	-0.00029200	-2.09657900	-1.81004900
C	0.00142600	3.84209300	-0.76448200
C	0.00124000	4.47762800	0.47643600
C	0.00067300	3.70536000	1.62102200
C	0.00028200	2.30890200	1.49648200
C	0.00101500	2.45687700	-0.81070500
H	0.00187400	4.40540800	-1.69475600
H	0.00157100	5.56315400	0.54541000
H	0.00053500	4.13601200	2.61822400
C	0.00117100	1.72127800	-2.10563800
H	-0.87448200	2.00417000	-2.71222200
H	0.87772700	2.00312500	-2.71141100
C	0.00032100	0.20948600	-1.89862800
O	0.00025000	-0.48455500	-2.93410900
N	0.00045600	1.67914200	0.30584500
O	-0.00022100	1.60891300	2.62139000
H	-0.00057100	0.63086300	2.44554800
Cl	-0.00033200	-1.33296400	2.20862700

$TS_{1,2}$

G_{solv} = -3107.829062

Fe	-0.00006100	-0.40262500	0.00442600
P	-2.26905800	-0.63657000	-0.03248000
P	2.26888900	-0.63704200	-0.03272000
N	-0.00032500	-2.43739800	-0.44332500
C	-2.43080800	-2.41471900	-0.54243300
H	-3.36406300	-2.87048400	-0.18797200
H	-2.45242700	-2.43303700	-1.64224200
C	-1.21365000	-3.17271000	-0.05442100
H	-1.20962700	-3.26536300	1.04067200
H	-1.19203600	-4.19315000	-0.47187500
C	1.21301300	-3.17304900	-0.05508700
H	1.19109300	-4.19331100	-0.47295700
H	1.20926100	-3.26618500	1.03996000
C	2.43023000	-2.41512700	-0.54305900
H	2.45182800	-2.43323700	-1.64286900
H	3.36341500	-2.87112300	-0.18870400
C	3.35718400	-0.53121300	1.49165500
H	4.38556700	-0.68336500	1.12523900
C	3.26305400	0.82961900	2.17530300
H	3.99397800	0.88447400	2.99397700
H	2.26537900	0.97960000	2.60702500
H	3.46162600	1.67023700	1.50132100
C	3.04076900	-1.62936500	2.50010000
H	3.68757300	-1.51776500	3.38118200
H	3.20556400	-2.63763900	2.10182500
H	2.00055000	-1.56123800	2.84780200
C	3.29025300	0.19971000	-1.36366400
H	2.65984300	0.04168900	-2.25388600
C	3.45816300	1.70270900	-1.15360000
H	3.76143000	2.18017500	-2.09556000
H	4.25026000	1.91077700	-0.42233000
H	2.54370800	2.20063500	-0.80621800
C	4.64941500	-0.43918900	-1.62642000
H	5.13696100	0.06521200	-2.47249700
H	4.58296400	-1.50397600	-1.87757800
H	5.32113900	-0.33440900	-0.76362500
C	-3.29063800	0.20008000	-1.36333700
H	-2.66027600	0.04239000	-2.25365400
C	-4.64963700	-0.43917300	-1.62611200
H	-5.13745300	0.06534600	-2.47196200
H	-5.32130200	-0.33493100	-0.76320500
H	-4.58285800	-1.50384700	-1.87764500
C	-3.45896800	1.70296700	-1.15297200
H	-3.76338100	2.18037400	-2.09459200
H	-2.54435100	2.20121900	-0.80647800
H	-4.25041100	1.91066000	-0.42087900
C	-3.35700200	-0.52991200	1.49209200
H	-4.38562600	-0.68073600	1.12580200
C	-3.04173900	-1.62860500	2.50030600
H	-3.68830000	-1.51642500	3.38149600
H	-2.00140300	-1.56171100	2.84789600
H	-3.20772500	-2.63662200	2.10188700
C	-3.26109500	0.83068500	2.17597300
H	-3.99280300	0.88683200	2.99385500
H	-3.45731200	1.67176700	1.50187600
H	-2.26358600	0.97875000	2.60873200
H	-0.00056400	-2.35051000	-1.47060600
C	0.00021500	3.67009900	-0.96331000
C	0.00074600	4.31806400	0.27677100
C	0.00101500	3.58048200	1.44780600
C	0.00075000	2.17154100	1.37405800
C	-0.00005600	2.28278100	-0.97989000
H	0.00002400	4.22531200	-1.89853500
H	0.00096700	5.40585500	0.32299200
H	0.00145300	4.05280400	2.42681400
H	-0.00006800	-0.72486700	1.66843100
C	-0.00056000	1.44938800	-2.22115900
H	-0.87797800	1.67316600	-2.85002100
H	0.87602600	1.67353500	-2.85103500
C	-0.00026400	-0.04852100	-1.86698400
O	-0.00040900	-0.84411400	-2.82660200
N	0.00018200	1.55842500	0.15982500
O	0.00106500	1.41299900	2.42462800
H	0.00048200	0.24804600	1.97165700

2

G_{solv} = -3107.843909

Fe	-0.00010100	-0.41946700	0.01517000
P	-2.27530900	-0.64602400	-0.03892100
P	2.27490300	-0.64720300	-0.03899000
N	-0.00064600	-2.44012700	-0.47631000
C	-2.43522300	-2.41550800	-0.57790800
H	-3.36672300	-2.87711300	-0.22663300
H	-2.46244700	-2.41674500	-1.67759500

C	-1.21663700	-3.18369200	-0.10630600
H	-1.21470400	-3.30629700	0.98607600
H	-1.19316000	-4.19268400	-0.54915800
C	1.21492800	-3.18432500	-0.10620300
H	1.19093000	-4.19334100	-0.54897500
H	1.21289700	-3.30683400	0.98619100
C	2.43392800	-2.41681900	-0.57783200
H	2.46114800	-2.41815900	-1.67751800
H	3.36518700	-2.87888000	-0.22651900
C	3.32319100	-0.56239900	1.51097900
H	4.36286400	-0.69668300	1.17041600
C	3.18484800	0.78436500	2.21379500
H	3.85223100	0.81709800	3.08632900
H	2.15565700	0.93865300	2.56622000
H	3.44249800	1.63441500	1.57227100
C	2.99084200	-1.68503200	2.48757400
H	3.61947000	-1.58969300	3.38321800
H	3.16847100	-2.68371000	2.07123600
H	1.94518600	-1.62899800	2.82119700
C	3.29975300	0.22096700	-1.34123700
H	2.68294300	0.07810400	-2.24352000
C	3.45681700	1.71980900	-1.09679700
H	3.77260300	2.21668200	-2.02427700
H	4.23626000	1.91555500	-0.34878400
H	2.53415200	2.20531800	-0.75432200
C	4.66398900	-0.41076900	-1.59493000
H	5.16468800	0.11438100	-2.42017100
H	4.60257700	-1.46928600	-1.87249900
H	5.31958700	-0.32553700	-0.71778800
C	-3.29997100	0.22262200	-1.34102700
H	-2.68275800	0.08049900	-2.24315200
C	-4.66383500	-0.40953100	-1.59564400
H	-5.16435700	0.11579400	-2.42088100
H	-5.31988000	-0.32497300	-0.71877100
H	-4.60184800	-1.46789800	-1.87366800
C	-3.45781300	1.72125500	-1.09583700
H	-3.77293600	2.21854300	-2.02332100
H	-2.53567300	2.20692000	-0.75221400
H	-4.23804000	1.91626400	-0.34845600
C	-3.32344300	-0.56099100	1.51116300
H	-4.36326500	-0.69399000	1.17055700
C	-2.99229700	-1.68457000	2.48707200
H	-3.62084600	-1.58911700	3.38275900
H	-1.94659200	-1.62985100	2.82075500
H	-3.17097800	-2.68280100	2.07011100
C	-3.18366700	0.78517500	2.21485000
H	-3.85101100	0.81803600	3.08741000
H	-3.44040900	1.63592900	1.57390900
H	-2.15432000	0.93813500	2.56739200
H	-0.00058700	-2.33297500	-1.50220400
C	0.00137800	3.65733700	-1.04069200
C	0.00163200	4.37100600	0.16713800
C	0.00137900	3.69024300	1.36280800
C	0.00087400	2.25713600	1.40174500
C	0.00084100	2.27310100	-0.97696200
H	0.00155800	4.15697300	-2.00708800
H	0.00204000	5.46086300	0.15934700
H	0.00157300	4.21081700	2.31822500
H	-0.00035200	-1.02303000	1.60170200
C	0.00049500	1.42355200	-2.20713500
H	-0.87618000	1.64001400	-2.83969200
H	0.87732400	1.63936700	-2.83970300
C	-0.00002000	-0.05973500	-1.85317600
O	-0.00029500	-0.86672600	-2.80068200
N	0.00058500	1.58310800	0.18635800
O	0.00061100	1.61219700	2.48371000
H	-0.00010300	-0.20904300	1.72865000

$TS_{2,3}$

G_{solv} = -3107.834688

Fe	-0.00006100	-0.40262500	0.00442600
P	-2.26905800	-0.63657000	-0.03248000
P	2.26888900	-0.63704200	-0.03272000
N	-0.00032500	-2.43739800	-0.44332500
C	-2.43080800	-2.41471900	-0.54243300
H	-3.36406300	-2.87048400	-0.18797200
H	-2.45242700	-2.43303700	-1.64224200
C	-1.21365000	-3.17271000	-0.05442100
H	-1.20962700	-3.26536300	1.04067200
H	-1.19203600	-4.19315000	-0.47187500
C	1.21301300	-3.17304900	-0.05508700
H	1.19109300	-4.19331100	-0.47295700
H	1.20926100	-3.26618500	1.03996000
C	2.43023000	-2.41512700	-0.54305900
H	2.45182800	-2.43323700	-1.64286900
H	3.36341500	-2.87112300	-0.18870400
C	3.35718400	-0.53121300	1.49165500
H	4.38556700	-0.68336500	1.12523900
C	3.26305400	0.82961900	2.17530300
H	3.99397800	0.88447400	2.99397700
H	2.26537900	0.97960000	2.60702500
H	3.46162600	1.67023700	1.50132100
C	3.04076900	-1.62936500	2.50010000
H	3.68757300	-1.51776500	3.38118200
H	3.20556400	-2.63763900	2.10182500
H	2.00055000	-1.56123800	2.84780200
C	3.29025300	0.19971000	-1.36366400
H	2.65984300	0.04168900	-2.25388600
C	3.45816300	1.70270900	-1.15360000
H	3.76143000	2.18017500	-2.09556000
H	4.25026000	1.91077700	-0.42233000
H	2.54370800	2.20063500	-0.80621800
C	4.64941500	-0.43918900	-1.62642000
H	5.13696100	0.06521200	-2.47249700
H	4.58296400	-1.50397600	-1.87757800
H	5.32113900	-0.33440900	-0.76362500
C	-3.29063800	0.20008000	-1.36333700
H	-2.66027600	0.04239000	-2.25365400
C	-4.64963700	-0.43917300	-1.62611200
H	-5.13745300	0.06534600	-2.47196200
H	-5.32130200	-0.33493100	-0.76320500
H	-4.58285800	-1.50384700	-1.87764500
C	-3.45896800	1.70296700	-1.15297200
H	-3.76338100	2.18037400	-2.09459200

H	-2.54435100	2.20121900	-0.80647800
H	-4.25041100	1.91066000	-0.42087900
C	-3.35700200	-0.52991200	1.49209200
H	-4.38562600	-0.68073600	1.12580200
C	-3.04173900	-1.62860500	2.50030600
H	-3.68830000	-1.51642500	3.38149600
H	-2.00140300	-1.56171100	2.84789600
H	-3.20772500	-2.63662200	2.10188700
C	-3.26109500	0.83068500	2.17597300
H	-3.99280300	0.88683200	2.99385500
H	-3.45731200	1.67176700	1.50187600
H	-2.26358600	0.97875000	2.60873200
H	-0.00056400	-2.35051000	-1.47060600
C	0.00021500	3.67009900	-0.96331000
C	0.00074600	4.31806400	0.27677100
C	0.00101500	3.58048200	1.44780600
C	0.00075000	2.17154100	1.37405800
C	-0.00005600	2.28278100	-0.97989000
H	0.00002400	4.22531200	-1.89853500
H	0.00096700	5.40585500	0.32299200
H	0.00145300	4.05280400	2.42681400
H	-0.00006800	-0.72486700	1.66843100
C	-0.00056000	1.44938800	-2.22115900
H	-0.87797800	1.67316600	-2.85002100
H	0.87602600	1.67353500	-2.85103500
C	-0.00026400	-0.04852100	-1.86698400
O	-0.00040900	-0.84411400	-2.82660200
N	0.00018200	1.55842500	0.15982500
O	0.00106500	1.41299900	2.42462800
H	0.00048200	0.24804600	1.97165700

3

G_{solv} = -3107.833536

Fe	-0.00007000	-0.40758600	-0.00607000
P	-2.25888200	-0.64346200	-0.02592000
P	2.25868100	-0.64392100	-0.02643300
N	-0.00032000	-2.42687500	-0.51945500
C	-2.42884300	-2.39709500	-0.61217200
H	-3.36328700	-2.86529100	-0.27742600
H	-2.45036500	-2.36791100	-1.71176500
C	-1.21275100	-3.17610200	-0.15716600
H	-1.20753400	-3.31297100	0.93306400
H	-1.19269500	-4.17868000	-0.61666800
C	1.21196000	-3.17635300	-0.15717600
H	1.19162100	-4.17899200	-0.61653300
H	1.20681800	-3.31305600	0.93307500
C	2.42818600	-2.39769700	-0.61241700
H	2.44961100	-2.36870300	-1.71201700
H	3.36255900	-2.86604600	-0.27768800
C	3.35123700	-0.60878000	1.50017500
H	4.37938700	-0.72816100	1.12136400
C	3.24847100	0.71139300	2.25789900
H	4.01141300	0.74717900	3.04792500
H	2.26889900	0.80584100	2.74232600
H	3.39035100	1.59353700	1.62346400
C	3.05558500	-1.76126000	2.45246100
H	3.70087000	-1.68301000	3.33852900
H	3.23723800	-2.74578500	2.00510100
H	2.01375300	-1.72788400	2.80072800
C	3.29570600	0.24480200	-1.31444300
H	2.67087200	0.12437900	-2.21453500
C	3.46201700	1.73769900	-1.04215900
H	3.78678800	2.25200200	-1.95736100
H	4.23723000	1.91623700	-0.28511800
H	2.53984300	2.22300900	-0.69725400
C	4.65638500	-0.38203600	-1.59718000
H	5.14554800	0.15249500	-2.42376900
H	4.59126700	-1.43724400	-1.88648200
H	5.32649600	-0.30847900	-0.72981400
C	-3.29603700	0.24568000	-1.31354800
H	-2.67151500	0.12512400	-2.21383900
C	-4.65697600	-0.38074800	-1.59594600
H	-5.14626300	0.15405200	-2.42228900
H	-5.32679600	-0.30718100	-0.72835500
H	-4.59221500	-1.43591900	-1.88545800
C	-3.46180100	1.73862500	-1.04119000
H	-3.78656200	2.25305000	-1.95632800
H	-2.53939700	2.22361900	-0.69645100
H	-4.23682100	1.91741400	-0.28401500
C	-3.35112300	-0.60845700	1.50093400
H	-4.37940600	-0.72707000	1.12224400
C	-3.05599500	-1.76161300	2.45256000
H	-3.70108800	-1.68344900	3.33877500
H	-2.01408500	-1.72903700	2.80067100
H	-3.23830700	-2.74579200	2.00470500
C	-3.24751000	0.71124300	2.25937000
H	-4.01038100	0.74704700	3.04946500
H	-3.38889500	1.59383200	1.62545200
H	-2.26786300	0.80483200	2.74380200
H	-0.00031600	-2.30571700	-1.54384600
C	0.00013900	3.69054500	-0.97629500
C	0.00053800	4.36214300	0.24731100
C	0.00083200	3.63593900	1.42672500
C	0.00068600	2.23819600	1.34804600
C	-0.00000200	2.30277100	-0.97880100
H	-0.00006600	4.22942000	-1.92100000
H	0.00066900	5.44974700	0.27781200
H	0.00123100	4.11098100	2.40376000
H	0.00008900	-0.77772800	1.62265500
C	-0.00041300	1.47695700	-2.22162100
H	-0.87845800	1.70953400	-2.84670300
H	0.87706600	1.70967500	-2.84743600
C	-0.00026800	-0.02165500	-1.88015300
O	-0.00034400	-0.80145200	-2.85572900
N	0.00022400	1.58420600	0.17072600
O	0.00119000	1.51154600	2.45354400
H	0.00129300	0.53183500	2.14765700

$TS_{3,4}$

G_{solv} = -3296.329534

Fe	0.00178300	-0.17476800	-0.30578100
P	-2.27762100	-0.35509100	-0.47911200
P	2.28173500	-0.35001800	-0.47485100
N	0.00525700	-1.81144500	-1.58936700

C	-2.41153500	-1.71103200	-1.73850900
H	-3.36260700	-2.25382800	-1.68005600
H	-2.36915400	-1.23054600	-2.72717600
C	-1.21753400	-2.63149700	-1.57951800
H	-1.24992800	-3.18195800	-0.63090200
H	-1.18310100	-3.37271400	-2.39518600
C	1.22837800	-2.63092700	-1.57370300
H	1.19742300	-3.37315900	-2.38859500
H	1.25755900	-3.18013400	-0.62431600
C	2.42263200	-1.71024500	-1.72916700
H	2.38612700	-1.23314300	-2.71974200
H	3.37348400	-2.25255000	-1.66344100
C	3.44761000	-0.86485100	0.90793200
H	4.45375700	-0.61330900	0.53776800
C	3.18349500	-0.07600300	2.18650200
H	3.98461900	-0.26503800	2.91426500
H	2.23867000	-0.38648300	2.64910800
H	3.13185100	1.00768200	2.02641000
C	3.42638200	-2.35737400	1.21174100
H	4.13010500	-2.57483800	2.02693200
H	3.71858200	-2.97663700	0.35594500
H	2.43692400	-2.69096600	1.54734300
C	3.25856000	1.01642300	-1.31081300
H	2.59433400	1.30844400	-2.13916500
C	3.46761200	2.22629400	-0.40444200
H	3.80695300	3.08632700	-0.99817500
H	4.24537700	2.02860800	0.34570900
H	2.55806900	2.53066200	0.12953300
C	4.58976300	0.58040800	-1.91322800
H	5.05583000	1.43149000	-2.42932900
H	4.48339400	-0.22536500	-2.64838000
H	5.30082400	0.24698500	-1.14529700
C	-3.25441700	1.01328200	-1.31222500
H	-2.58503200	1.31507300	-2.13275300
C	-4.57854200	0.57529500	-1.92858900
H	-5.04856900	1.42983200	-2.43530100
H	-5.29139500	0.22483500	-1.16991200
H	-4.46110900	-0.21898400	-2.67444500
C	-3.47607200	2.21548800	-0.39875800
H	-3.81793700	3.07709900	-0.98871700
H	-2.57091500	2.52220100	0.14135300
H	-4.25632300	2.00787400	0.34603000
C	-3.44713400	-0.87894000	0.89728300
H	-4.45285200	-0.63293400	0.52206700
C	-3.41858500	-2.37177900	1.19892500
H	-4.12580200	-2.59460400	2.00963000
H	-2.42903800	-2.69966000	1.53998500
H	-3.70195400	-2.99170500	0.34065100
C	-3.19487500	-0.09142500	2.17917300
H	-4.00140700	-0.28354400	2.90011400
H	-3.14401200	0.99258400	2.02170000
H	-2.25323300	-0.40074600	2.64895900
H	0.00707700	-1.28409600	-2.47497100
C	-0.00921500	3.99422000	0.39965300
C	-0.01405100	4.15628800	1.78545900
C	-0.01384200	3.03706000	2.59865700
C	-0.00883500	1.77529200	1.99363300
C	-0.00378300	2.71093200	-0.12623700
H	-0.00941600	4.84802600	-0.27401000
H	-0.01808200	5.15103800	2.22541000
H	-0.01769700	3.10066700	3.68293400
H	0.00360400	-1.24682900	1.06845600
C	0.00279000	2.43313500	-1.58960800
H	-0.86969700	2.89544100	-2.07966000
H	0.88371000	2.89051600	-2.06931600
C	0.00215300	0.92537400	-1.86365300
O	0.00273800	0.58999700	-3.06391100
N	-0.00329200	1.60518200	0.66073800
O	-0.00996400	0.69758300	2.76494300
H	-0.00671500	-0.10202500	2.17102500
C	0.00147700	-2.64815500	2.15863800
O	0.00636100	-3.57855700	1.42124000
O	-0.00397200	-2.13261400	3.22807900

4

G_{solv} = -3296.348236

Fe	0.00104100	-0.42318400	-0.08858200
P	2.27967600	-0.70045800	0.04937200
P	-2.27481700	-0.68416600	0.14577900
N	0.00659200	-2.53361800	-0.06344900
C	2.47551700	-2.52819400	-0.23168400
H	3.28613500	-2.73640900	-0.93549800
H	2.75074900	-3.00260600	0.71633900
C	1.17568500	-3.10598300	-0.76768400
H	1.04774000	-2.84512100	-1.82030000
H	1.17498000	-4.20093800	-0.67750700
C	-1.23522400	-3.12066800	-0.61254800
H	-1.21989300	-4.21390000	-0.50492900
H	-1.24139000	-2.87756300	-1.67816500
C	-2.45275500	-2.53085400	0.07678300
H	-2.53455800	-2.91132000	1.10083400
H	-3.36345300	-2.83294900	-0.44727100
C	-3.48419200	-0.11076500	-1.15134200
C	-3.41100400	1.39551100	-1.43333800
H	-3.86477500	1.61031700	-2.40751900
H	-2.38840300	1.77283800	-1.44737700
H	-3.96000000	1.97084800	-0.68275800
C	-3.03493600	-0.31246900	1.80522800
C	-3.39113900	1.16581600	1.98636900
H	-3.68320700	1.34723100	3.02759600
H	-4.22845200	1.46943900	1.35346300
H	-2.53334300	1.80988400	1.76909900
C	3.00867600	-0.54693400	1.76035800
C	3.38550700	0.88174600	2.15821400
H	3.69815000	0.89306500	3.20962100
H	2.52743100	1.55368200	2.06216400
H	4.21766600	1.27101400	1.56695400
C	3.50599800	0.03756900	-1.14228000
C	3.43539400	1.56718200	-1.22949000
H	3.97632100	1.90742300	-2.12006500
H	3.90208000	2.04247200	-0.36244200
H	2.41273000	1.93990900	-1.29475400
H	0.06886800	-2.81859500	0.91707200
C	-0.00817800	3.52934800	-1.42977200

C	0.00952800	4.29470100	-0.25017100
C	0.04352800	3.67828600	0.98233000
C	0.05866700	2.24749200	1.07643900
C	0.00073900	2.14974700	-1.29938900
H	-0.02466300	3.99093800	-2.41145900
H	0.00039300	5.38087600	-0.31051300
H	0.06291900	4.25021200	1.90490100
C	0.01000700	1.18187000	-2.44739900
H	-0.82176500	1.36580000	-3.13879800
H	0.93110100	1.29469000	-3.03550100
C	-0.05546600	-0.28475800	-1.94911900
O	-0.13443400	-1.14690200	-2.83590200
N	0.01901100	1.54130000	-0.10047100
O	0.10873200	1.60342300	2.16106100
C	-2.06513200	-0.75859100	2.90715900
H	-2.55140600	-0.67731100	3.88642700
H	-1.73597800	-1.79794900	2.79313300
H	-1.18542600	-0.10565400	2.90284200
C	1.99906300	-1.12382500	2.76139600
H	1.11446300	-0.47844200	2.80393600
H	1.68458200	-2.14221600	2.50526800
H	2.44225300	-1.16204900	3.76332700
C	4.95127700	-0.41750100	-0.91350400
H	5.58806300	-0.04444800	-1.72412800
H	5.34878800	-0.01810600	0.02565100
H	5.05674700	-1.50619500	-0.88870500
C	-4.93503600	-0.53216400	-0.89860800
H	-5.34980600	-0.02070800	-0.02335700
H	-5.55264700	-0.25762300	-1.76188100
H	-5.04854300	-1.60935000	-0.74594200
H	-3.11750300	-0.63638000	-2.04390300
H	3.15921100	-0.36967000	-2.10265800
H	-3.95377600	-0.91094100	1.86651700
H	3.91492700	-1.16737300	1.76463700

$TS_{4,5}$

G_{solv} = -3296.350028

Fe	-0.01095000	-0.20591000	-0.30016100
P	-2.31569500	-0.41010100	-0.45768600
P	2.29805500	-0.39538400	-0.48948600
N	-0.01333200	-1.98255800	-1.39305000
C	-2.43734600	-1.91669900	-1.53335600
H	-3.38225200	-2.45673800	-1.39944700
H	-2.40975900	-1.56472900	-2.57509800
C	-1.23413600	-2.80279000	-1.27484200
H	-1.25427800	-3.24413100	-0.26841200
H	-1.20003100	-3.63520500	-1.99553400
C	1.21654300	-2.79127800	-1.29081600
H	1.17725800	-3.62837100	-2.00600400
H	1.25841700	-3.22388100	-0.28167200
C	2.40697300	-1.89628400	-1.57463500
H	2.35432100	-1.54251400	-2.61482500
H	3.35837200	-2.42983600	-1.46184900
C	3.49572700	-0.72854400	0.91754500
H	4.49243700	-0.55061900	0.48398900
C	3.27862200	0.24176300	2.07489700
H	4.07612100	0.11418800	2.81956900
H	2.32260400	0.05019300	2.57680100
H	3.27976300	1.29342600	1.76627500
C	3.45899000	-2.16442700	1.42569700
H	4.19828200	-2.28233500	2.22949900
H	3.70229800	-2.90099400	0.65143400
H	2.48376000	-2.42767700	1.85274800
C	3.21661100	0.87652300	-1.51441700
H	2.51795300	1.06671300	-2.34354900
C	3.44955200	2.18487000	-0.76383000
H	3.73911900	2.97295500	-1.47211700
H	4.27082100	2.08541000	-0.04170300
H	2.56396000	2.53664100	-0.21850600
C	4.52480200	0.37403800	-2.11601500
H	4.97056600	1.16590000	-2.73361300
H	4.38891700	-0.50170400	-2.76036400
H	5.26315300	0.11758100	-1.34464100
C	-3.27486900	0.84928000	-1.45832200
H	-2.60062400	1.04956700	-2.30534000
C	-4.59186300	0.32946200	-2.02456700
H	-5.07096800	1.11975100	-2.61872200
H	-5.30094300	0.05014500	-1.23376700
H	-4.45967700	-0.53621600	-2.68315500
C	-3.50267500	2.15251400	-0.69757700
H	-3.82648700	2.93740700	-1.39441100
H	-2.60485000	2.51578800	-0.18052800
H	-4.29857200	2.04055500	0.05076200
C	-3.46741200	-0.74328100	0.98917500
H	-4.47596700	-0.54563100	0.59328400
C	-3.44402100	-2.18235700	1.48916300
H	-4.18422700	-2.29651100	2.29254500
H	-2.47225900	-2.45758500	1.91642200
H	-3.69310000	-2.91459900	0.71271600
C	-3.19366100	0.21474900	2.14449100
H	-3.95601800	0.08276900	2.92443400
H	-3.20699900	1.26896900	1.84410900
H	-2.21367700	0.02209600	2.59962100
H	-0.02187700	-1.56239600	-2.33199100
C	-0.02225800	3.95352400	0.17516000
C	-0.00624300	4.21770000	1.54974000
C	0.01271600	3.16537200	2.43684700
C	0.01511600	1.82222500	1.96949400
C	-0.02018200	2.63303200	-0.23715400
H	-0.03593200	4.75044800	-0.56508300
H	-0.00771300	5.24335800	1.91506500
H	0.02675200	3.31806500	3.51315600
H	-0.34176900	-1.60056500	1.16716500
C	-0.03597400	2.26501800	-1.68519900
H	-0.92104800	2.68745600	-2.18793200
H	0.83120800	2.69745100	-2.20989000
C	-0.03057600	0.75320800	-1.88875200
O	-0.04109700	0.32573000	-3.05304200
N	-0.00475200	1.58304800	0.62329600
O	0.02890100	0.86881800	2.82627700
H	0.14027100	-0.42963400	2.88510800
C	-0.00659800	-2.20831100	2.06038900
O	0.06365200	-3.42027800	1.96644300
O	0.24248700	-1.50155700	3.10967000

5

G_{solv} = -3296.349377

Fe	0.00069500	-0.08357800	-0.37036100
P	-2.30534200	-0.26676400	-0.55541900
P	2.30704200	-0.26710700	-0.55382100
N	0.00095800	-1.64734000	-1.76151800
C	-2.42227400	-1.54383900	-1.89637200
H	-3.36898900	-2.09698100	-1.87211800
H	-2.38407700	-1.00611100	-2.85537200
C	-1.22366100	-2.46705400	-1.79525400
H	-1.25660600	-3.07482000	-0.87935900
H	-1.19225600	-3.16497000	-2.64724500
C	1.22534300	-2.46736800	-1.79432900
H	1.19443200	-3.16524800	-2.64637400
H	1.25726200	-3.07520800	-0.87845500
C	2.42430900	-1.54449500	-1.89451700
H	2.38699000	-1.00683100	-2.85360000
H	3.37085500	-2.09791700	-1.86948200
C	3.47328500	-0.87785900	0.78526700
H	4.48193000	-0.65284400	0.40398700
C	3.25288200	-0.13229000	2.09767900
H	3.99926100	-0.45391600	2.83691600
H	2.25647900	-0.34519100	2.50759400
H	3.33662900	0.95574100	1.99547000
C	3.39190300	-2.37937300	1.02586500
H	4.13824100	-2.66770100	1.77810500
H	3.58665000	-2.97701400	0.12823300
H	2.41466500	-2.67417500	1.42722100
C	3.25503800	1.16063000	-1.30977200
H	2.57413300	1.50380800	-2.10384300
C	3.47697000	2.30760300	-0.32808700
H	3.78838000	3.20861800	-0.87391800
H	4.28100100	2.06880900	0.38051400
H	2.58118000	2.56300900	0.25301500
C	4.57455300	0.76662700	-1.96402700
H	5.02985700	1.65216200	-2.42860900
H	4.45448300	0.01298900	-2.75045400
H	5.29838300	0.38281900	-1.23259200
C	-3.25318600	1.16126000	-1.31117100
H	-2.57167400	1.50607700	-2.10398900
C	-4.57152000	0.76677800	-1.96756000
H	-5.02765100	1.65267100	-2.43064100
H	-5.29551300	0.38025400	-1.23771000
H	-4.44952300	0.01509800	-2.75554600
C	-3.47745600	2.30681500	-0.32839100
H	-3.79022400	3.20779800	-0.87349600
H	-2.58228100	2.56325300	0.25316400
H	-4.28129000	2.06604000	0.37976400
C	-3.47199600	-0.87650000	0.78394400
H	-4.48043600	-0.64754100	0.40449800
C	-3.39547000	-2.37863200	1.02221100
H	-4.14151400	-2.66531700	1.77537000
H	-2.41868400	-2.67799200	1.42122600
H	-3.59417200	-2.97407900	0.12398700
C	-3.24751600	-0.13318100	2.09695900
H	-3.99408000	-0.45313800	2.83674100
H	-3.32780600	0.95523000	1.99592300
H	-2.25142500	-0.34973800	2.50565400
H	0.00133800	-1.06574100	-2.60994400
C	-0.00302800	3.87184900	0.93305000
C	-0.00428700	3.80587600	2.33364600
C	-0.00295300	2.58048200	2.96589900
C	-0.00007500	1.37415500	2.20679400
C	-0.00109400	2.67901700	0.22934200
H	-0.00379600	4.82029600	0.40039400
H	-0.00619400	4.72185800	2.92315700
H	-0.00348000	2.49448500	4.05021900
H	0.00128400	-2.18088800	0.95020200
C	0.00022800	2.60363500	-1.26484900
H	-0.87523700	3.11928300	-1.69149500
H	0.87687600	3.11893600	-1.68952600
C	0.00077900	1.14980500	-1.75265100
O	0.00108100	0.95142800	-2.97719000
N	-0.00008300	1.47338900	0.83982000
O	0.00340400	0.22927200	2.76067800
H	-0.00140000	-1.30695300	2.86677700
C	-0.00286200	-2.89624000	1.81091800
O	-0.00441100	-4.09641500	1.64492000
O	-0.00622000	-2.31133000	2.98383700

$TS_{4,4'}$

G_{solv} = -3296.342909

Fe	0.00922900	-0.20330600	-0.24899600
P	-2.30782900	-0.43284200	-0.43677500
P	2.33286500	-0.40741700	-0.41086400
N	0.02519700	-2.01551500	-1.28850400
C	-2.39033200	-1.96701400	-1.47653900
H	-3.33661500	-2.50637800	-1.35168300
H	-2.33568300	-1.64630200	-2.52737400
C	-1.19239300	-2.83989300	-1.15809800
H	-1.23281800	-3.24003400	-0.13563200
H	-1.14032000	-3.69755500	-1.84751800
C	1.26345400	-2.81583100	-1.21098800
H	1.22132500	-3.63803000	-1.94262200
H	1.32532600	-3.27242000	-0.21395900
C	2.44215100	-1.90558800	-1.49816700
H	2.37546500	-1.54187200	-2.53415600
H	3.39793600	-2.43256600	-1.40126900
C	3.51807800	-0.70659400	1.02657300
H	4.47533300	-0.29201600	0.67582100
C	3.08436800	0.07985900	2.25882900
H	3.87375600	0.04258500	3.02181400
H	2.17548700	-0.34325700	2.70493000
H	2.88376100	1.13640200	2.04096700
C	3.76714200	-2.16844300	1.38053200
H	4.49819100	-2.21652700	2.19920700
H	4.18080200	-2.74380200	0.54456100
H	2.86159000	-2.67893800	1.73178800
C	3.27628700	0.86683900	-1.40419600
H	2.60204700	1.08573600	-2.24603100
C	3.49901400	2.14776400	-0.60545000
H	3.87736900	2.93954200	-1.26593900
H	4.24935500	2.00138900	0.18355600

H	2.58298200	2.52143000	-0.12939400
C	4.59147500	0.35530700	-1.98150800
H	5.07987200	1.15801300	-2.55083600
H	4.45207000	-0.48941100	-2.66543100
H	5.29577300	0.04481600	-1.19780600
C	-3.22278400	0.79638100	-1.51740100
H	-2.51701500	0.96312700	-2.34542700
C	-4.52143200	0.26978400	-2.11906200
H	-4.94833500	1.03055900	-2.78714200
H	-5.27826300	0.05872800	-1.35201600
H	-4.37818200	-0.63969500	-2.71316000
C	-3.47110800	2.12697700	-0.81211600
H	-3.77122900	2.88752400	-1.54575700
H	-2.58905300	2.50692500	-0.27984600
H	-4.28904900	2.04262300	-0.08416900
C	-3.53645100	-0.73388900	0.95035500
H	-4.51533900	-0.55589900	0.47774700
C	-3.52455200	-2.15996700	1.48900800
H	-4.28670100	-2.25023500	2.27578300
H	-2.55641000	-2.40649600	1.94174000
H	-3.76324200	-2.90835100	0.72425000
C	-3.35497100	0.25885100	2.09543600
H	-4.22416800	0.21255900	2.76582700
H	-3.25146300	1.29847000	1.76183200
H	-2.46873500	-0.00138200	2.68337300
H	0.00631900	-1.60586200	-2.23190300
C	0.01835500	3.99280300	0.01802300
C	0.02129100	4.33758200	1.37062800
C	0.00070600	3.33329100	2.31571600
C	-0.02364600	1.99113600	1.89703200
C	0.00269500	2.65275800	-0.32751000
H	0.03288100	4.74641100	-0.76592500
H	0.03666500	5.38094800	1.67778400
H	-0.00383200	3.53594800	3.38289500
H	0.98712900	-1.89195500	1.38478600
C	0.01092200	2.21099500	-1.75057100
H	-0.86916300	2.60243200	-2.28555000
H	0.88177100	2.62504800	-2.28329100
C	0.02465600	0.69080200	-1.87667800
O	0.04416200	0.21603900	-3.02257800
N	-0.01357900	1.65002600	0.59159800
O	-0.04444500	1.07615700	2.84136400
H	-0.19473900	0.10547700	2.56309600
C	0.13650800	-2.27998200	2.00888500
O	-0.01615000	-3.50429200	2.07102300
O	-0.56059900	-1.37328300	2.55675400

4′

G_{solv} = -3296.369764

Fe	0.00002200	-0.22688800	-0.24202100
P	-2.29964700	-0.43810300	-0.39344300
P	2.29970300	-0.43792500	-0.39342900
N	0.00008900	-2.02468500	-1.28226300
C	-2.41789600	-1.95220900	-1.45578300
H	-3.36766400	-2.48630400	-1.33295300
H	-2.36817800	-1.61052300	-2.50048100
C	-1.22263700	-2.83720300	-1.15791300
H	-1.24964500	-3.24328800	-0.13854000
H	-1.18280100	-3.68670000	-1.85979100
C	1.22291800	-2.83705900	-1.15797200
H	1.18314900	-3.68656900	-1.85983900
H	1.25002500	-3.24313500	-0.13859800
C	2.41806200	-1.95192200	-1.45589300
H	2.36822500	-1.61018100	-2.50056300
H	3.36790400	-2.48591200	-1.33314900
C	3.44485800	-0.78717200	1.05689200
H	4.45505900	-0.56276200	0.67954600
C	3.15091400	0.13351300	2.23721400
H	3.94851700	0.04449200	2.98772200
H	2.20694200	-0.14604300	2.72039400
H	3.07959700	1.19134000	1.95611300
C	3.43536800	-2.24037500	1.51746600
H	4.10651300	-2.35148400	2.38052100
H	3.78548100	-2.93560100	0.74590200
H	2.43804600	-2.56675000	1.83675700
C	3.28202500	0.80512800	-1.38967800
H	2.61867900	1.00414600	-2.24630600
C	3.49982300	2.11014300	-0.62895400
H	3.86475000	2.88761100	-1.31402100
H	4.25994500	1.99068200	0.15514900
H	2.58520900	2.48845000	-0.15351400
C	4.60550800	0.28157100	-1.93610500
H	5.09205100	1.06294300	-2.53637900
H	4.47982800	-0.59394700	-2.58317900
H	5.30605900	0.01212600	-1.13410700
C	-3.28214400	0.80474200	-1.38978000
H	-2.61860300	1.00419600	-2.24615900
C	-4.60524600	0.28074700	-1.93671000
H	-5.09188300	1.06201100	-2.53704900
H	-5.30595300	0.01095400	-1.13496800
H	-4.47904200	-0.59465000	-2.58384400
C	-3.50074500	2.10949400	-0.62884200
H	-3.86587300	2.88692900	-1.31383900
H	-2.58644600	2.48814100	-0.15307400
H	-4.26101600	1.98950300	0.15503800
C	-3.44471700	-0.78719800	1.05698500
H	-4.45497500	-0.56304800	0.67963800
C	-3.43498300	-2.24028900	1.51794100
H	-4.10600700	-2.35124700	2.38111000
H	-2.43759400	-2.56649400	1.83719700
H	-3.78513600	-2.93574600	0.74660600
C	-3.15089000	0.13384900	2.23704100
H	-3.94847900	0.04494000	2.98758000
H	-3.07970800	1.19160400	1.95561900
H	-2.20687400	-0.14544100	2.72028900
H	0.00005500	-1.62316600	-2.23076100
C	-0.00010000	4.01347400	-0.12430700
C	-0.00016200	4.40950400	1.21299600
C	-0.00019700	3.44093300	2.19718500
C	-0.00014800	2.08866000	1.82159600
C	-0.00007400	2.65992800	-0.42366600
H	-0.00008600	4.73846800	-0.93505300
H	-0.00018500	5.46409700	1.48000800
H	-0.00026300	3.68246500	3.25630700

H	-0.00030100	-2.04432300	3.45942900
C	-0.00007000	2.17282300	-1.83193800
H	-0.87603800	2.56230100	-2.37604200
H	0.87576400	2.56248600	-2.37612200
C	0.00004300	0.64709300	-1.90871200
O	0.00019300	0.15972300	-3.05697400
N	-0.00007400	1.69284700	0.53174300
O	-0.00023200	1.18723400	2.78777800
H	-0.00028700	0.25069600	2.40476500
C	0.00001200	-2.19515800	2.35118200
O	0.00024100	-3.34656900	1.91078800
O	0.00012000	-1.10076500	1.69096300

1b (R1=H, R2=Me)

G_{solv} = -3145.934428

Fe	-0.00110600	-0.57105800	-0.06936700
P	-2.28118200	-0.82533200	-0.02185500
P	2.27935700	-0.82785600	-0.02080700
N	-0.00195100	-2.63460300	-0.44524700
C	-2.44970600	-2.61349400	-0.49681500
H	-3.36315600	-3.06577600	-0.08874800
H	-2.52676300	-2.65230100	-1.59350800
C	-1.21456000	-3.36819900	-0.04591400
H	-1.18913600	-3.47326700	1.04773800
H	-1.20149200	-4.38604100	-0.46897400
C	1.20862000	-3.36826800	-0.03993100
H	1.19497600	-4.38823600	-0.45786900
H	1.18107600	-3.46753500	1.05430000
C	2.44516500	-2.61705200	-0.49261700
H	2.52122600	-2.65802600	-1.58928200
H	3.35806700	-3.07013200	-0.08428800
C	3.23763800	-0.73089700	1.58233600
H	4.25866400	-1.07182600	1.34604300
C	3.28287900	0.68919300	2.13488900
H	3.87019600	0.70525100	3.06356500
H	2.26839600	1.03845400	2.37300400
H	3.74341200	1.40485400	1.44542400
C	2.64023900	-1.66976000	2.62577700
H	3.17034700	-1.54700300	3.58011900
H	2.72012700	-2.72655500	2.34600300
H	1.58144500	-1.43649100	2.81064700
C	3.36462300	-0.01839500	-1.30992700
H	2.82265300	-0.27923800	-2.23427000
C	3.43189200	1.50501700	-1.21086400
H	3.71393400	1.92922400	-2.18411000
H	4.19957600	1.81997400	-0.49330200
H	2.48453700	1.96613500	-0.90565700
C	4.76934100	-0.60327100	-1.39821900
H	5.30566400	-0.15349000	-2.24532200
H	4.77320300	-1.68954200	-1.54821700
H	5.35298500	-0.38038600	-0.49472700
C	-3.36852900	-0.01241700	-1.30682400
H	-2.82898300	-0.27266700	-2.23284200
C	-4.77411200	-0.59561100	-1.39241600
H	-5.31270000	-0.14278900	-2.23643900
H	-5.35450700	-0.37501100	-0.48627900
H	-4.77941600	-1.68142900	-1.54558100
C	-3.43337300	1.51102300	-1.20600700
H	-3.71573100	1.93667900	-2.17850500
H	-2.48501300	1.97036300	-0.90117500
H	-4.19973100	1.82655800	-0.48730800
C	-3.23505800	-0.73130300	1.58411100
H	-4.25650600	-1.07275600	1.35026300
C	-2.63425200	-1.67163000	2.62432900
H	-3.16073300	-1.54969800	3.58078500
H	-1.57460500	-1.43935400	2.80548400
H	-2.71601300	-2.72792800	2.34336200
C	-3.28051200	0.68785000	2.13899200
H	-3.86342800	0.70117300	3.07046900
H	-3.74603200	1.40330300	1.45274400
H	-2.26572500	1.03889800	2.37312300
H	0.00061500	-2.56437500	-1.47236900
C	0.00153700	3.46979300	-1.05833900
C	0.00388100	4.15377800	0.17668900
C	0.00433100	3.41706600	1.34728600
C	0.00232100	1.98492800	1.33232700
C	-0.00043700	2.08559200	-1.04479800
H	0.00136300	4.01238200	-2.00351300
H	0.00639300	3.91179500	2.31862000
C	-0.00279400	1.22416400	-2.27008000
H	-0.88266200	1.42622900	-2.90216600
H	0.87134900	1.42967500	-2.90888400
C	0.00043100	-0.26930300	-1.90120800
O	0.00451500	-1.08733900	-2.83649000
N	-0.00007100	1.37595300	0.09833100
O	0.00204100	1.26149900	2.36556500
C	0.00477900	5.65205600	0.19955000
H	0.87942200	6.05337000	-0.32882400
H	-0.88238200	6.05348100	-0.30757400
H	0.01685800	6.04149200	1.22335000

2b (R1=H, R2=Me)

G_{solv} = -3147.106745

Fe	0.00005300	-0.59751700	0.01914200
P	-2.27491500	-0.82549400	-0.03295900
P	2.27507500	-0.82501700	-0.03299700
N	0.00025700	-2.62467500	-0.44620400
C	-2.43459100	-2.60279500	-0.54600500
H	-3.36539200	-3.06000600	-0.18715400
H	-2.46329400	-2.61949200	-1.64551800
C	-1.21512800	-3.36373600	-0.06542900
H	-1.21221100	-3.47139500	1.02856700
H	-1.19153900	-4.37881400	-0.49427500
C	1.21587300	-3.36348200	-0.06565900
H	1.19246800	-4.37852000	-0.49460900
H	1.21312500	-3.47125700	1.02832500
C	2.43510100	-2.60220500	-0.54630100
H	2.46367100	-2.61874200	-1.64582000
H	3.36605100	-3.05925200	-0.18762300
C	3.32435900	-0.71545700	1.51476000
H	4.36417500	-0.85452800	1.17644400
C	3.18488400	0.64225700	2.19598700
H	3.84872900	0.68763500	3.07070100
H	2.15440200	0.80365900	2.54187200

H	3.44652800	1.48193000	1.54251300
C	2.99261000	-1.82280600	2.50879000
H	3.62259300	-1.71436100	3.40199400
H	3.16896500	-2.82784300	2.10735400
H	1.94745600	-1.76090100	2.84292400
C	3.29872900	0.02334000	-1.34931500
H	2.68069700	-0.13334400	-2.24853200
C	3.45638500	1.52557200	-1.12799000
H	3.77052900	2.00826800	-2.06352300
H	4.23737000	1.73242500	-0.38459700
H	2.53447800	2.01618200	-0.79103500
C	4.66270400	-0.61212300	-1.59491800
H	5.16249900	-0.09973200	-2.42870300
H	4.60146600	-1.67485600	-1.85597400
H	5.31944000	-0.51306600	-0.72009700
C	-3.29865700	0.02248200	-1.34944700
H	-2.68059200	-0.13431600	-2.24862400
C	-4.66257900	-0.61314400	-1.59493800
H	-5.16238800	-0.10099900	-2.42886700
H	-5.31935300	-0.51391300	-0.72016600
H	-4.60125400	-1.67593700	-1.85572700
C	-3.45646100	1.52473700	-1.12840800
H	-3.77050700	2.00725000	-2.06406700
H	-2.53464500	2.01547700	-0.79138600
H	-4.23757300	1.73163700	-0.38515900
C	-3.32424800	-0.71590300	1.51475600
H	-4.36398100	-0.85577600	1.17651700
C	-2.99177200	-1.82259500	2.50927600
H	-3.62184200	-1.71417900	3.40242300
H	-1.94666200	-1.75984000	2.84339400
H	-3.16745000	-2.82792700	2.10828700
C	-3.18560500	0.64220100	2.19536800
H	-3.84932900	0.68749500	3.07017900
H	-3.44796800	1.48139600	1.54156600
H	-2.15517100	0.80446000	2.54100400
H	0.00016400	-2.53090100	-1.47343400
C	-0.00024300	3.46697700	-1.08031600
C	-0.00031200	4.21511500	0.11036500
C	-0.00035300	3.52890700	1.31002000
C	-0.00037900	2.10052100	1.37115900
C	-0.00020500	2.08291000	-1.00171700
H	-0.00017400	3.95456700	-2.05460000
H	-0.00035900	4.06353500	2.26005700
H	0.00022300	-1.17730500	1.61418700
C	-0.00008800	1.22099000	-2.22351300
H	-0.87680000	1.43018900	-2.85854100
H	0.87663400	1.43033900	-2.85848000
C	0.00002200	-0.25875600	-1.85313300
O	0.00007800	-1.07637100	-2.79157500
N	-0.00021700	1.40560600	0.16589800
O	-0.00041500	1.46859600	2.46198000
H	-0.00013300	-0.36098800	1.72876300
C	-0.00048200	5.71429900	0.08090100
H	-0.88344100	6.11893100	0.59177400
H	0.87881000	6.11931800	0.59772900
H	0.00283600	6.09843700	-0.94525300

$TS_{3,4}$b (R1=H, R2=Me)

G_{solv} = -3335.593343

Fe	0.00009300	-0.39648400	-0.29690500
P	-2.27910900	-0.60678800	-0.42696400
P	2.27925600	-0.60644100	-0.42683000
N	0.00023200	-2.25941100	-1.22496000
C	-2.41608800	-2.18865400	-1.38674000
H	-3.36720100	-2.70871000	-1.22031900
H	-2.37554500	-1.91685400	-2.45193700
C	-1.22265100	-3.06036700	-1.04981200
H	-1.25357900	-3.41199000	-0.01079500
H	-1.19085400	-3.94863600	-1.70246600
C	1.22327100	-3.06013500	-1.04978700
H	1.19162600	-3.94844300	-1.70239300
H	1.25427700	-3.41172100	-0.01075300
C	2.41650000	-2.18817300	-1.38678500
H	2.37571300	-1.91622300	-2.45193700
H	3.36777000	-2.70801000	-1.22058900
C	3.44548800	-0.84377300	1.02958800
H	4.45236500	-0.67387200	0.61686900
C	3.18621200	0.18195900	2.12813300
H	3.98496000	0.13384800	2.88119100
H	2.23848600	-0.02333300	2.64074800
H	3.14247900	1.21323400	1.75779500
C	3.41937500	-2.24782800	1.61984700
H	4.12269500	-2.30310500	2.46210100
H	3.71061700	-3.02310800	0.90187700
H	2.42890000	-2.50770800	2.01307000
C	3.26102200	0.56243000	-1.51808900
H	2.59353600	0.69386500	-2.38403200
C	3.48673100	1.92399600	-0.86704700
H	3.83798700	2.64482800	-1.61823000
H	4.26150400	1.86824700	-0.09030200
H	2.58015200	2.33890100	-0.40743300
C	4.58256600	0.00210600	-2.03228500
H	5.05702000	0.73468300	-2.70026300
H	4.45796600	-0.92481600	-2.60348900
H	5.29340500	-0.19437700	-1.21832100
C	-3.26080600	0.56184600	-1.51854700
H	-2.59328100	0.69302800	-2.38450500
C	-4.58237900	0.00150500	-2.03265400
H	-5.05663500	0.73391700	-2.70095600
H	-5.29331500	-0.19451600	-1.21866400
H	-4.45790400	-0.92565400	-2.60350500
C	-3.48649400	1.92360000	-0.86787400
H	-3.83721900	2.64438000	-1.61935300
H	-2.58003200	2.33837700	-0.40791200
H	-4.26164700	1.86815400	-0.09148600
C	-3.44565800	-0.84418100	1.02919400
H	-4.45249100	-0.67487400	0.61610800
C	-3.41899600	-2.24804000	1.61988700
H	-4.12228300	-2.30336700	2.46216300
H	-2.42841700	-2.50735700	2.01321500
H	-3.70982200	-3.02370600	0.90216400
C	-3.18716900	0.18195000	2.12755900
H	-3.98626400	0.13386000	2.88025000
H	-3.14347000	1.21314300	1.75700800

H	-2.23965700	-0.02303400	2.64069600
H	0.00021000	-1.91901500	-2.19796100
C	0.00002200	3.83089500	-0.45442700
C	-0.00012100	4.29762200	0.86816200
C	-0.00016800	3.35297100	1.88388700
C	-0.00023300	1.99337200	1.55484900
C	-0.00000500	2.47029500	-0.70608800
H	0.00019800	4.52934700	-1.29074800
H	-0.00010900	3.63877000	2.93326100
H	0.00066800	-1.16029200	1.26571200
C	0.00009800	1.89911000	-2.08232100
H	-0.87660000	2.24815600	-2.65170800
H	0.87681400	2.24825100	-2.65162700
C	0.00012300	0.36742100	-2.04465500
O	0.00021700	-0.20248400	-3.15335500
N	-0.00011100	1.54630900	0.28946300
O	-0.00038400	1.10087100	2.53630600
H	-0.00025600	0.19664500	2.12013500
C	-0.00007300	-2.31830100	2.62061500
O	0.00039500	-3.37751200	2.08490000
O	-0.00068800	-1.59697000	3.56326400
C	-0.00071000	5.76303600	1.16264600
H	0.87562200	6.25151900	0.71867900
H	-0.88573100	6.24752800	0.73162900
H	0.00641500	5.95954000	2.23950400

1c (R1=H, R2=OH)

G_{solv} = -3181.875789

Fe	0.00088000	-0.57357700	-0.08134600
P	-2.27491300	-0.82552100	-0.01525800
P	2.27762600	-0.81945300	-0.01647000
N	0.00389800	-2.63935800	-0.43324700
C	-2.44812300	-2.62286900	-0.45482800
H	-3.35211800	-3.06883400	-0.01953700
H	-2.54904100	-2.67956600	-1.54877900
C	-1.20463500	-3.37142000	-0.01742700
H	-1.16536200	-3.47124700	1.07615700
H	-1.19509100	-4.39179900	-0.43435500
C	1.21589400	-3.36839100	-0.02207800
H	1.20850800	-4.38783500	-0.44129600
H	1.17974300	-3.47078500	1.07138000
C	2.45593200	-2.61496100	-0.46076400
H	2.55455700	-2.66857600	-1.55507600
H	3.36232500	-3.05911500	-0.02861500
C	3.19783900	-0.70108000	1.60681600
H	4.19630000	-1.13129600	1.42586400
C	3.34017100	0.73845600	2.08701500
H	3.86299500	0.75358900	3.05338800
H	2.35140000	1.19311100	2.23790000
H	3.91374900	1.36591500	1.39710800
C	2.48914800	-1.53056700	2.67328200
H	3.00294400	-1.41263400	3.63719100
H	2.47687800	-2.60250700	2.44403400
H	1.45348100	-1.18561900	2.81109600
C	3.38164600	-0.02758100	-1.29926800
H	2.86254800	-0.32079000	-2.22717900
C	3.42588400	1.49960000	-1.24314400
H	3.68655400	1.90175200	-2.23144000
H	4.19777900	1.84847000	-0.54650000
H	2.47620800	1.95423800	-0.93583800
C	4.79433900	-0.59816500	-1.33868800
H	5.35029600	-0.15628100	-2.17726100
H	4.81272500	-1.68660600	-1.47081200
H	5.34888900	-0.35631000	-0.42177700
C	-3.38081000	-0.04015700	-1.30012100
H	-2.86123400	-0.33524300	-2.22716800
C	-4.79230200	-0.61385300	-1.33789200
H	-5.34959900	-0.17452000	-2.17692100
H	-5.34698100	-0.37185900	-0.42108800
H	-4.80831600	-1.70252200	-1.46838000
C	-3.42763200	1.48722500	-1.24887900
H	-3.68521900	1.88610700	-2.23928400
H	-2.47979200	1.94441700	-0.93931800
H	-4.20270500	1.83687000	-0.55610900
C	-3.19520700	-0.70639500	1.60780300
H	-4.19071500	-1.14435500	1.42915900
C	-2.48019500	-1.52648900	2.67734800
H	-2.99567600	-1.41003100	3.64054600
H	-1.44775900	-1.17177600	2.81441500
H	-2.45838800	-2.59899900	2.45156400
C	-3.34721400	0.73403200	2.08226800
H	-3.86836300	0.74922800	3.04953700
H	-3.92655300	1.35457700	1.39087700
H	-2.36139600	1.19616600	2.22997500
H	0.00200100	-2.58148800	-1.46102600
C	-0.00590700	3.46052900	-1.10447400
C	-0.00722000	4.12506700	0.13366500
C	-0.00578100	3.41512200	1.32154300
C	-0.00328700	1.98611800	1.30690500
C	-0.00316000	2.07545300	-1.07303500
H	-0.00630300	4.01326200	-2.04058700
H	-0.00682500	3.92644900	2.28412100
C	-0.00140000	1.20740600	-2.29342500
H	-0.87820400	1.40823000	-2.92988000
H	0.87623100	1.40980300	-2.92828600
C	-0.00006800	-0.28444500	-1.91457700
O	-0.00011500	-1.10823500	-2.84460100
N	-0.00235200	1.37350100	0.07125200
O	-0.00131000	1.26142300	2.33755300
O	-0.00957100	5.48266100	0.10329600
H	-0.01436900	5.82441600	1.00881200

2c (R1=H, R2=OH)

G_{solv} = -3183.048455

Fe	-0.00016900	-0.58952900	0.02068200
P	-2.27537500	-0.81655600	-0.03247600
P	2.27492300	-0.81757400	-0.03247100
N	-0.00061600	-2.61664400	-0.44324100
C	-2.43515700	-2.59370000	-0.54572500
H	-3.36674800	-3.05054800	-0.18855400
H	-2.46192200	-2.61045000	-1.64528900
C	-1.21665300	-3.35493100	-0.06292600
H	-1.21509300	-3.46156000	1.03116500
H	-1.19296100	-4.37034800	-0.49087000

C	1.21500900	-3.35547400	-0.06266700
H	1.19089000	-4.37093600	-0.49048000
H	1.21325000	-3.46195500	1.03143800
C	2.43393500	-2.59488600	-0.54541000
H	2.46084500	-2.61183500	-1.64496500
H	3.36526400	-3.05210900	-0.18803500
C	3.32479400	-0.70794200	1.51495300
H	4.36482500	-0.84376900	1.17613500
C	3.18218600	0.64858100	2.19788000
H	3.84951100	0.69651700	3.06978000
H	2.15255400	0.80510400	2.54803000
H	3.43670200	1.48996600	1.54377100
C	2.99608000	-1.81719100	2.50782800
H	3.62459600	-1.70710700	3.40186600
H	3.17652800	-2.82128200	2.10596000
H	1.95025900	-1.75949100	2.84072000
C	3.29809500	0.03129900	-1.34879100
H	2.67933100	-0.12356600	-2.24776800
C	3.45674600	1.53309400	-1.12521700
H	3.77122700	2.01719900	-2.05985900
H	4.23768200	1.73837000	-0.38131100
H	2.53519000	2.02398300	-0.78767100
C	4.66130900	-0.60488900	-1.59637500
H	5.16082500	-0.09155700	-2.42973400
H	4.59886600	-1.66711200	-1.85916100
H	5.31894800	-0.50790800	-0.72200700
C	-3.29827700	0.03297500	-1.34858200
H	-2.67960800	-0.12191300	-2.24762100
C	-4.66171100	-0.60269600	-1.59627100
H	-5.16110500	-0.08896100	-2.42945500
H	-5.31927400	-0.50576900	-0.72183900
H	-4.59961600	-1.66486100	-1.85937300
C	-3.45639300	1.53478100	-1.12469800
H	-3.77078600	2.01917600	-2.05922000
H	-2.53463500	2.02528400	-0.78714700
H	-4.23719500	1.74018900	-0.38068900
C	-3.32517600	-0.70677900	1.51500100
H	-4.36528800	-0.84182500	1.17612000
C	-2.99722400	-1.81658700	2.50749800
H	-3.62568100	-1.70638100	3.40156300
H	-1.95137200	-1.75971300	2.84043300
H	-3.17834500	-2.82041900	2.10528500
C	-3.18174600	0.64941700	2.19840900
H	-3.84914200	0.69749000	3.07024800
H	-3.43562800	1.49119800	1.54456500
H	-2.15205800	0.80516300	2.54872800
H	-0.00049600	-2.52364900	-1.47050700
C	0.00081700	3.47241700	-1.10232600
C	0.00117400	4.20335600	0.09511600
C	0.00116000	3.54533100	1.30751900
C	0.00074600	2.11682300	1.36691300
C	0.00044400	2.09157000	-1.00629100
H	0.00087200	3.97168000	-2.06820300
H	0.00147000	4.09297300	2.24932300
H	-0.00038400	-1.16962000	1.61666900
C	0.00009500	1.22588000	-2.22520200
H	-0.87671000	1.43513000	-2.85975300
H	0.87673400	1.43485200	-2.86007100
C	-0.00010300	-0.25302800	-1.85175100
O	-0.00021400	-1.07144000	-2.78939000
N	0.00037800	1.41739500	0.16368800
O	0.00088300	1.49156000	2.45930100
H	0.00000400	-0.35360300	1.72892000
O	0.00155400	5.55627300	-0.00199100
H	0.00182800	5.94277900	0.88553400

$TS_{3,4}$c (R1=H, R2=OH)

G_{solv} = -3371.531770

Fe	-0.00003800	-0.38763400	-0.29977600
P	-2.27931800	-0.59641500	-0.42982000
P	2.27921000	-0.59685700	-0.42974300
N	-0.00019500	-2.24363000	-1.23988500
C	-2.41665800	-2.17099800	-1.40134500
H	-3.36789100	-2.69212300	-1.23915300
H	-2.37588800	-1.89095800	-2.46440200
C	-1.22336700	-3.04548200	-1.07063700
H	-1.25445400	-3.40466500	-0.03416800
H	-1.19165300	-3.92897500	-1.72972500
C	1.22275400	-3.04577000	-1.07039300
H	1.19091200	-3.92933000	-1.72938600
H	1.25362600	-3.40484600	-0.03388000
C	2.41628100	-2.17159900	-1.40106200
H	2.37566800	-1.89167200	-2.46415600
H	3.36738900	-2.69291500	-1.23873800
C	3.44423700	-0.84591500	1.02593200
H	4.45154900	-0.67179600	0.61611600
C	3.18323500	0.17018800	2.13302600
H	3.98214400	0.11724200	2.88559800
H	2.23605800	-0.04140600	2.64411100
H	3.13773400	1.20442900	1.77112100
C	3.41832000	-2.25502200	1.60402600
H	4.11900800	-2.31669500	2.44803700
H	3.71313200	-3.02351500	0.88025000
H	2.42694100	-2.51991400	1.99162400
C	3.26211000	0.58022700	-1.51086500
H	2.59557300	0.71824100	-2.37653800
C	3.48627200	1.93678800	-0.84889700
H	3.83712300	2.66406700	-1.59396000
H	4.26055300	1.87573900	-0.07204100
H	2.57907700	2.34726300	-0.38647500
C	4.58427500	0.02402600	-2.02784800
H	5.05997300	0.76205900	-2.68887700
H	4.45999900	-0.89796000	-2.60704400
H	5.29387800	-0.17974700	-1.21458000
C	-3.26194700	0.58103500	-1.51077700
H	-2.59541800	0.71899700	-2.37646500
C	-4.58426700	0.02525000	-2.02780700
H	-5.05961600	0.76336300	-2.68900100
H	-5.29402500	-0.17812900	-1.21457800
H	-4.46028000	-0.89687500	-2.60684800
C	-3.48575700	1.93755500	-0.84859700
H	-3.83610100	2.66513800	-1.59360100
H	-2.57853900	2.34756800	-0.38581500
H	-4.26028400	1.87662800	-0.07197400

C	-3.44446200	-0.84540600	1.02577800
H	-4.45169500	-0.67082700	0.61596700
C	-3.41907300	-2.25465000	1.60355800
H	-4.11963900	-2.31618900	2.44768000
H	-2.42774400	-2.52009600	1.99090800
H	-3.71437600	-3.02283900	0.87965900
C	-3.18312700	0.17037400	2.13309600
H	-3.98214800	0.11766300	2.88556600
H	-3.13706200	1.20466200	1.77139600
H	-2.23611400	-0.04174400	2.64426200
H	-0.00006500	-1.89689600	-2.21065100
C	0.00048900	3.84452500	-0.44678500
C	0.00049100	4.28238900	0.88098100
C	0.00029800	3.35008600	1.90929700
C	0.00013500	1.99676900	1.56632600
C	0.00028000	2.48384400	-0.69325500
H	0.00064700	4.55876900	-1.26646600
H	0.00028400	3.63913700	2.95781300
H	0.00000400	-1.15610500	1.25992300
C	0.00019600	1.91969700	-2.07205300
H	-0.87649000	2.27347900	-2.63825000
H	0.87681100	2.27342500	-2.63839200
C	0.00008900	0.38730000	-2.04254200
O	0.00009200	-0.17477100	-3.15515100
N	0.00012000	1.55585800	0.29715000
O	-0.00000300	1.09857800	2.54029400
H	-0.00006300	0.19690300	2.11649300
C	-0.00030000	-2.31951400	2.60777200
O	-0.00064400	-3.37630200	2.06738900
O	-0.00000200	-1.60249700	3.55383600
O	0.00068800	5.61114200	1.10452400
H	0.00053400	5.79003700	2.05668400

1d (R1=H, R2=OMe)

G_{solv} = -3221.115723

Fe	-0.03680300	-0.75071500	-0.05761900
P	-2.32706200	-0.88150000	0.01972900
P	2.22718300	-1.11191500	0.02161800
N	-0.14425800	-2.83778400	-0.23471100
C	-2.58893300	-2.69262200	-0.29735200
H	-3.52423900	-3.06013700	0.14472700
H	-2.66754300	-2.82263800	-1.38693800
C	-1.39459300	-3.46756400	0.22302600
H	-1.37471100	-3.47547500	1.32166300
H	-1.43578400	-4.51859900	-0.10646400
C	1.02453800	-3.58763500	0.25475900
H	0.96362800	-4.64187800	-0.06166500
H	0.98169400	-3.57831200	1.35304600
C	2.30326200	-2.94913000	-0.25035700
H	2.39435800	-3.11407000	-1.33436600
H	3.18449900	-3.40059700	0.22422300
C	3.18587100	-0.89728700	1.61279400
H	4.15560400	-1.39530800	1.44961200
C	3.41593800	0.56777100	1.96441100
H	3.97641300	0.63499500	2.90740100
H	2.45594700	1.08115800	2.11146700
H	3.99111900	1.10762600	1.20519200
C	2.46086200	-1.59166900	2.76100000
H	3.00703800	-1.42652000	3.69986500
H	2.37943100	-2.67599900	2.62172900
H	1.45216500	-1.17281600	2.89039900
C	3.35287200	-0.50231700	-1.33955600
H	2.80845600	-0.85269800	-2.23231700
C	3.47178700	1.01951200	-1.42475600
H	3.73537400	1.31759000	-2.44850600
H	4.27033600	1.39186000	-0.77162700
H	2.55014200	1.54648300	-1.14952500
C	4.73677700	-1.14099700	-1.33976500
H	5.29668300	-0.81262200	-2.22659500
H	4.70471300	-2.23693400	-1.36041900
H	5.31907800	-0.83403600	-0.46027100
C	-3.38141400	-0.12878300	-1.32863500
H	-2.85613300	-0.48446200	-2.23065000
C	-4.81201200	-0.65272400	-1.37096200
H	-5.32774100	-0.25105000	-2.25423300
H	-5.38286200	-0.32737800	-0.49061000
H	-4.86738400	-1.74630400	-1.42858600
C	-3.38000500	1.39917400	-1.34605600
H	-3.63977500	1.76177600	-2.34984300
H	-2.41375300	1.83865800	-1.07024900
H	-4.13456900	1.80179800	-0.65872800
C	-3.26683300	-0.59334400	1.61068000
H	-4.31145400	-0.87604000	1.40216100
C	-2.73419800	-1.48943100	2.72437100
H	-3.25671700	-1.26209200	3.66347900
H	-1.66292200	-1.31107400	2.89814400
H	-2.88233200	-2.55682200	2.52287300
C	-3.20487200	0.86438900	2.05368700
H	-3.78716600	0.99304600	2.97688700
H	-3.61245500	1.55895700	1.31140100
H	-2.16623500	1.15410900	2.26649200
H	-0.13431400	-2.86971100	-1.26326900
C	0.14754700	3.18475400	-1.37979900
C	0.19756300	3.94211800	-0.19015900
C	0.18844700	3.31390100	1.04521400
C	0.12607600	1.88549300	1.11997500
C	0.08104600	1.80991100	-1.25674600
H	0.15848500	3.67466900	-2.35055000
H	0.23062000	3.86270600	1.98170900
C	0.02232000	0.85176400	-2.40649700
H	-0.85499900	1.04214500	-3.04535700
H	0.89728900	0.96312800	-3.06689100
C	-0.03702000	-0.60646300	-1.90959900
O	-0.07797700	-1.49945400	-2.77231600
N	0.06512200	1.19170100	-0.06360700
O	0.12544300	1.22798700	2.19635000
O	0.25451800	5.28451400	-0.35932000
C	0.27416700	6.09872400	0.79933300
H	0.30599200	7.13284600	0.44878200
H	-0.62966900	5.95196500	1.40567000
H	1.16168200	5.90081200	1.41506600

2d (R1=H, R2=OMe)

G_{solv} = -3222.288377

Fe	0.00397400	-0.77341300	0.04176700
P	-2.27035900	-1.01468200	0.00171800
P	2.28066600	-0.99186000	0.00163700
N	0.01420900	-2.82991000	-0.27100000
C	-2.42094100	-2.82781500	-0.37023400
H	-3.34910800	-3.26114000	0.02357300
H	-2.45003100	-2.93049900	-1.46498800
C	-1.19763500	-3.54282000	0.16717100
H	-1.19400900	-3.56413200	1.26635500
H	-1.16944800	-4.58834800	-0.18038900
C	1.23331800	-3.53072300	0.16650800
H	1.21555600	-4.57634800	-0.18147500
H	1.23023100	-3.55250200	1.26568500
C	2.44919200	-2.80326300	-0.37103300
H	2.47884900	-2.90520200	-1.46585400
H	3.38177000	-3.22750600	0.02222700
C	3.33568100	-0.75609200	1.53066500
H	4.37430300	-0.92748400	1.20392500
C	3.20250400	0.65463600	2.09575700
H	3.86895100	0.77034400	2.96188600
H	2.17356500	0.84617900	2.43072100
H	3.46487700	1.43593200	1.37400500
C	3.00369100	-1.77394100	2.61613300
H	3.63378600	-1.58824400	3.49652600
H	3.18089800	-2.80982600	2.30330600
H	1.95850100	-1.68431600	2.94360500
C	3.29291200	-0.24431400	-1.38373700
H	2.67254000	-0.48141100	-2.26363300
C	3.43686800	1.27299200	-1.28897100
H	3.72927600	1.68057500	-2.26633300
H	4.22828400	1.54719000	-0.57924600
H	2.51612200	1.78147800	-0.97641800
C	4.66248800	-0.88346800	-1.58400700
H	5.14890300	-0.44119500	-2.46459200
H	4.61339500	-1.96578700	-1.74995300
H	5.32513700	-0.69857900	-0.72785400
C	-3.28994100	-0.27768700	-1.38391100
H	-2.66703200	-0.50860700	-2.26365600
C	-4.65295700	-0.93069700	-1.58418400
H	-5.14366800	-0.49379200	-2.46506200
H	-5.31753400	-0.75205100	-0.72819100
H	-4.59292500	-2.01255200	-1.74956700
C	-3.44928000	1.23808700	-1.28930100
H	-3.74524900	1.64264100	-2.26685200
H	-2.53388100	1.75583300	-0.97621300
H	-4.24387600	1.50427900	-0.58008600
C	-3.32761600	-0.78892500	1.53064900
H	-4.36441900	-0.97145500	1.20412400
C	-2.98467800	-1.80253200	2.61670500
H	-3.61668700	-1.62313600	3.49703400
H	-1.94047900	-1.70153500	2.94405200
H	-3.15074700	-2.84043400	2.30444700
C	-3.20931100	0.62345100	2.09498900
H	-3.87677700	0.73244600	2.96119700
H	-3.48012500	1.40159700	1.37294800
H	-2.18237900	0.82616800	2.42958200
H	0.01383700	-2.81625100	-1.30222100
C	-0.01608500	3.20090900	-1.34834100
C	-0.02029600	4.01860700	-0.20184700
C	-0.01744200	3.43786200	1.05135500
C	-0.01038200	2.01250200	1.19628400
C	-0.00906900	1.83205000	-1.16670800
H	-0.01826100	3.63811000	-2.34421300
H	-0.02043700	4.01920600	1.96829600
H	0.00621000	-1.23831300	1.67484500
C	-0.00420400	0.88488700	-2.32397500
H	-0.88179700	1.04514000	-2.97159400
H	0.87228800	1.05353800	-2.97095800
C	0.00276100	-0.56623200	-1.84998100
O	0.00673600	-1.44725100	-2.72906000
N	-0.00614900	1.23490500	0.04720200
O	-0.00763800	1.46256300	2.32971900
H	0.00247800	-0.41659700	1.73176100
O	-0.02712900	5.35208100	-0.42947000
C	-0.03265400	6.21354400	0.69546500
H	0.86370000	6.06965700	1.31323800
H	-0.03730700	7.23294300	0.30291900
H	-0.92891200	6.06064400	1.31121300

$TS_{3,4}$d (R1=H, R2=OMe)

G_{solv} = -3410.772566

Fe	-0.59775800	-0.05503000	-0.27883900
P	-1.01708000	2.19650800	-0.38253100
P	-0.62894700	-2.34378200	-0.36885000
N	-2.56839400	-0.22497400	-0.92599300
C	-2.72426600	2.18650300	-1.10908600
H	-3.29329700	3.09452300	-0.87611600
H	-2.60260000	2.14827300	-2.20169400
C	-3.43492800	0.93110700	-0.64234300
H	-3.63259500	0.95179900	0.43691200
H	-4.40308500	0.81482500	-1.15732900
C	-3.22934700	-1.50694100	-0.62999500
H	-4.20128500	-1.56094300	-1.14820700
H	-3.42471400	-1.54825200	0.44926700
C	-2.31782500	-2.63079700	-1.08232800
H	-2.20996200	-2.59119500	-2.17643600
H	-2.72490100	-3.61783500	-0.83176400
C	-0.54567200	-3.50058800	1.11186500
H	-0.35481400	-4.49713200	0.68321200
C	0.60642000	-3.13625200	2.04249200
H	0.74143400	-3.92338700	2.79719100
H	0.39696000	-2.20166400	2.57725100
H	1.56314100	-3.00953700	1.52182400
C	-1.84125600	-3.58052700	1.90879100
H	-1.71361100	-4.28267300	2.74419200
H	-2.69303800	-3.93216600	1.31531300
H	-2.11179800	-2.61074100	2.34404200
C	0.44844200	-3.23924300	-1.61664500
H	0.38665300	-2.57950000	-2.49610800
C	1.90728200	-3.32547100	-1.17675300
H	2.53903700	-3.61801500	-2.02683900
H	2.04242500	-4.08953600	-0.39899800
H	2.29768500	-2.37676400	-0.78594600
C	-0.05540600	-4.61700900	-2.03228800

H	0.60718200	-5.03378000	-2.80384300
H	-1.06706100	-4.59257400	-2.45303700
H	-0.05368400	-5.32749400	-1.19451800
C	-0.09559400	3.25330100	-1.62837600
H	-0.02305800	2.58434600	-2.49997600
C	-0.83079400	4.51395400	-2.06934600
H	-0.23432800	5.04263500	-2.82603900
H	-0.98457500	5.21519300	-1.23803800
H	-1.80804200	4.30142500	-2.51743100
C	1.31532800	3.60322800	-1.16425000
H	1.89673000	4.00955000	-2.00333500
H	1.86529400	2.74019900	-0.76697100
H	1.29431400	4.37638800	-0.38406000
C	-1.13895200	3.36188500	1.08978300
H	-1.08500900	4.37358900	0.65802000
C	-2.45173400	3.25517200	1.85542000
H	-2.44035000	3.95729700	2.70038200
H	-2.60076000	2.25198700	2.27378300
H	-3.32802600	3.49776300	1.24358700
C	0.03302600	3.17762300	2.04834600
H	0.02814400	3.97829300	2.80092000
H	1.00913200	3.19834000	1.54887300
H	-0.04483600	2.22333500	2.58334200
H	-2.37262600	-0.21259500	-1.93803800
C	3.54538600	0.30094400	-1.06295900
C	4.18576500	0.35583800	0.18452600
C	3.41866800	0.29154200	1.34173200
C	2.03198800	0.17291900	1.20032900
C	2.17156100	0.18313200	-1.10450000
H	4.12778500	0.34887500	-1.97991200
H	3.83727700	0.32799300	2.34181200
H	-1.11603600	-0.10115300	1.38093600
C	1.40732300	0.11324400	-2.38199700
H	1.59453500	1.00581200	-3.00077900
H	1.74418500	-0.74131500	-2.99115300
C	-0.09787200	-0.01510600	-2.11960900
O	-0.82029200	-0.07766500	-3.13385100
N	1.40461100	0.11818400	0.01630800
O	1.29495800	0.11192500	2.30030200
H	0.34294800	0.03162500	2.01766500
C	-2.06920600	-0.14485700	2.88805700
O	-3.18590200	-0.27024900	2.50685500
O	-1.22579300	-0.03085100	3.71513300
O	5.52317800	0.46813400	0.16651500
C	6.20911600	0.52062700	1.41043500
H	6.03323800	-0.38899200	1.99833100
H	7.27121600	0.59311000	1.16883300
H	5.90945300	1.40181100	1.99175100

1e (R1=Me, R2=H)

G_{solv} = -3185.195815

Fe	0.00057300	-0.65316700	-0.08989300
P	-2.27297700	-0.89684800	-0.02469700
P	2.27431300	-0.89467900	-0.02489700
N	0.00159300	-2.72250500	-0.41731900
C	-2.45111400	-2.70099100	-0.43575600
H	-3.35462500	-3.13878300	0.00886400
H	-2.55461000	-2.77456800	-1.52851700
C	-1.20809600	-3.44531000	0.01065800
H	-1.16737400	-3.52698700	1.10575900
H	-1.20180000	-4.47246300	-0.38951900
C	1.21243800	-3.44447800	0.00878400
H	1.20688900	-4.47112500	-0.39265600
H	1.17265300	-3.52753900	1.10379500
C	2.45433100	-2.69825600	-0.43759300
H	2.55745100	-2.77069200	-1.53046600
H	3.35858000	-3.13530000	0.00626600
C	3.19522400	-0.74564100	1.59559000
H	4.18524800	-1.20088100	1.42925600
C	3.36877700	0.70349000	2.03577600
H	3.89265600	0.73369000	3.00128900
H	2.39001000	1.18212600	2.17664100
H	3.95504400	1.29948800	1.32890000
C	2.46413900	-1.52783000	2.68272700
H	2.97942800	-1.39736300	3.64442000
H	2.42552400	-2.60502300	2.48216100
H	1.43836900	-1.14830400	2.80433900
C	3.37476300	-0.12488300	-1.32483800
H	2.85964900	-0.44626800	-2.24552600
C	3.40617500	1.40431400	-1.30925200
H	3.65542300	1.78312400	-2.31000500
H	4.18035500	1.77837900	-0.62834900
H	2.45467100	1.85753100	-1.00517200
C	4.79203800	-0.68502400	-1.34722900
H	5.34529200	-0.26447900	-2.19851300
H	4.81867200	-1.77687500	-1.44626300
H	5.34379700	-0.41200000	-0.43742200
C	-3.37380400	-0.12915700	-1.32553200
H	-2.85807100	-0.45044900	-2.24589600
C	-4.79038800	-0.69110200	-1.34808700
H	-5.34389100	-0.27164700	-2.19974500
H	-5.34284400	-0.41843500	-0.43858600
H	-4.81556100	-1.78301900	-1.44672900
C	-3.40716100	1.40001700	-1.31075800
H	-3.65703700	1.77787700	-2.31171700
H	-2.45617500	1.85473000	-1.00711700
H	-4.18181000	1.77339600	-0.62999500
C	-3.19472400	-0.74726900	1.59523200
H	-4.18461800	-1.20259600	1.42846500
C	-2.46421300	-1.52897800	2.68308300
H	-2.98017900	-1.39833700	3.64439000
H	-1.43864500	-1.14911800	2.80520800
H	-2.42505600	-2.60620700	2.48288100
C	-3.36854100	0.70200700	2.03479500
H	-3.89427800	0.73260600	2.99929100
H	-3.95301300	1.29826400	1.32664000
H	-2.38977300	1.18001300	2.17748600
H	0.00082000	-2.67906200	-1.44565000
C	-0.00227700	3.37497900	-1.06968600
C	-0.00293300	3.98394500	0.20140100
C	-0.00243000	3.25847100	1.38064800
C	-0.00103100	1.82421200	1.30699900
C	-0.00095300	1.98695100	-1.07977200
C	-0.00009500	1.12381000	-2.30383000

H	-0.87650300	1.31979100	-2.94479900
H	0.87632200	1.32064900	-2.94446500
C	0.00036400	-0.37099600	-1.92356700
O	0.00037200	-1.19700900	-2.85184200
N	-0.00073700	1.26999100	0.05892100
O	-0.00053600	1.04703600	2.30818000
C	-0.00318800	3.90178000	2.72928300
H	0.87397900	3.60014800	3.31954100
H	-0.00283900	4.99547500	2.64942900
H	-0.88121900	3.60011600	3.31814200
C	-0.00324600	4.16595800	-2.34357800
H	-0.00345600	5.24263100	-2.13635600
H	0.87870100	3.95217200	-2.96633300
H	-0.88618600	3.95181900	-2.96491500
H	-0.00391700	5.07602600	0.25777000

2e (R1=Me, R2=H)

G_{solv} = -3186.368677

Fe	0.00159600	-0.68190000	0.03395600
P	-2.27160100	-0.90319600	-0.02290100
P	2.27532800	-0.89615100	-0.02242400
N	0.00482900	-2.71662700	-0.38366400
C	-2.43237700	-2.69726500	-0.47797400
H	-3.36069300	-3.14438400	-0.10034000
H	-2.46739500	-2.74812100	-1.57619000
C	-1.21040600	-3.44436900	0.01912900
H	-1.20517700	-3.52179200	1.11569300
H	-1.18835100	-4.47107800	-0.38120600
C	1.22191700	-3.44059000	0.02027600
H	1.20331500	-4.46745700	-0.37981100
H	1.21609400	-3.51775000	1.11686600
C	2.44200500	-2.68999000	-0.47617900
H	2.47827900	-2.74150800	-1.57431700
H	3.37142400	-3.13381900	-0.09735700
C	3.33869900	-0.72465800	1.50915700
H	4.37352500	-0.89587000	1.17045100
C	3.22500900	0.66740000	2.12380100
H	3.89801500	0.74536600	2.98909600
H	2.20016800	0.85784700	2.47255100
H	3.49266700	1.47006300	1.42752400
C	2.99914900	-1.77703400	2.55854100
H	3.63996300	-1.63651000	3.43954100
H	3.15500600	-2.80293500	2.20373800
H	1.95855900	-1.68185000	2.89869300
C	3.28113400	-0.08993500	-1.38021300
H	2.66411100	-0.30589800	-2.26773500
C	3.40992100	1.42570000	-1.24013600
H	3.69127200	1.86543000	-2.20723000
H	4.20399000	1.68739200	-0.52871200
H	2.48598900	1.91402800	-0.90557100
C	4.65742400	-0.70900000	-1.59713200
H	5.14118200	-0.23722200	-2.46375400
H	4.61905700	-1.78684600	-1.79281700
H	5.31620000	-0.54166700	-0.73434500
C	-3.27988400	-0.09909700	-1.38026300
H	-2.66171600	-0.31123300	-2.26788300
C	-4.65361600	-0.72338800	-1.59876700
H	-5.13930800	-0.25146000	-2.46422500
H	-5.31325600	-0.56103500	-0.73569600
H	-4.61088700	-1.80055500	-1.79716400
C	-3.41510600	1.41581200	-1.23820200
H	-3.70014400	1.85535300	-2.20431700
H	-2.49283700	1.90802300	-0.90480700
H	-4.20910200	1.67303500	-0.52503800
C	-3.33562200	-0.73554200	1.50873700
H	-4.37020700	-0.90707400	1.16955200
C	-2.99530600	-1.78948200	2.55633200
H	-3.63614000	-1.65095400	3.43762800
H	-1.95480400	-1.69394700	2.89662300
H	-3.15035100	-2.81492400	2.19985300
C	-3.22349300	0.65550800	2.12595200
H	-3.89764900	0.73150700	2.99051000
H	-3.49071000	1.45928300	1.43074700
H	-2.19918200	0.84606200	2.47615300
H	0.00522400	-2.65037700	-1.41288900
C	-0.00747300	3.36185600	-1.13405000
C	-0.01002000	4.08111600	0.07513700
C	-0.00836000	3.44722500	1.29889700
C	-0.00274400	2.00870600	1.34820100
C	-0.00367700	1.97849500	-1.03284900
H	0.00128400	-1.24014000	1.63710000
C	-0.00139800	1.09383500	-2.23664500
H	-0.87645700	1.28556800	-2.88177100
H	0.87324100	1.28957700	-2.88116400
C	0.00180500	-0.37849800	-1.84080800
O	0.00431300	-1.21343900	-2.76447800
N	-0.00154800	1.31922300	0.15281000
O	-0.00003400	1.38393500	2.44766400
H	0.00357900	-0.42302800	1.74604100
C	-0.01173200	4.19247300	2.59435100
H	0.86519400	3.93959700	3.20641200
H	-0.01444200	5.27627500	2.42645600
H	-0.88910800	3.93524300	3.20406000
C	-0.00929300	4.04689600	-2.46798100
H	-0.01359900	5.13644200	-2.34526500
H	0.87412300	3.78837700	-3.07164200
H	-0.89016300	3.78147400	-3.07231600
H	-0.01370400	5.17393400	0.04192300

$TS_{3,4}$e (R1=Me, R2=H)

G_{solv} = -3374.854651

Fe	0.00117800	-0.45755400	-0.33171800
P	-2.27573600	-0.66175600	-0.46842400
P	2.27845500	-0.65197600	-0.47339300
N	0.00404400	-2.27764100	-1.33688700
C	-2.41446200	-2.20542300	-1.48930900
H	-3.36354100	-2.73391800	-1.33844200
H	-2.38144500	-1.88999400	-2.54266300
C	-1.21723400	-3.08793400	-1.19489500
H	-1.24444600	-3.48672300	-0.17296600
H	-1.18477800	-3.94555200	-1.88730400
C	1.22904200	-3.08274700	-1.19725000
H	1.19874500	-3.94067000	-1.88937700
H	1.26011100	-3.48125200	-0.17526500

C	2.42179300	-2.19511400	-1.49448600
H	2.38511800	-1.88004300	-2.54783400
H	3.37360200	-2.71927600	-1.34566600
C	3.44985000	-0.93725000	0.97034600
H	4.45534700	-0.75341800	0.56043700
C	3.19503900	0.04924600	2.10581400
H	3.99745000	-0.02604100	2.85275400
H	2.24966800	-0.17487200	2.61488900
H	3.15021100	1.09359500	1.77319100
C	3.42405000	-2.36065500	1.51182100
H	4.12975200	-2.44656500	2.34945100
H	3.71107600	-3.11130600	0.76652400
H	2.43413500	-2.63106300	1.89915900
C	3.24828400	0.56469900	-1.52256300
H	2.58027900	0.71424200	-2.38514600
C	3.45216500	1.90851500	-0.82785500
H	3.77958900	2.66240600	-1.55755600
H	4.23595300	1.84354300	-0.06081200
H	2.54163600	2.28627000	-0.34484100
C	4.57803200	0.03978400	-2.05277700
H	5.04339800	0.79973300	-2.69609400
H	4.46618600	-0.86966900	-2.65397300
H	5.29109800	-0.17414700	-1.24519200
C	-3.25412300	0.55021500	-1.51529800
H	-2.58923900	0.70296700	-2.37970800
C	-4.58262500	0.01875200	-2.04213200
H	-5.05306300	0.77639500	-2.68448700
H	-5.29268500	-0.19828700	-1.23272900
H	-4.46795100	-0.89027400	-2.64343000
C	-3.46320200	1.89318600	-0.82045700
H	-3.79589000	2.64516300	-1.54976800
H	-2.55360900	2.27569700	-0.33939900
H	-4.24514500	1.82464900	-0.05185500
C	-3.44221500	-0.95158200	0.97832800
H	-4.44945200	-0.77076600	0.57133900
C	-3.41077400	-2.37508300	1.51924200
H	-4.11354700	-2.46319100	2.35910600
H	-2.41895100	-2.64329100	1.90320100
H	-3.69834900	-3.12608700	0.77449900
C	-3.18719700	0.03579200	2.11298400
H	-3.98717200	-0.04185900	2.86229400
H	-3.14673400	1.08018700	1.77992500
H	-2.23955400	-0.18507300	2.61928000
H	0.00227100	-1.89675600	-2.29474700
C	-0.01255600	3.77884900	-0.31559300
C	-0.00785200	4.13416600	1.03757400
C	-0.00027200	3.17547100	2.03831200
C	0.00081600	1.83295000	1.62381500
C	-0.00776800	2.42121100	-0.62038900
H	0.00532400	-1.30283300	1.18950500
C	-0.00907200	1.90757900	-2.01758900
H	-0.88620000	2.27600800	-2.57669900
H	0.86374000	2.28152000	-2.57984600
C	-0.00380500	0.37714300	-2.04421500
O	-0.00399100	-0.14651000	-3.17589900
N	-0.00181400	1.45891800	0.33791700
O	0.00483500	0.88755500	2.55936900
H	0.00505200	0.00716000	2.09621300
C	0.00730400	-2.51522800	2.49341100
O	0.00897000	-3.55110200	1.91354700
O	0.00656200	-1.83397700	3.46543300
C	0.00540300	3.51018000	3.49447900
H	0.00542800	4.59523400	3.64258100
H	-0.87178500	3.09383200	4.00635900
H	0.88720700	3.09482300	3.99917700
C	-0.02807900	4.80886600	-1.40260600
H	-0.93361600	4.73229100	-2.02138900
H	0.00429800	5.82053900	-0.98379600
H	0.82926600	4.69942000	-2.08137700
H	-0.01008800	5.18943700	1.31532700

1f (R1=Me, R2=Me)

G_{solv} = -3224.453422

Fe	0.02551500	-0.80555200	-0.09002100
P	-2.23776800	-1.12413100	-0.00891900
P	2.30530900	-0.97510700	-0.02531200
N	0.09245300	-2.88293800	-0.37308700
C	-2.35924400	-2.94149300	-0.38222600
H	-3.24667900	-3.39940000	0.07448400
H	-2.46403000	-3.04032100	-1.47293400
C	-1.09138500	-3.63692000	0.07265500
H	-1.04456800	-3.69769100	1.16890500
H	-1.05333700	-4.67054300	-0.30887100
C	1.32765300	-3.55601400	0.06279600
H	1.35448900	-4.59070000	-0.31661100
H	1.29498200	-3.61673700	1.15951700
C	2.54252000	-2.77916900	-0.40479100
H	2.64100600	-2.86864800	-1.49691300
H	3.46286100	-3.17902000	0.04105800
C	3.23380600	-0.76470200	1.58454100
H	4.24915000	-1.15384400	1.40348500
C	3.31717600	0.69293600	2.02519600
H	3.88809100	0.76057900	2.96189600
H	2.31124900	1.08990500	2.21983000
H	3.81471000	1.33718700	1.29285700
C	2.57465800	-1.59333800	2.68286000
H	3.09003900	-1.42128600	3.63793300
H	2.61213600	-2.67126400	2.48633200
H	1.52507500	-1.29115400	2.81591200
C	3.37999800	-0.19798900	-1.34284300
H	2.86896600	-0.54452500	-2.25663100
C	3.37378300	1.33083700	-1.34769500
H	3.62069900	1.70221700	-2.35168200
H	4.13417900	1.73246300	-0.66679800
H	2.40905300	1.76370400	-1.05654500
C	4.81156100	-0.72047800	-1.36490300
H	5.34664300	-0.30404200	-2.22972200
H	4.86778400	-1.81311700	-1.43954300
H	5.36265400	-0.41160300	-0.46610700
C	-3.36898300	-0.42054800	-1.32008300
H	-2.84488700	-0.74095800	-2.23600700
C	-4.76631900	-1.02928100	-1.32975200
H	-5.33367900	-0.64469500	-2.18878600
H	-5.32728500	-0.75744100	-0.42515400

H	-4.75614300	-2.12308500	-1.40753700
C	-3.45356700	1.10638500	-1.33312400
H	-3.72198900	1.45704100	-2.33911500
H	-2.51623500	1.59828700	-1.04479700
H	-4.23662100	1.46578300	-0.65438600
C	-3.15910000	-0.97060000	1.61087900
H	-4.13906800	-1.45000000	1.45265600
C	-2.40955700	-1.71961200	2.70885500
H	-2.92508200	-1.58467900	3.66982400
H	-1.39141800	-1.31749000	2.82089200
H	-2.34888500	-2.79872300	2.52476000
C	-3.36400800	0.48111000	2.02899800
H	-3.89997500	0.51483800	2.98781800
H	-3.95187600	1.05745100	1.30730800
H	-2.39528700	0.97843300	2.17415400
H	0.08774300	-2.85939800	-1.40197100
C	-0.11998600	3.21014200	-1.11991300
C	-0.14576100	3.85207800	0.14904300
C	-0.08332600	3.11137800	1.32777100
C	-0.04216900	1.67760600	1.25738800
C	-0.06262700	1.82421100	-1.12472200
C	-0.03898300	0.93435400	-2.33463100
H	-0.92352600	1.08621600	-2.97531700
H	0.82953900	1.13920500	-2.98242400
C	0.01065600	-0.55455800	-1.92700400
O	0.03585600	-1.39436500	-2.84297400
N	-0.03175500	1.11556500	0.01727700
O	-0.01634800	0.89398400	2.25645100
C	-0.23567900	5.35127800	0.19929600
H	0.75356400	5.81800900	0.08064500
H	-0.86798100	5.74344800	-0.60537600
H	-0.65122500	5.70886600	1.14619800
C	-0.05906300	3.73714300	2.69059700
H	0.56314800	4.63976500	2.72770000
H	-1.06342100	4.02040800	3.04237900
H	0.33738400	3.01733000	3.41508300
C	-0.15830800	3.99314300	-2.40119800
H	-1.14694100	4.43779100	-2.59485600
H	0.56424900	4.82050300	-2.40120700
H	0.08082600	3.36109900	-3.26342100

2f (R1=Me, R2=Me)

G_{solv} = -3225.623750

Fe	-0.25868700	-0.79525600	0.02801200
P	-2.49686300	-0.34982300	-0.02187500
P	1.85437000	-1.66960100	-0.02806100
N	-0.84864200	-2.74449800	-0.39790600
C	-3.17108400	-2.00965100	-0.50866800
H	-4.19499500	-2.16859200	-0.14736600
H	-3.20380800	-2.03155200	-1.60795400
C	-2.22809700	-3.08790300	-0.01313100
H	-2.25765900	-3.17541900	1.08228300
H	-2.50480000	-4.07126900	-0.42719500
C	0.09923100	-3.79298400	0.01371500
H	-0.21759000	-4.77056600	-0.38507600
H	0.06522800	-3.86205800	1.11047200
C	1.48831100	-3.43569500	-0.47642400
H	1.51571300	-3.50401300	-1.57389400
H	2.24389300	-4.13016100	-0.08715900
C	2.92564900	-1.82906000	1.49908200
H	3.84266100	-2.33902800	1.16207900
C	3.28167200	-0.46760200	2.08779500
H	3.94654500	-0.60128000	2.95261500
H	2.37725800	0.05439800	2.43157400
H	3.79639900	0.18801100	1.37678300
C	2.26611800	-2.69327300	2.56765100
H	2.92716800	-2.76450900	3.44205700
H	2.06617800	-3.71684700	2.22885700
H	1.32104700	-2.25163800	2.91256500
C	3.04758400	-1.19942600	-1.39282000
H	2.39105700	-1.24780700	-2.27696400
C	3.59398400	0.22276600	-1.27970100
H	3.96044400	0.56072300	-2.25925700
H	4.44694300	0.26326300	-0.59010500
H	2.84867300	0.94896200	-0.93235100
C	4.19496200	-2.18183500	-1.59904000
H	4.77377100	-1.89120000	-2.48690700
H	3.85695200	-3.21317000	-1.75359600
H	4.89102300	-2.17452100	-0.74924600
C	-3.23858000	0.74110600	-1.34964000
H	-2.69686700	0.40047100	-2.24699200
C	-4.72913100	0.52397700	-1.58628000
H	-5.06282300	1.14796500	-2.42701700
H	-5.32702900	0.81793900	-0.71296400
H	-4.97759200	-0.51431100	-1.83413600
C	-2.95161500	2.22731500	-1.14949700
H	-3.11678000	2.76876500	-2.09151000
H	-1.92376100	2.43050000	-0.82328700
H	-3.63294200	2.66335600	-0.40704400
C	-3.45798300	0.08945500	1.52475300
H	-4.49134000	0.27621900	1.18961400
C	-3.48157300	-1.05715700	2.52931800
H	-4.04176100	-0.75025300	3.42301500
H	-2.46722300	-1.32058600	2.85997400
H	-3.96442000	-1.96110200	2.13909100
C	-2.90298900	1.34321800	2.19388600
H	-3.52105400	1.60176700	3.06515300
H	-2.88851800	2.21636900	1.53182100
H	-1.87358300	1.17917900	2.54185100
H	-0.81748100	-2.67674900	-1.42660300
C	0.93944400	3.07941500	-1.12736300
C	1.21815600	3.76767500	0.08175200
C	1.01175900	3.13802600	1.30104900
C	0.56193800	1.76896300	1.34224400
C	0.50866800	1.76518300	-1.03218000
H	-0.43048000	-1.32796200	1.63051900
C	0.22835800	0.92119000	-2.23646800
H	-0.58187500	1.34716400	-2.85280000
H	1.10004400	0.86860700	-2.91097200
C	-0.17365000	-0.49551400	-1.84304800
O	-0.40769300	-1.29339400	-2.77055700
N	0.32612100	1.12266500	0.14773600
O	0.39002800	1.15063700	2.43355500
H	-0.17300200	-0.55179700	1.74063600

C	1.73593500	5.17666600	0.02192300
H	0.94234200	5.88486000	-0.25704600
H	2.14666600	5.50812500	0.97932400
H	2.52832000	5.27953600	-0.72967600
C	1.25425400	3.82511800	2.61439900
H	2.32411800	3.98971700	2.81183800
H	0.76481900	4.80649800	2.66768800
H	0.86541400	3.20573700	3.42747100
C	1.14372500	3.72281300	-2.47036300
H	0.97769000	4.80553200	-2.43788100
H	2.16386500	3.56749500	-2.85900500
H	0.45509500	3.32142700	-3.22300300

$TS_{3,4}$f (R1=Me, R2=Me)

G_{solv} = -3414.114136

Fe	-0.59893200	0.21964900	-0.30693700
P	0.03544600	2.41716700	-0.44343800
P	-1.62852200	-1.82409300	-0.42455400
N	-2.37650100	0.91301300	-1.14062500
C	-1.43394400	3.13994800	-1.31655500
H	-1.56036000	4.21174300	-1.12194000
H	-1.25019400	3.02336500	-2.39490400
C	-2.66372400	2.34187700	-0.93015700
H	-2.92722200	2.48382500	0.12552500
H	-3.53353500	2.64669600	-1.53569300
C	-3.55926900	0.06482600	-0.91756000
H	-4.40563200	0.42682300	-1.52493200
H	-3.84692800	0.15173600	0.13801200
C	-3.20259200	-1.36050500	-1.29203000
H	-2.99423600	-1.40867100	-2.37121400
H	-4.02432300	-2.05781700	-1.08932000
C	-2.18952700	-2.86028500	1.04187000
H	-2.41542900	-3.85289500	0.62144600
C	-1.07986400	-3.00812700	2.07796400
H	-1.36825300	-3.75601300	2.82948900
H	-0.90651700	-2.06175300	2.60453100
H	-0.12211500	-3.32428300	1.64667900
C	-3.45593300	-2.34310900	1.71163100
H	-3.70634900	-2.98488700	2.56759700
H	-4.32491400	-2.33916200	1.04373000
H	-3.32694400	-1.32608000	2.10184900
C	-0.95321200	-3.13501300	-1.58481800
H	-0.65205000	-2.53978800	-2.46093200
C	0.28158400	-3.83528200	-1.02437500
H	0.78436700	-4.40307300	-1.81984900
H	0.00690300	-4.55431500	-0.24059600
H	1.01607100	-3.13961500	-0.59817600
C	-1.97258400	-4.16760500	-2.05319500
H	-1.49940600	-4.85113600	-2.77215000
H	-2.83695100	-3.71775700	-2.55481900
H	-2.34444300	-4.78576900	-1.22497500
C	1.42312900	2.91207200	-1.60607400
H	1.23751100	2.26557300	-2.47801600
C	1.37893800	4.35945500	-2.08354000
H	2.18339700	4.53109200	-2.81253000
H	1.53946100	5.07024700	-1.26182300
H	0.43496400	4.61875200	-2.57630700
C	2.80557400	2.58851000	-1.04586200
H	3.55809800	2.64676500	-1.84510900
H	2.86811300	1.58551200	-0.60475200
H	3.09948900	3.31313000	-0.27410500
C	0.32317800	3.56745700	1.01683800
H	0.82961900	4.44848600	0.59234700
C	-0.95990200	4.04782000	1.68261400
H	-0.71063900	4.70116600	2.53009600
H	-1.54804900	3.21322200	2.08326200
H	-1.60641500	4.62179600	1.00888700
C	1.23740900	2.93017500	2.05834600
H	1.52317600	3.67712200	2.81178600
H	2.16099700	2.51966700	1.63217100
H	0.72604100	2.11272600	2.58157300
H	-2.10908700	0.80254200	-2.13002700
C	3.35102800	-1.28461900	-0.67657600
C	3.84032900	-1.41836800	0.63973300
C	3.00559900	-1.11677300	1.71873700
C	1.71033300	-0.65570700	1.42835900
C	2.05539300	-0.81246200	-0.85462600
H	-1.24159800	0.48592400	1.29070200
C	1.44654000	-0.59434100	-2.19851700
H	2.05993900	0.08903900	-2.81008500
H	1.40335200	-1.53393300	-2.77475900
C	0.02839800	-0.03061300	-2.08528200
O	-0.55129200	0.19763900	-3.16591400
N	1.24260500	-0.49408900	0.18364100
O	0.89685100	-0.35074100	2.43779200
H	0.04253500	-0.02645900	2.04331800
C	-2.26855000	0.87576900	2.69602300
O	-3.26615100	1.28735700	2.20134100
O	-1.56995400	0.57878100	3.60787800
C	5.24912200	-1.87474200	0.87130300
H	5.57351800	-1.70964800	1.90158400
H	5.36118400	-2.94717300	0.65913000
H	5.95011800	-1.34736600	0.21359700
C	3.44156400	-1.26555200	3.14680900
H	3.81840400	-2.27598700	3.34918500
H	4.24734300	-0.56416700	3.40198600
H	2.61209000	-1.07487400	3.83135900
C	4.20344800	-1.60513400	-1.87014000
H	4.74407100	-0.71778700	-2.23462600
H	4.95313400	-2.37066100	-1.64610300
H	3.60293000	-1.97765000	-2.70724500

1g (R1=Me, R2=OH)

G_{solv} = -3260.397876

Fe	0.05032300	-0.80047000	-0.09153100
P	-2.20636200	-1.17340500	-0.01324800
P	2.33334700	-0.91641700	-0.01810100
N	0.16680500	-2.87557100	-0.37667900
C	-2.28245600	-2.99415200	-0.38212300
H	-3.15795200	-3.47305600	0.07607700
H	-2.38519700	-3.09858300	-1.47254200
C	-0.99758400	-3.65705800	0.07321800
H	-0.94792900	-3.71360800	1.16969300
H	-0.93524000	-4.69055400	-0.30544900

C	1.41912900	-3.52090500	0.05275900
H	1.47119200	-4.55181600	-0.33416100
H	1.38932200	-3.59028700	1.14894900
C	2.61430500	-2.71135700	-0.41005100
H	2.71500600	-2.79051000	-1.50277700
H	3.54404900	-3.09194100	0.03318100
C	3.24609400	-0.69650200	1.59931900
H	4.27081300	-1.06288100	1.42357000
C	3.29449200	0.76072300	2.04587700
H	3.85145300	0.83663600	2.99030900
H	2.27835900	1.13712800	2.22752200
H	3.78893900	1.41706900	1.32225700
C	2.59774300	-1.54383200	2.68996400
H	3.09969300	-1.36089400	3.65015300
H	2.66444500	-2.62009500	2.49213900
H	1.53964500	-1.26903400	2.81459500
C	3.39792300	-0.10259200	-1.32140500
H	2.90392800	-0.45686600	-2.24155800
C	3.35046800	1.42554700	-1.31659200
H	3.58645200	1.81049200	-2.31800500
H	4.09993400	1.84317200	-0.63325300
H	2.37498800	1.83053500	-1.02165800
C	4.84322800	-0.58601500	-1.33422500
H	5.37457200	-0.14909100	-2.19121100
H	4.93011000	-1.67609800	-1.41536700
H	5.37742000	-0.26811200	-0.42839300
C	-3.34994500	-0.50167200	-1.33047300
H	-2.81317000	-0.80951900	-2.24338900
C	-4.73132700	-1.14568000	-1.34635900
H	-5.30414800	-0.77482600	-2.20784100
H	-5.30325600	-0.88834900	-0.44439600
H	-4.69381300	-2.23879600	-1.42473500
C	-3.47379000	1.02231800	-1.34663500
H	-3.74658100	1.36440600	-2.35429600
H	-2.55084200	1.53871300	-1.05541100
H	-4.26842900	1.36304300	-0.67176300
C	-3.13753100	-1.03972500	1.60277400
H	-4.10376000	-1.54491100	1.44050500
C	-2.37414100	-1.76736100	2.70553700
H	-2.89979000	-1.64835500	3.66309600
H	-1.36873200	-1.33661900	2.82483100
H	-2.28034500	-2.84399100	2.52093300
C	-3.38258100	0.40669700	2.01709200
H	-3.92219900	0.42822000	2.97420700
H	-3.98339800	0.96557100	1.29239700
H	-2.42821000	0.93061300	2.16362600
H	0.15751500	-2.85106300	-1.40547100
C	-0.19102200	3.21179400	-1.14190700
C	-0.24074900	3.82980600	0.12880300
C	-0.19847300	3.12094000	1.32289800
C	-0.09759600	1.69289600	1.25808300
C	-0.10003900	1.82829100	-1.12817000
C	-0.04112400	0.93941900	-2.33637000
H	-0.91937300	1.07332500	-2.98896600
H	0.83214700	1.16550200	-2.97041300
C	0.03655800	-0.54825700	-1.92794300
O	0.08143500	-1.38629700	-2.84459900
N	-0.05786800	1.12465300	0.01701400
O	-0.04634000	0.91943000	2.26138600
C	-0.25962000	3.80423700	2.65464500
H	0.59640300	4.47323500	2.83396800
H	-1.17569400	4.40019600	2.78894000
H	-0.24842800	3.04623400	3.44431500
C	-0.24519500	4.02812000	-2.39682200
H	-1.20419700	4.55457600	-2.50591300
H	0.53524000	4.80065000	-2.41415700
H	-0.11118200	3.40280500	-3.28578200
O	-0.33784600	5.18915500	0.11950800
H	-0.36411800	5.52133200	1.02761100

2g (R1=Me, R2=OH)

G_{solv} = -3261.566559

Fe	-0.04317200	-0.83330900	0.03667000
P	-2.32417200	-0.94232400	-0.01426000
P	2.21644200	-1.16291600	-0.02596400
N	-0.14301800	-2.86603400	-0.38447400
C	-2.57614800	-2.72483900	-0.47239100
H	-3.52504700	-3.12480200	-0.09282100
H	-2.61714200	-2.77155000	-1.57056500
C	-1.39190100	-3.53387500	0.01908600
H	-1.38761700	-3.61579600	1.11541100
H	-1.42258400	-4.55888400	-0.38512300
C	1.03748400	-3.65172300	0.01260200
H	0.96639500	-4.67496600	-0.39101900
H	1.03094300	-3.73260400	1.10894100
C	2.29210300	-2.96156100	-0.48529200
H	2.32391100	-3.01241500	-1.58362600
H	3.19871200	-3.45208500	-0.10865200
C	3.29130600	-1.05577500	1.50365900
H	4.31334400	-1.29006700	1.16404000
C	3.26269300	0.34088700	2.11616300
H	3.93332100	0.37730300	2.98622000
H	2.24957600	0.59650400	2.45761100
H	3.58715700	1.12280800	1.42069100
C	2.88959400	-2.08511100	2.55384900
H	3.54220400	-1.98734100	3.43193400
H	2.97713900	-3.11840600	2.19725000
H	1.85897800	-1.92321900	2.89880000
C	3.25920700	-0.40570300	-1.38468500
H	2.63258500	-0.59567800	-2.27142500
C	3.45757100	1.10305700	-1.25092100
H	3.75455700	1.52618000	-2.22073500
H	4.26500900	1.33182500	-0.54328600
H	2.55844700	1.63422100	-0.91475300
C	4.60548300	-1.08823100	-1.59927800
H	5.10867400	-0.64464100	-2.46973100
H	4.51833900	-2.16461000	-1.78740500
H	5.27247100	-0.94506200	-0.73844300
C	-3.30091300	-0.08754800	-1.36375200
H	-2.70084900	-0.32904200	-2.25631500
C	-4.70582600	-0.64171600	-1.57311100
H	-5.17324700	-0.14489900	-2.43468300
H	-5.34996600	-0.44752100	-0.70489300
H	-4.71758600	-1.71945100	-1.77275100

C	-3.35767400	1.43179100	-1.21788900
H	-3.61961900	1.88919900	-2.18223800
H	-2.41112600	1.87393300	-0.88304900
H	-4.13681200	1.72771400	-0.50337600
C	-3.37232200	-0.73060100	1.52247900
H	-4.41511900	-0.85594100	1.18806300
C	-3.07390500	-1.80001600	2.56711000
H	-3.70527500	-1.63567300	3.45083400
H	-2.02896400	-1.75024700	2.90361500
H	-3.27412400	-2.81715300	2.20952000
C	-3.19423200	0.65306300	2.14000100
H	-3.85354500	0.75636500	3.01317300
H	-3.43575500	1.46834100	1.44881100
H	-2.15838900	0.79994300	2.47738400
H	-0.14145800	-2.79612500	-1.41347800
C	0.14790000	3.20697500	-1.15728200
C	0.20611800	3.93168100	0.05021000
C	0.18876500	3.30419500	1.28510600
C	0.10336100	1.87226900	1.34357300
C	0.07766800	1.82801000	-1.03150300
H	-0.06923900	-1.38530700	1.64270600
C	0.01825400	0.94160700	-2.23328500
H	-0.86372100	1.16946000	-2.85670800
H	0.88339400	1.10276600	-2.89907200
C	-0.03557100	-0.52937600	-1.83704800
O	-0.07299700	-1.36232200	-2.76208300
N	0.05705500	1.17166100	0.15193300
O	0.07341400	1.24637500	2.44186800
H	-0.02530400	-0.56892800	1.74648400
C	0.25553800	4.09493300	2.55675400
H	1.17229000	4.70010300	2.63468300
H	-0.60001900	4.77715500	2.68145400
H	0.24764600	3.40806300	3.40771900
C	0.16340200	3.87204200	-2.50101900
H	0.18487800	4.96123500	-2.40435200
H	1.04101900	3.57830700	-3.09673000
H	-0.72392300	3.61217700	-3.09744700
O	0.28340500	5.28744100	-0.04748100
H	0.31730000	5.67551500	0.83783300

$TS_{3,4}$g (R1=Me, R2=OH)

G_{solv} = -3450.055357

Fe	0.63325600	0.00507900	-0.30851300
P	0.86580100	-2.27135200	-0.43226500
P	0.82430900	2.28603400	-0.43505700
N	2.53763100	0.02210400	-1.14496300
C	2.49960600	-2.39737900	-1.30461700
H	3.01854400	-3.34219700	-1.10273500
H	2.28506200	-2.36717900	-2.38313500
C	3.33982600	-1.19320200	-0.92729300
H	3.63715200	-1.21981900	0.12838700
H	4.26060200	-1.15261400	-1.53282400
C	3.31730600	1.25257600	-0.92967500
H	4.23795100	1.22940800	-1.53635000
H	3.61598800	1.28561800	0.12578400
C	2.45414300	2.43961000	-1.30935500
H	2.23946700	2.40129700	-2.38759300
H	2.95649300	3.39425300	-1.11148200
C	0.96431100	3.45892900	1.02833500
H	0.80419000	4.46355100	0.60642300
C	-0.11822700	3.18279000	2.06654600
H	-0.12084100	3.97716500	2.82583100
H	0.06980200	2.23357700	2.58329100
H	-1.12685600	3.13093100	1.63873000
C	2.33197400	3.44902300	1.69821300
H	2.33184300	4.15284800	2.54181500
H	3.14427100	3.74727300	1.02539500
H	2.57713300	2.46077500	2.10567100
C	-0.29698600	3.24713800	-1.59349200
H	-0.35869300	2.58027000	-2.46749700
C	-1.70280000	3.43550000	-1.03005000
H	-2.38429500	3.76785400	-1.82583700
H	-1.71914600	4.20947900	-0.25054800
H	-2.11926800	2.51634700	-0.59806200
C	0.26063700	4.58398100	-2.06959400
H	-0.43692000	5.03730600	-2.78788700
H	1.22809700	4.48706300	-2.57529700
H	0.37921900	5.30084400	-1.24569900
C	-0.23662300	-3.25259800	-1.59232200
H	-0.30759500	-2.58485100	-2.46514100
C	0.34697100	-4.57849500	-2.06843500
H	-0.34366000	-5.04974000	-2.78178700
H	0.48533700	-5.28988300	-1.24304400
H	1.30969500	-4.46111100	-2.57868500
C	-1.63995800	-3.46980700	-1.03184100
H	-2.31568200	-3.80497800	-1.83136500
H	-2.07324600	-2.56403400	-0.58839900
H	-1.64309800	-4.25334200	-0.26171600
C	1.02453500	-3.44118600	1.03174400
H	0.89298000	-4.44899700	0.60778400
C	2.38818200	-3.39715900	1.70904900
H	2.39965300	-4.09424900	2.55817000
H	2.60952200	-2.40054900	2.10965100
H	3.21007800	-3.68248800	1.04244500
C	-0.07106900	-3.19415000	2.06369300
H	-0.06523200	-3.99463800	2.81641300
H	-1.07716800	-3.15761200	1.62885400
H	0.09333200	-2.24562000	2.58970600
H	2.24645400	0.01863200	-2.13371000
C	-3.59474100	-0.03393500	-0.68834600
C	-4.07504800	-0.03262500	0.63100600
C	-3.20719400	-0.02602800	1.72299500
C	-1.83744500	-0.01696700	1.43255700
C	-2.21535500	-0.02200300	-0.85102500
H	1.32887200	0.00906900	1.28772600
C	-1.57550000	-0.01697400	-2.19622700
H	-1.88591400	-0.89581400	-2.78693200
H	-1.90378700	0.85322200	-2.78984000
C	-0.04763300	-0.00224100	-2.08624400
O	0.57292000	0.00101500	-3.16819700
N	-1.34167400	-0.01352500	0.18648700
O	-0.97384700	-0.01041800	2.44355700
H	-0.05825500	-0.00454200	2.05212400
C	2.42483200	0.02260100	2.69208900

O	3.50443900	0.04203800	2.19892600
O	1.66506900	0.00696900	3.60360300
C	-3.71863500	-0.02512800	3.13067200
H	-4.31498900	0.87143100	3.35376500
H	-4.34488100	-0.90362000	3.34315200
H	-2.89194300	-0.04391700	3.84405100
C	-4.51219400	-0.04203700	-1.87218600
H	-4.30067000	-0.88944400	-2.53895400
H	-5.55929400	-0.11218600	-1.56706300
H	-4.40119200	0.87139100	-2.47388600
O	-5.41629500	-0.03841900	0.80744700
H	-5.63289600	-0.03941700	1.75092300

1h (R1=Me, R2=OMe)

G_{solv} = -3299.632178

Fe	-0.85345600	0.44292600	-0.08255100
P	0.12501800	2.51337900	-0.02177200
P	-2.24289200	-1.37271800	0.00209900
N	-2.63040900	1.52421300	-0.35336500
C	-1.33310500	3.60557500	-0.39022200
H	-1.22515800	4.60268300	0.05672100
H	-1.37103600	3.73768800	-1.48184900
C	-2.60351000	2.92928400	0.08614000
H	-2.66386700	2.92678300	1.18341800
H	-3.49345600	3.46397400	-0.28448200
C	-3.86320900	0.86262400	0.10625600
H	-4.74959700	1.40422500	-0.26283800
H	-3.87780500	0.93167000	1.20296500
C	-3.88758600	-0.58237400	-0.35217300
H	-4.03856800	-0.62224300	-1.44118600
H	-4.71706900	-1.13047600	0.11384300
C	-2.55169200	-2.25763700	1.62039300
H	-3.44227700	-2.88665700	1.45842100
C	-1.37694800	-3.13445000	2.04040300
H	-1.60395800	-3.61592600	3.00185000
H	-0.47389800	-2.52470000	2.18147700
H	-1.15607900	-3.93093500	1.32245000
C	-2.85478400	-1.24371600	2.71949700
H	-2.98031400	-1.76242500	3.67984100
H	-3.77538000	-0.67735300	2.53624500
H	-2.01835300	-0.53824500	2.83410200
C	-2.19489900	-2.70027900	-1.31242500
H	-2.21997300	-2.08720800	-2.22884300
C	-0.90824600	-3.52629800	-1.32972600
H	-0.73931700	-3.93391600	-2.33573400
H	-0.97890300	-4.38362600	-0.64937800
H	-0.01674800	-2.95379100	-1.04537900
C	-3.41216200	-3.61741200	-1.31266300
H	-3.35540200	-4.31269100	-2.16176900
H	-4.35919300	-3.07109600	-1.39816900
H	-3.45254700	-4.22796700	-0.40021500
C	1.32393400	3.06490900	-1.34663600
H	0.76603800	2.79057300	-2.25759400
C	1.57538000	4.56809800	-1.37090000
H	2.20262700	4.82640700	-2.23549100
H	2.11555500	4.89612800	-0.47231800
H	0.65381100	5.15708500	-1.44851800
C	2.65280600	2.30746700	-1.36074700
H	3.08771800	2.33719100	-2.36925100
H	2.56051800	1.25468500	-1.06706400
H	3.38271800	2.77505300	-0.68867700
C	0.77359600	3.21892400	1.58440600
H	0.91612900	4.29752900	1.40705200
C	-0.25804900	3.03111800	2.69236400
H	0.14808800	3.39907000	3.64467300
H	-0.49061100	1.96382300	2.82490800
H	-1.18943500	3.57872000	2.50669700
C	2.09709300	2.59143000	2.00840600
H	2.42805400	3.04161800	2.95478500
H	2.89968400	2.74132400	1.27888500
H	1.97102400	1.51353400	2.18132300
H	-2.62307600	1.50983400	-1.38230600
C	2.60034100	-1.58572100	-1.18303600
C	3.17013400	-1.88025800	0.07871600
C	2.56271400	-1.54937900	1.27959400
C	1.31705100	-0.83758600	1.23198100
C	1.39108100	-0.90697900	-1.15489100
C	0.60123600	-0.46273000	-2.35080400
H	1.19196500	0.18787700	-3.01643400
H	0.28859500	-1.31502400	-2.97643500
C	-0.66547200	0.30870300	-1.92316400
O	-1.40058400	0.73663300	-2.82917100
N	0.79990100	-0.55432700	0.00211500
O	0.67540700	-0.45178500	2.25309900
C	3.13443200	-1.89016400	2.61702700
H	3.97635400	-2.58510800	2.53263300
H	3.47782300	-0.99359200	3.15439600
H	2.36671200	-2.34915000	3.25403000
C	3.28220000	-1.99624000	-2.45326700
H	4.32080400	-1.64201200	-2.50039500
H	3.32296100	-3.08893800	-2.56301900
H	2.76255100	-1.59877500	-3.33157100
O	4.37890700	-2.54338300	0.08260500
C	5.48588900	-1.66934100	0.23099000
H	5.47836900	-1.16836700	1.21038600
H	6.39413500	-2.27308700	0.14579400
H	5.49212300	-0.89648600	-0.55319800

2h (R1=Me, R2=OMe)

G_{solv} = -3300.802162

Fe	-0.87426800	0.46175900	0.03108700
P	0.23104000	2.46300300	-0.03469200
P	-2.33282000	-1.29017100	-0.01682400
N	-2.55189100	1.60727300	-0.40196900
C	-1.15742400	3.60421300	-0.50445800
H	-1.00162300	4.62685200	-0.13782800
H	-1.17871100	3.64981000	-1.60334200
C	-2.46537700	3.02274700	-0.00476500
H	-2.53341600	3.06703700	1.09159100
H	-3.32307300	3.58470100	-0.40909800
C	-3.84118500	1.01486300	-0.00681300
H	-4.67393800	1.60503300	-0.42271500
H	-3.91411200	1.07414700	1.08854300
C	-3.90524600	-0.42091300	-0.49010100

H	-3.96297200	-0.43367300	-1.58840300
H	-4.79747500	-0.93489500	-0.11013600
C	-2.80737900	-2.24496400	1.52165100
H	-3.53907000	-2.99832300	1.18708200
C	-1.60281000	-2.94089100	2.14797500
H	-1.92307200	-3.51276800	3.03019800
H	-0.85247400	-2.20582400	2.47229400
H	-1.10808200	-3.64170400	1.46641300
C	-3.48256700	-1.35422500	2.55827000
H	-3.74985200	-1.95385100	3.43895300
H	-4.40556500	-0.89111900	2.18978000
H	-2.80857500	-0.55789500	2.90318000
C	-2.21840400	-2.58796900	-1.36070400
H	-2.04987500	-1.96172100	-2.25188000
C	-1.02788100	-3.53299500	-1.20790800
H	-0.81098500	-4.01723200	-2.17025800
H	-1.25054100	-4.33475500	-0.49206700
H	-0.11225000	-3.03037700	-0.87164200
C	-3.49622500	-3.38994200	-1.58099100
H	-3.37160600	-4.04653300	-2.45332900
H	-4.37302800	-2.75981400	-1.77029300
H	-3.72105000	-4.03849900	-0.72354300
C	1.47494600	2.83540900	-1.38584700
H	0.97200900	2.41482800	-2.27196100
C	1.70935000	4.32127200	-1.63534600
H	2.38858500	4.44735600	-2.48996300
H	2.18723800	4.80759600	-0.77415000
H	0.78931600	4.86916200	-1.86842300
C	2.81451500	2.12221200	-1.20955000
H	3.35858900	2.11366400	-2.16473800
H	2.71506600	1.08233000	-0.87352300
H	3.44862100	2.65113000	-0.48573700
C	0.95875900	3.25916300	1.49704400
H	1.41257000	4.20230000	1.15129500
C	-0.11482000	3.59435100	2.52652100
H	0.35247100	4.05499300	3.40749900
H	-0.63295400	2.68895900	2.87206500
H	-0.86492300	4.30067300	2.15111100
C	2.02993600	2.38490600	2.14405700
H	2.46630800	2.91428500	3.00262600
H	2.85123800	2.13112000	1.46422800
H	1.59852300	1.44257700	2.51039200
H	-2.48967700	1.56513700	-1.43053800
C	2.56563500	-1.66979200	-1.12620800
C	3.21711800	-1.97221800	0.08949100
C	2.65891400	-1.66463000	1.31502800
C	1.38892800	-0.99105000	1.35414700
C	1.36283400	-0.98885800	-1.02090600
H	-1.33499000	0.78940200	1.63214600
C	0.60620100	-0.54201100	-2.22952600
H	1.23959100	0.05913700	-2.90439300
H	0.27591200	-1.40051600	-2.83966100
C	-0.61861200	0.27874800	-1.84215900
O	-1.30815000	0.73758600	-2.77194000
N	0.79254200	-0.64483100	0.15880400
O	0.83827900	-0.69249500	2.45162400
H	-0.66559500	0.32204300	1.74371600
C	3.32701100	-1.96969900	2.61599200
H	2.66523700	-2.55176300	3.27055300
H	4.25349300	-2.53389900	2.46964100
H	3.56308000	-1.04757400	3.16714400
C	3.15810500	-2.00593000	-2.46151700
H	4.02645400	-2.66322800	-2.35106800
H	2.43509500	-2.52039300	-3.10991600
H	3.48877900	-1.10786400	-3.00764100
O	4.44676900	-2.59160900	0.03997700
C	5.51532500	-1.66299300	-0.04211300
H	5.41610900	-1.01149100	-0.92457700
H	5.56182400	-1.02832900	0.85631600
H	6.44343000	-2.23625000	-0.12420400

$TS_{3,4}$h (R1=Me, R2=OMe)

G_{solv} = -3489.288883

Fe	-0.75626300	0.24049800	-0.30272600
P	0.03492700	2.38377400	-0.48636500
P	-1.92810800	-1.72228000	-0.35315800
N	-2.50580300	1.05172900	-1.07857200
C	-1.41150300	3.20336100	-1.31194500
H	-1.45373600	4.28326200	-1.12530900
H	-1.27668600	3.06485200	-2.39481500
C	-2.68139400	2.49952000	-0.87368100
H	-2.89728400	2.66956600	0.18860700
H	-3.54687400	2.86232900	-1.45284200
C	-3.73646200	0.29073700	-0.80413400
H	-4.57723300	0.70673800	-1.38389900
H	-3.97700300	0.40555300	0.26021800
C	-3.49576500	-1.16042400	-1.17285400
H	-3.33147900	-1.23684300	-2.25787500
H	-4.35618700	-1.79557000	-0.92963200
C	-2.50565300	-2.69283000	1.14974500
H	-2.82055800	-3.67085700	0.75322700
C	-1.36885600	-2.90911900	2.14391700
H	-1.67675300	-3.63090000	2.91295600
H	-1.11277400	-1.97300500	2.65503900
H	-0.45145100	-3.29063000	1.67938000
C	-3.70235500	-2.07382100	1.86030100
H	-3.97714000	-2.69377500	2.72474900
H	-4.58946300	-1.99437300	1.22161000
H	-3.47408900	-1.07214200	2.24463600
C	-1.38168400	-3.09321300	-1.51178800
H	-1.07460300	-2.53305000	-2.40873600
C	-0.17452400	-3.86331100	-0.98257900
H	0.26635200	-4.46933500	-1.78641300
H	-0.46728600	-4.55634500	-0.18215800
H	0.61480200	-3.21070000	-0.58699700
C	-2.48310500	-4.06320200	-1.92439500
H	-2.08422200	-4.78798800	-2.64797900
H	-3.33353500	-3.56384400	-2.40239400
H	-2.86436200	-4.64167900	-1.07216100
C	1.41312300	2.76461800	-1.70427900
H	1.16517600	2.11057300	-2.55477200
C	1.43915500	4.20150400	-2.21430600
H	2.23606600	4.31106700	-2.96329900
H	1.65642700	4.92014700	-1.41257300

H	0.50111900	4.50246700	-2.69429200
C	2.79292900	2.37460800	-1.17894900
H	3.52181100	2.37832500	-2.00214800
H	2.81584300	1.37737500	-0.72114800
H	3.15118900	3.09544400	-0.43110500
C	0.46766700	3.52454500	0.94502500
H	1.02214300	4.35839600	0.48678500
C	-0.74772900	4.11023800	1.65171600
H	-0.41694700	4.74881400	2.48236900
H	-1.38494900	3.32846200	2.08265200
H	-1.37162800	4.72735400	0.99501600
C	1.37173300	2.83500400	1.96262600
H	1.75356200	3.57263700	2.68195900
H	2.23784800	2.33654800	1.50948100
H	0.81758200	2.07775900	2.53053500
H	-2.28244900	0.91390500	-2.07538000
C	3.10124100	-1.42902100	-0.81432000
C	3.62567200	-1.52424900	0.48583300
C	2.86533600	-1.19292400	1.60277800
C	1.56476900	-0.72725900	1.35478200
C	1.80741300	-0.93754300	-0.93808600
H	-1.31506400	0.56121600	1.31623900
C	1.15554700	-0.72881400	-2.26059700
H	1.78300700	-0.10587300	-2.92049200
H	1.03664000	-1.68421900	-2.79980900
C	-0.21898600	-0.07361400	-2.10264900
O	-0.82473600	0.17772100	-3.16339000
N	1.04852700	-0.57889800	0.12807500
O	0.81518500	-0.39217000	2.40024700
H	-0.04625300	-0.03749800	2.04900400
C	-2.24548700	1.06140600	2.74829300
O	-3.23490500	1.52828500	2.28728900
O	-1.52818800	0.74050700	3.63788400
C	3.37660100	-1.27321100	3.00447800
H	4.36841200	-1.73252000	3.03548400
H	3.44139500	-0.27604600	3.46107900
H	2.70350700	-1.86349700	3.63775500
C	3.90561300	-1.78912500	-2.02497200
H	4.82629700	-2.31054700	-1.74714200
H	3.33942800	-2.44297500	-2.70089400
H	4.18514800	-0.89707700	-2.60568600
O	4.91382300	-1.95189000	0.65836900
C	5.85372300	-0.88481300	0.60048000
H	5.78973700	-0.34872200	-0.35840500
H	5.68699300	-0.16794500	1.41821200
H	6.84944800	-1.32391700	0.70275700

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