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Supporting Information

Mechanistic understanding of [Rh(NHC)]-catalyzed intramolecular [5+2] cycloadditions of vinyloxiranes and vinylcyclopropanes with alkynes

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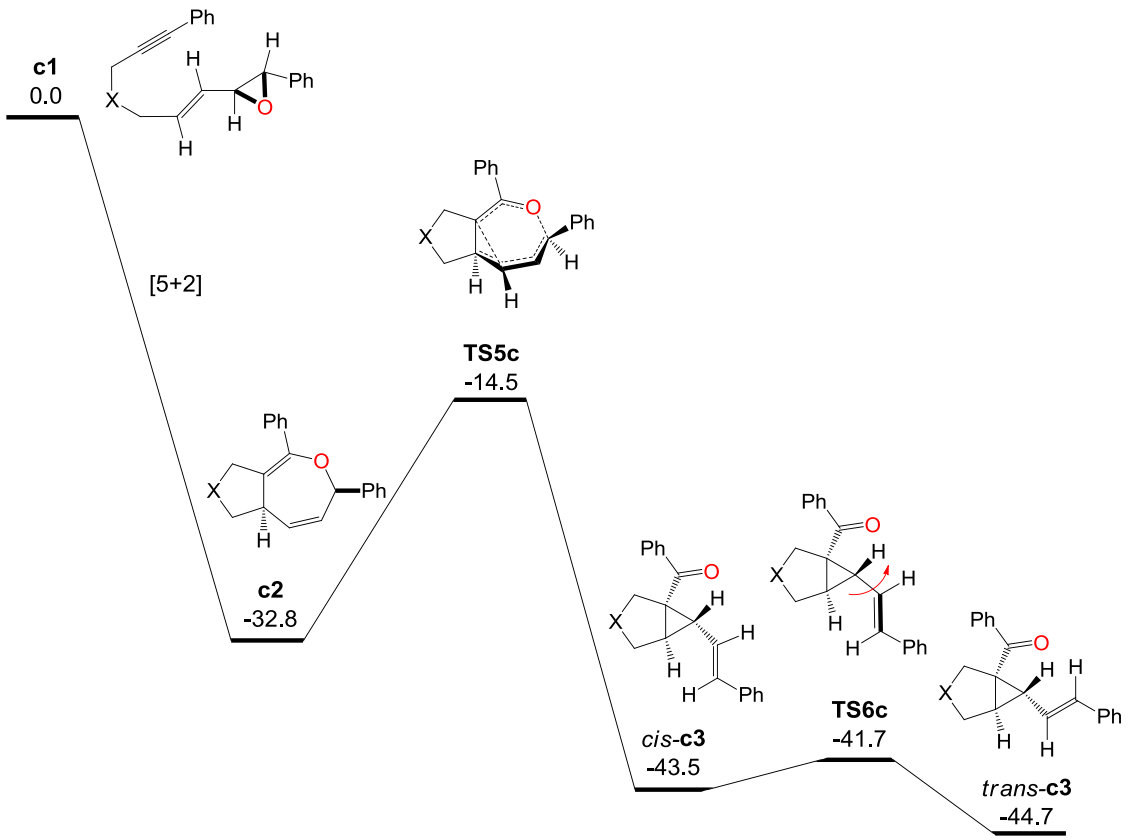


Fig. S1 Free energy profile for the [3,3]-sigmatropic rearrangement process from **c2** to c**3**.

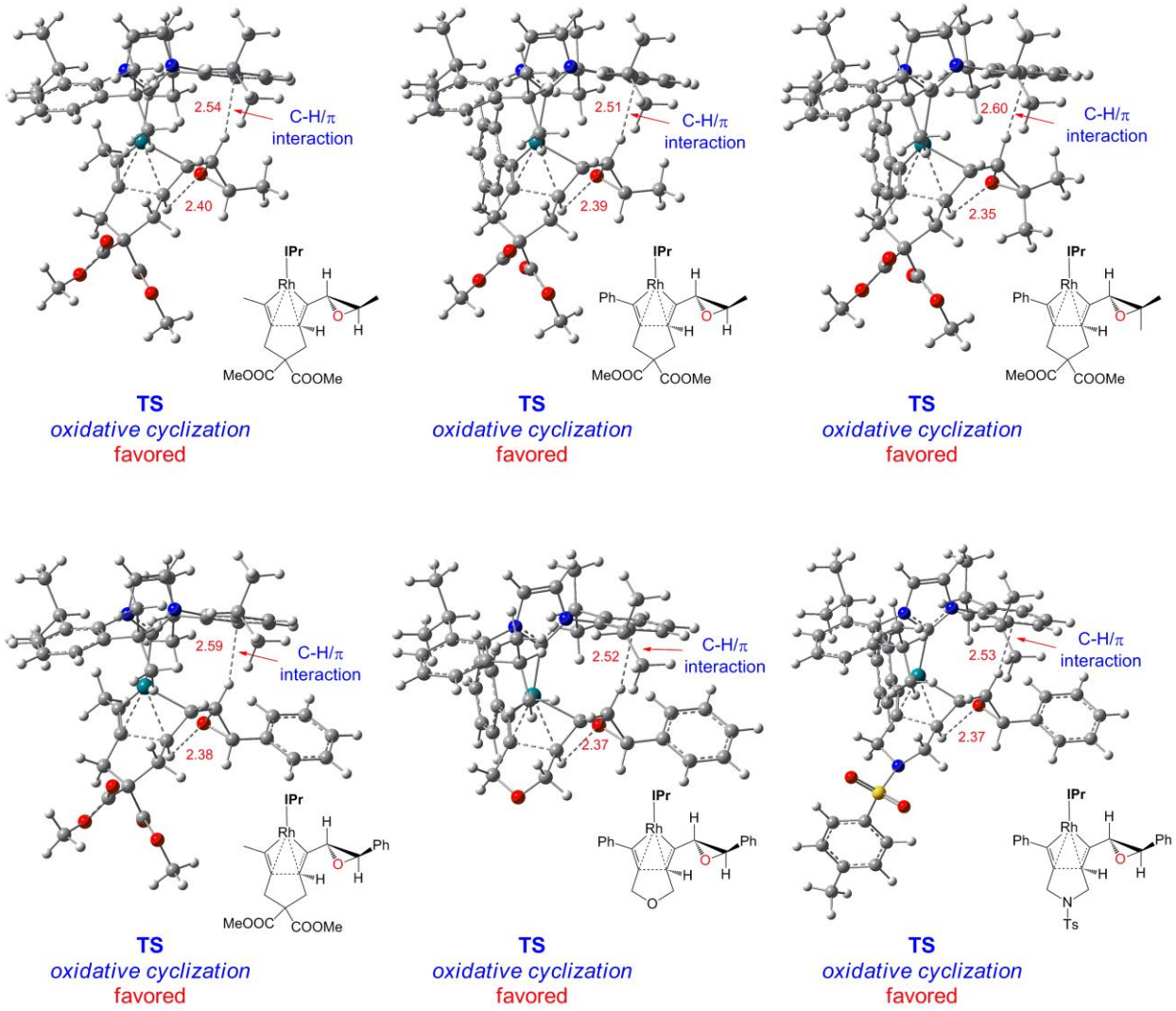


Fig. S2 Optimized geometries for the alkyne–alkene oxidative cyclization transiton states in [Rh(IPr)]-catalyzed [5+2] cycloadditions of experimenatal VOR–alkynes, with selected bond distances given in angstrom.

Noncovalent Interaction Analysis

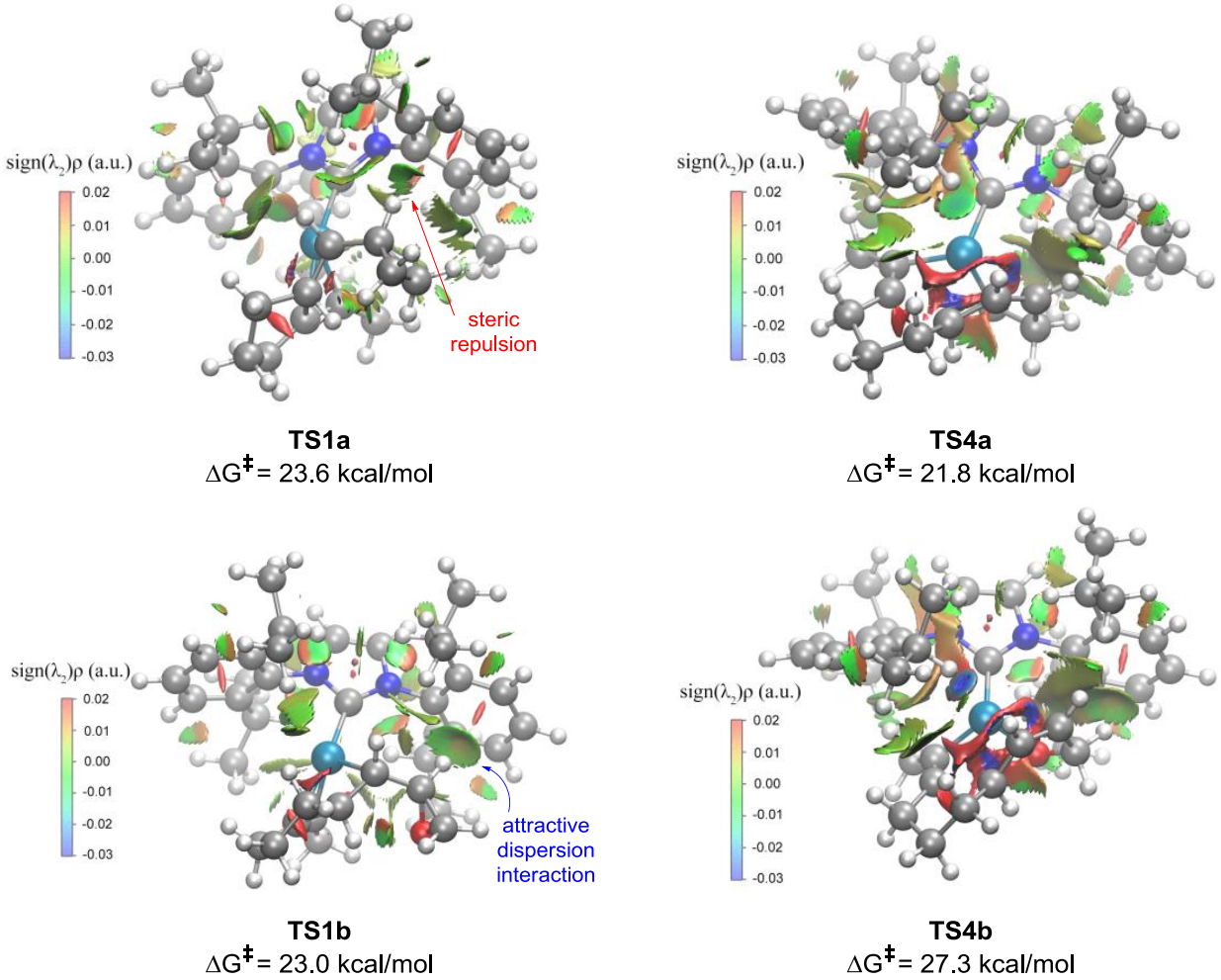
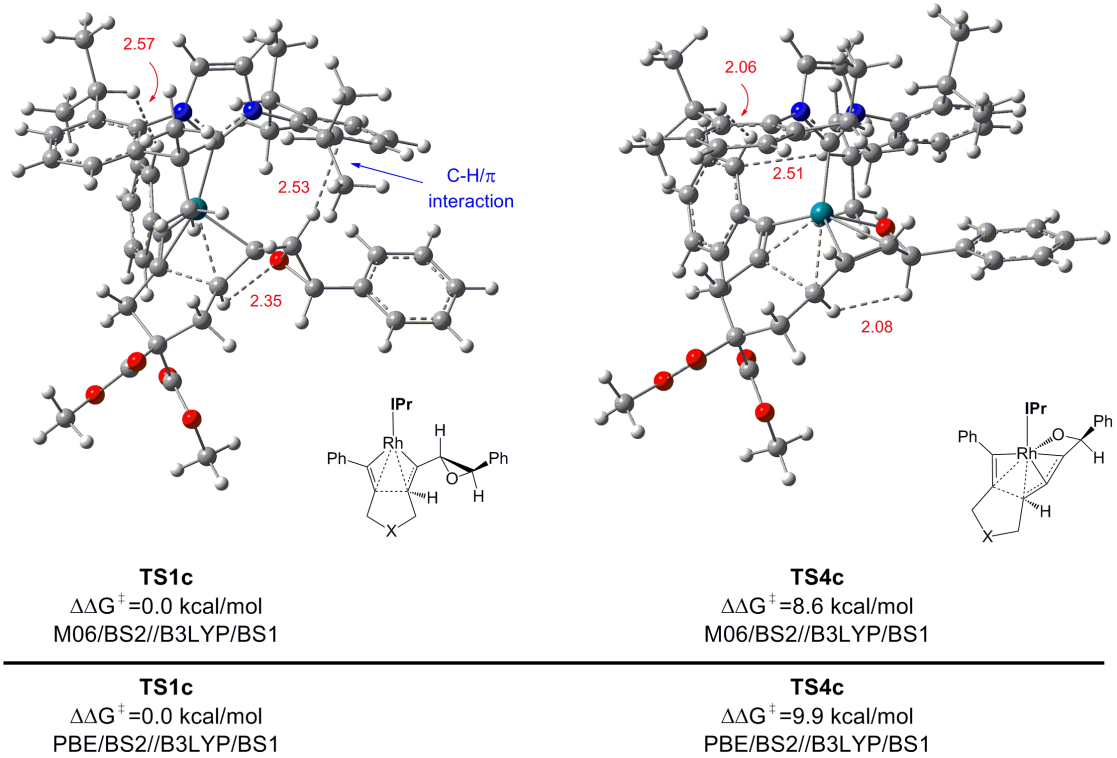


Fig. S3 Non-Covalent Interaction (NCI) analysis for the key structures in the main text.



TS1c
$\Delta\Delta G^{\ddagger}$=0.0 kcal/mol
M06/BS2//B3LYP/BS1

TS4c
$\Delta\Delta G^{\ddagger}$=8.6 kcal/mol
M06/BS2//B3LYP/BS1

TS1c
$\Delta\Delta G^{\ddagger}$=0.0 kcal/mol
PBE/BS2//B3LYP/BS1

TS4c
$\Delta\Delta G^{\ddagger}$=9.9 kcal/mol
PBE/BS2//B3LYP/BS1

Fig. S4 Comparisons of the key TSs **TS1c** and **TS4c** with calculations M06/BS2//B3LYP/BS1 and PBE/BS2//B3LYP/BS1.

M06/BS1-optimized geometries and M06/BS2//M06/BS1-calculated energies

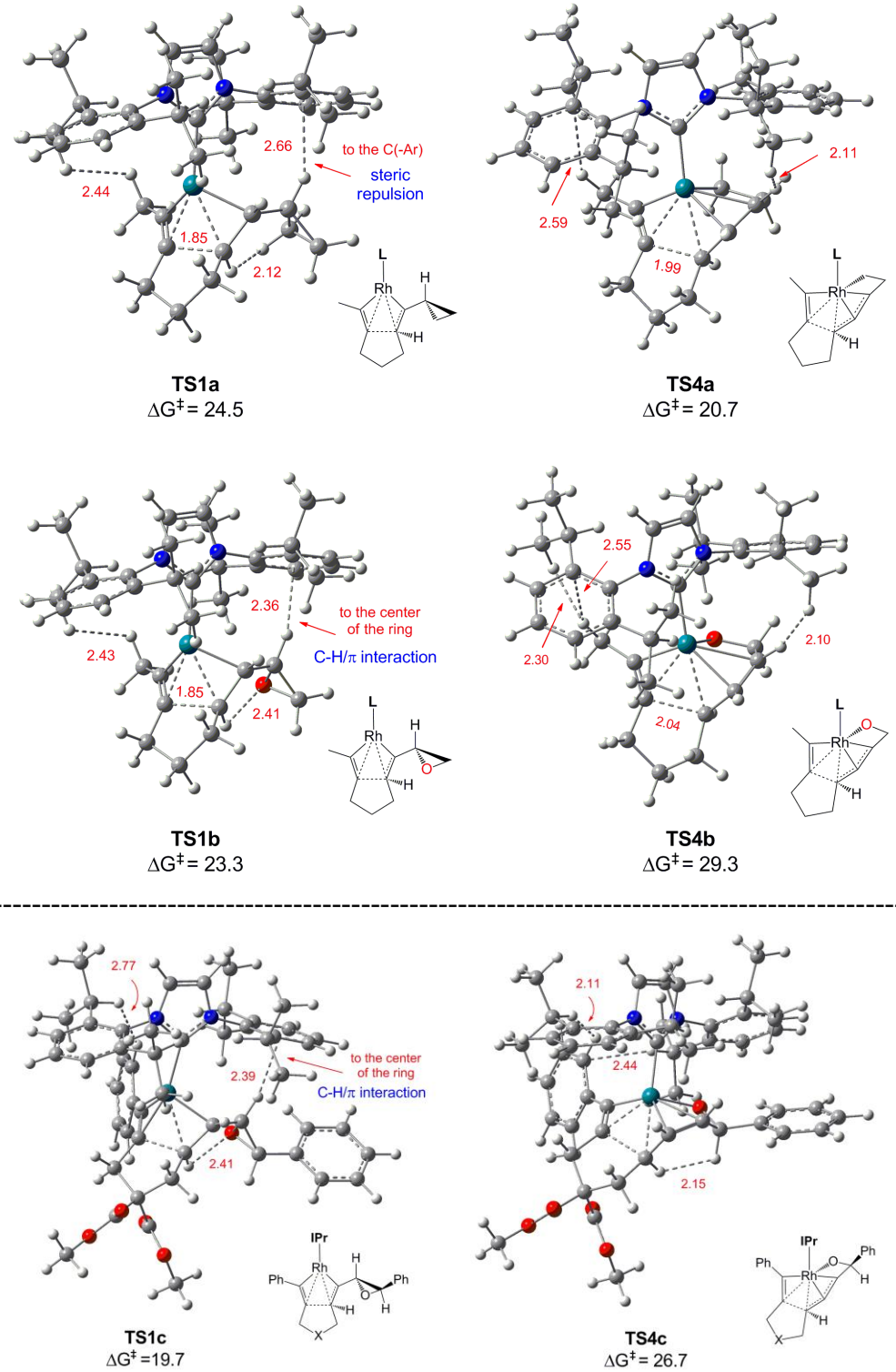


Fig. S5 M06/BS1-optimized geomtries and M06/BS2//M06/BS1-calculated energies for key transition strates **TS1a, TS4a, TS1b, TS4b, TS1c** and **TS4c**.

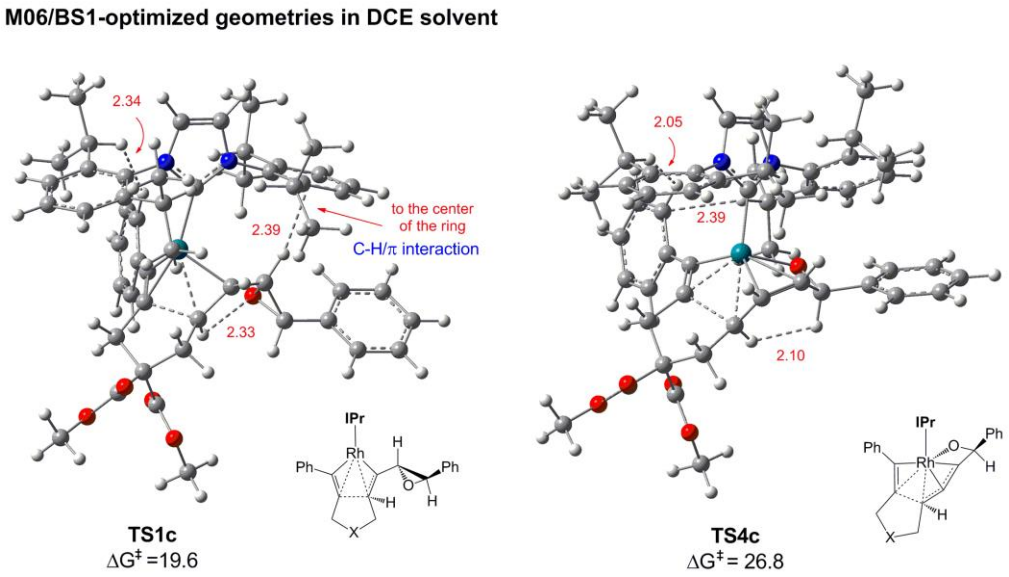


Fig. S6 M06/BS1-optimized geomtries in DCE solvent and M06/BS2//M06/BS1-calculated energies for key transition strates **TS1c** and **TS4c**.

Cartesian Coordinates (Å), SCF Energies and Free Energies at 298.15 K and 1 atm for the Optimized Structures

trans-**a1** (X = CH_2)

B3LYP SCF energy in gas phase: -428.6970338 a.u.

M06 SCF energy in solution: -428.4793234 a.u.

M06 Free energy in solution: -428.2828194 a.u.

C	3.05083000	0.91630100	0.66184500
C	2.34798800	0.03723900	-0.35948600
C	1.29824300	-0.91117100	0.07233300
C	0.20421100	-1.22267200	-0.63092800
H	0.04900800	-0.74949800	-1.60227600
H	1.45351000	-1.37894100	1.04776900
C	-0.84589300	-2.21076000	-0.20200700
C	-2.61344600	-0.54860200	0.75850600
C	-2.13861700	0.77592400	0.34906200
C	-1.78619300	1.88058600	0.00399900
H	2.17890500	0.48815900	-1.33556900
H	3.29089600	1.93644400	0.37402900
H	2.75914200	0.80677500	1.70326300
H	-2.19707700	-0.80389100	1.74415200
H	-3.70275900	-0.50139500	0.89796900
H	-0.80283200	-3.09092800	-0.86327800
H	-0.61406600	-2.57726700	0.80783300
C	-1.33119300	3.20706100	-0.40614900
H	-1.81745100	3.53034900	-1.33509200
H	-1.55318100	3.96041000	0.36009200
H	-0.24750700	3.22048900	-0.57719600
C	-2.29775000	-1.69252100	-0.23390200
H	-2.96202300	-2.53435200	0.00160300
H	-2.55578600	-1.36594800	-1.24933200
C	3.80118300	-0.21067500	0.01107000
H	4.56168800	0.02714100	-0.72789200
H	4.02335900	-1.09180900	0.60787200

cis-**a1** (X = CH_2)

B3LYP SCF energy in gas phase: -428.6947261 a.u.

M06 SCF energy in solution: -428.47694 a.u.

M06 Free energy in solution: -428.280868 a.u.

C	3.75582100	-0.06443100	0.10518500
C	2.35181100	0.27562300	0.57724600
C	1.30119100	-0.77645000	0.65459500
C	0.41371100	-1.08193800	-0.29693100
H	0.41416500	-0.51294200	-1.22708100
H	1.27669200	-1.33744300	1.59195000
C	-0.60422900	-2.18627800	-0.19978000
C	-2.68729000	-0.75407400	0.44550500
C	-2.25106900	0.63121700	0.25041000
C	-1.92415100	1.78181500	0.06931800
H	2.32019900	0.99062300	1.40034800
H	4.59868200	0.38383700	0.62497400
H	3.93134600	-1.07725500	-0.24737800
H	-2.48277600	-1.06667000	1.48010200
H	-3.77968800	-0.79669100	0.33117700
H	-0.32881500	-2.99025500	-0.90082800
H	-0.56778800	-2.63201200	0.80400200
C	-1.50145500	3.16443300	-0.14133400
H	-2.04971800	3.63206300	-0.96874200
H	-1.67270600	3.77548700	0.75372800
H	-0.43180700	3.22036900	-0.37912200
C	-2.05447400	-1.77819100	-0.52613400
H	-2.67299200	-2.68503000	-0.50889800
H	-2.10994200	-1.38149800	-1.54785500
C	2.86519000	0.82014200	-0.73199700
H	3.09600200	1.88056100	-0.78864100
H	2.46881200	0.40564300	-1.65422700

a2 (X = CH_2)

B3LYP SCF energy in gas phase: -428.7739591 a.u.

M06 SCF energy in solution: -428.546354 a.u.

M06 Free energy in solution: -428.337343 a.u.

C	-2.29868100	-0.80405600	0.59483200
C	-1.67230200	-1.82742000	-0.31960000
C	-0.35127300	-1.89760300	-0.49216100
C	0.61819700	-1.00104200	0.24394200
H	0.51661100	-1.20501900	1.32501100
H	0.07292600	-2.63101000	-1.17774400
C	2.09746100	-1.24572000	-0.12423700
C	1.82212400	1.14879700	-0.06535900
C	0.43151600	0.51517900	0.03942900
C	-0.72144100	1.20107700	-0.04321600
H	-2.32949900	-2.49701600	-0.87243300
H	-3.36968800	-1.00496100	0.71389100
H	-1.85783700	-0.87792700	1.59996700
H	2.01989700	1.46536600	-1.10041600
H	1.93259000	2.04136400	0.56025000
H	2.49724600	-2.15881600	0.33078200
H	2.18877400	-1.35392500	-1.21437600
C	2.80711800	0.03283100	0.33353500
H	3.80024600	0.16174700	-0.10967800
H	2.93515700	0.01641700	1.42406800
C	-0.73742700	2.69520000	-0.29205000
H	0.24372000	3.10044200	-0.54808000
H	-1.42289000	2.94013600	-1.11566900
H	-1.10770600	3.24039500	0.58869400
C	-2.12852100	0.63749500	0.08229700
H	-2.62587000	0.72624500	-0.89708900
H	-2.69430000	1.30813800	0.74835800

trans-**b1** (X = CH_2)

B3LYP SCF energy in gas phase: -464.5929085 a.u.
M06 SCF energy in solution: -464.3880146 a.u.
M06 Free energy in solution: -464.2149676 a.u.

C	3.13862700	0.82808200	0.64470200
C	2.32900900	0.06802000	-0.32777700
C	1.31289900	-0.91600000	0.09808600
C	0.21336400	-1.19987300	-0.60726000
H	0.05289800	-0.69090600	-1.55937000
H	1.50363800	-1.41146800	1.05045200
C	-0.83613000	-2.19929700	-0.20770400
C	-2.60453000	-0.54393100	0.75873400
C	-2.12236300	0.77992700	0.35508200
C	-1.76349500	1.88257700	0.00976800
H	2.16677300	0.52056000	-1.30810700
H	3.51775700	1.81538100	0.37520200
H	2.98246800	0.66964100	1.71285500
H	-2.19337900	-0.80541100	1.74482800
H	-3.69409400	-0.49324500	0.89331700
H	-0.78180400	-3.05975900	-0.89287800
H	-0.60915000	-2.58994600	0.79347100
O	3.71036300	-0.27003200	-0.06418600
C	-1.30920500	3.20952300	-0.40008100
H	-1.84171500	3.55881300	-1.29341100
H	-1.47472900	3.95021100	0.39214500
H	-0.23687700	3.21056500	-0.63281300
C	-2.28814200	-1.68207700	-0.23980000
H	-2.95077100	-2.52656600	-0.01110900
H	-2.54412400	-1.34932900	-1.25359600

cis-**b1** (X = CH_2)
B3LYP SCF energy in gas phase: -464.5925827 a.u.
M06 SCF energy in solution: -464.3861752 a.u.
M06 Free energy in solution: -464.2108262 a.u.

C	3.35792000	-0.47799000	-0.33756600
C	2.28807200	-0.29906200	0.66856200
C	1.07514800	-1.15647500	0.72865700
C	0.15312700	-1.21496300	-0.23638600
H	0.30084700	-0.60268200	-1.12470800
H	0.95281500	-1.73017300	1.64789300
C	-1.09383000	-2.05419600	-0.18956900
C	-2.75887300	-0.13156100	0.39731700
C	-1.91072500	1.05169200	0.23196700
C	-1.19550800	2.01209700	0.05934300
H	2.58630500	0.14780300	1.62046400
H	4.38223200	-0.17943200	-0.10903100
H	3.25073000	-1.26834000	-1.08046400
H	-2.71621500	-0.47967900	1.44009100
H	-3.80719700	0.14509600	0.21698300
H	-0.99440500	-2.88566700	-0.90517800
H	-1.19367800	-2.51456700	0.80310300
O	2.41591800	0.59378200	-0.44777000
C	-0.26987700	3.12353200	-0.14729900
H	-0.57224700	3.74876800	-0.99666100
H	-0.21690300	3.77158300	0.73653100
H	0.74052600	2.74601100	-0.34946200
C	-2.39371000	-1.30315200	-0.54475500
H	-3.21990300	-2.02578000	-0.52695200
H	-2.33072700	-0.92273000	-1.57206000

b2 (X = CH_2)
B3LYP SCF energy in gas phase: -464.6691986 a.u.
M06 SCF energy in solution: -464.4557123 a.u.
M06 Free energy in solution: -464.2706993 a.u.

C	-2.20839200	-0.75452100	0.58093100
C	-1.61563000	-1.83059400	-0.29062200
C	-0.29323000	-1.92740300	-0.44121600
C	0.67106100	-1.00282200	0.26613000
H	0.65904300	-1.25098600	1.34324400
H	0.12925100	-2.68924800	-1.09648900
C	2.13607400	-1.13724900	-0.20225900
C	1.72176900	1.23753100	-0.00012800
C	0.38340000	0.49755400	0.09008200
C	-0.80283000	1.11874400	-0.04551200
H	-2.28986100	-2.49665600	-0.82479500
H	-3.28788400	-0.88123900	0.69347200
H	-1.75841300	-0.76896900	1.58474200
H	1.87267500	1.65272700	-1.00733600
H	1.79703000	2.07946200	0.69842500
H	2.61767800	-2.04377400	0.18166000
H	2.16527300	-1.18402100	-1.29983500
C	2.79012800	0.16060400	0.28517300
H	3.74784800	0.37318300	-0.20137100
H	2.97973300	0.09484800	1.36465900
C	-0.96235200	2.58907100	-0.32604300
H	-0.00951300	3.07760400	-0.53549600
H	-1.62364300	2.72824100	-1.18990800
H	-1.43700800	3.09658800	0.52356900
O	-2.06027500	0.56334500	0.03328000

cis-**b3** (X = CH_2)
B3LYP SCF energy in gas phase: -464.6672177 a.u.
M06 SCF energy in solution: -464.4648983 a.u.
M06 Free energy in solution: -464.2845063 a.u.

C	2.32929800	-1.91561500	0.04288600
C	1.41853300	-1.51742900	0.93394600
C	0.03987800	-1.03336400	0.66358600
C	-0.56013900	-0.89026100	-0.70188600
H	0.06952100	-1.11933800	-1.55634300
H	-0.65221400	-1.29315400	1.46434100
C	-2.07182100	-1.02544500	-0.83221000
C	-1.60224800	0.98981200	0.51298600
C	-0.26759100	0.38202200	0.06753600
C	0.88912300	1.24700600	-0.32155000
H	1.68312900	-1.53866700	1.99199600

H	3.31307200	-2.24818700	0.36225900
H	2.14264200	-1.91170100	-1.02586500
H	-1.59818500	1.34996100	1.54921000
H	-1.83194800	1.85319500	-0.12527100
H	-2.37585400	-0.65142100	-1.81811100
H	-2.42169300	-2.06191800	-0.75579800
C	1.01975500	2.59117200	0.37752000
H	1.93941100	3.08054800	0.05094900
H	1.03621100	2.45992100	1.46679400
H	0.16403300	3.23802500	0.14764700
O	1.71217000	0.88506500	-1.14785600
C	-2.65192400	-0.12854100	0.28917300
H	-2.78681600	-0.71002600	1.20766400
H	-3.63585700	0.27610600	0.03145900

trans-**b3** (X = CH_2)

B3LYP SCF energy in gas phase: -464.6724259 a.u.

M06 SCF energy in solution: -464.4685542 a.u.

M06 Free energy in solution: -464.2875702 a.u.

O	-1.26575700	1.62515200	1.14958000
C	-1.93349800	-1.07803500	-0.00060700
H	-2.35613000	-0.45137900	0.77994100
C	-0.46727000	-1.00393700	-0.18422600
H	-0.09622300	-1.65553800	-0.97437700
C	0.32034600	0.33510100	-0.06637500
C	0.45203300	-0.75915600	0.98131800
H	-0.01527400	-0.59489100	1.94851100
C	1.86570100	-1.31756500	0.91147200
H	2.47606700	-0.83753000	1.68727700
H	1.91024700	-2.39919000	1.08682200
C	1.62939800	0.37675200	-0.86309100
H	1.47970500	0.47720400	-1.94511000
H	2.21874100	1.24407900	-0.53903700
C	-0.44382800	1.58284100	0.24478100
C	-2.72609400	-1.87079300	-0.72771400
H	-2.33584900	-2.50775600	-1.51934100
C	-0.17801700	2.80587400	-0.61750100
H	-0.87542700	3.59867900	-0.34049700
H	0.84913500	3.16546100	-0.47874800
H	-0.29045000	2.56532500	-1.68171800
C	2.37540600	-0.93135100	-0.49808600
H	3.46253900	-0.80792800	-0.52965000
H	2.13112100	-1.72036900	-1.21753700
H	-3.79720700	-1.91577900	-0.55299800

1a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.18315 a.u.

M06 SCF energy in solution: -1698.432441 a.u.

M06 Free energy in solution: -1697.694179 a.u.

C	-2.55001300	-0.52898600	-3.96181600
C	-2.06112100	-0.48153000	-2.51439100
C	-0.62896600	-0.15676100	-2.23404700
C	0.43907400	-0.98726200	-2.64588000
H	0.15051800	-1.93511900	-3.10263800
H	-0.42417200	0.90489100	-2.10931400
C	-2.53846200	-1.77791300	-3.12569300
C	1.84457900	-0.57516900	-3.01790100
C	2.99104500	-2.33858400	-1.50934500
C	1.68047600	-2.65700900	-0.89643200
C	0.65316700	-3.32454600	-0.55347100
H	-2.75745200	-0.02182500	-1.82191900
H	-3.48660400	-2.16894100	-2.76762200
H	-1.81710000	-2.54987000	-3.37866700
H	-3.49973000	-0.05501600	-4.19315000
H	-1.80239100	-0.44163900	-4.74590500
H	3.52102300	-1.61644100	-0.87871600
H	3.60457400	-3.24815200	-1.55354800
H	1.82794100	-0.21897400	-4.06046700
H	2.18871600	0.26105300	-2.40143000
Rh	0.20653400	-1.28233600	-0.54544000
C	-0.08432800	0.46600800	0.55663000
N	-1.20591300	0.90932900	1.20935600
C	-0.87998400	1.86357600	2.16748900
C	-2.58532700	0.54192900	0.95111100
N	0.93557200	1.19200100	1.11654300
C	0.45948300	2.04548000	2.10399500
C	2.33992700	1.14094900	0.75919300
C	-3.08419600	-0.67195300	1.47243600
C	-3.39486500	1.46469400	0.25254700
C	-4.43073000	-0.96815600	1.22743100
C	-2.23852000	-1.59358200	2.35006800
C	-5.24850800	-0.08885200	0.52138800
C	-4.73744500	1.11601800	0.05025400
C	-2.89216600	2.82140800	-0.24303300
C	-2.62084200	-3.07830900	2.22840600
C	-2.31114300	-1.14709500	3.82743400
C	-3.21222200	3.07751300	-1.72925500
C	-3.46403800	3.96252800	0.62583000
C	3.18101800	0.24130600	1.44812400
C	2.81945500	2.06137700	-0.19923800
C	4.18637600	2.01382100	-0.50373300
C	1.93486300	3.14504300	-0.81707700
C	5.03519000	1.11007800	0.13026500
C	4.53916700	0.24344200	1.10176200
C	2.68145500	-0.63799300	2.59350600
C	2.17468400	3.36285400	-2.32234200
C	2.12247800	4.47905800	-0.05992600
C	2.98532300	0.03305700	3.95150400
C	3.25476400	-2.06650900	2.57107400
H	-1.63212500	2.31883800	2.79129900
H	1.11817900	2.69285800	2.65987700
H	-4.85272500	-1.89224200	1.60656200
H	-6.29198800	-0.33877000	0.35190800
H	-5.39100700	1.80122400	-0.48062300
H	-1.19215500	-1.50393200	2.02999400
H	-1.96307400	-0.11789000	3.96174900

H	-1.69061700	-1.79747300	4.45452500
H	-3.34135000	-1.20445400	4.19695300
H	-3.59700300	-3.28866300	2.67874400
H	-1.88717900	-3.69315300	2.76174000
H	-2.65252800	-3.40496600	1.18366200
H	-1.80207000	2.84486100	-0.14123000
H	-4.55617400	4.00531300	0.54873900
H	-3.06644500	4.92891800	0.29639600
H	-3.21365200	3.83677700	1.68471200
H	-4.29095900	3.13770800	-1.90995000
H	-2.80709500	2.29376300	-2.37721600
H	-2.77832800	4.03388600	-2.04159500
H	4.59551100	2.70511400	-1.23337400
H	6.09296500	1.09656400	-0.11716400
H	5.22111800	-0.42974900	1.61118000
H	0.88875400	2.84156200	-0.69624900
H	1.89742000	4.37975200	1.00693200
H	1.46200700	5.24931400	-0.47378300
H	3.15477200	4.83561300	-0.15026900
H	3.17442400	3.76084000	-2.52627500
H	1.45454700	4.09258900	-2.70820200
H	2.05776100	2.43842400	-2.89622100
H	1.59272200	-0.72568900	2.50495800
H	4.06568000	0.14517900	4.09740400
H	2.59501800	-0.57641800	4.77428500
H	2.53399100	1.02810200	4.02540800
H	4.33520200	-2.07904900	2.75059500
H	3.06099300	-2.56788400	1.61763100
H	2.79126200	-2.66161300	3.36578600
C	-0.09338900	-4.58345000	-0.32447100
H	0.57210900	-5.45019300	-0.41117300
H	-0.56073600	-4.60112900	0.66402400
H	-0.89398200	-4.68975200	-1.06560200
C	2.83023200	-1.75464600	-2.93560100
H	3.81767900	-1.43841600	-3.28843700
H	2.49319200	-2.55092400	-3.61158700

TS1a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.152299 a.u.

M06 SCF energy in solution: -1698.39497 a.u.

M06 Free energy in solution: -1697.656553 a.u.

C	3.25598900	3.42261200	-1.11457900
C	2.43543900	2.16105600	-0.84247900
C	0.98638000	2.11253000	-1.19818200
C	0.08314400	3.22521500	-0.84692700
H	0.60621400	3.96129400	-0.23264100
H	0.82485000	1.68972000	-2.19946100
C	3.00405500	2.97144700	0.29654800
C	-0.87074200	3.90867700	-1.80640600
C	-2.08970900	4.17535700	0.34986700
C	-1.12312300	3.06338300	0.65206000
C	-0.69528200	2.25243000	1.58831800
H	2.95589900	1.23299300	-1.05316700
H	3.82587400	2.52564200	0.84877500
H	2.33314900	3.56420500	0.91410900
H	4.24735400	3.29761900	-1.54023600
H	2.72763200	4.30416100	-1.46924400
H	-3.07948900	3.71710200	0.22755700
H	-2.16295600	4.86879000	1.19546000
H	-0.30373800	4.42995000	-2.58855400
H	-1.51720300	3.17519400	-2.30247800
Rh	-0.41400100	1.14761300	-0.05233900
C	-0.03950100	-0.88994800	0.10108600
N	1.05163100	-1.70264500	0.27169000
C	0.67200900	-3.03429400	0.37019900
C	2.45287100	-1.32930500	0.24612100
N	-1.09998200	-1.76523900	0.09080400
C	-0.67930800	-3.07438100	0.25251600
C	-2.48648600	-1.39941600	-0.13168100
C	3.08218500	-0.94477500	1.44774700
C	3.15152300	-1.47045900	-0.97215900
C	4.45544600	-0.67314200	1.39410500
C	2.33997100	-0.88906600	2.78024600
C	5.16989100	-0.78956700	0.20427900
C	4.52402000	-1.18723200	-0.96291800
C	2.49351500	-1.95243000	-2.26429900
C	2.75004800	0.31654500	3.64464000
C	2.53430400	-2.20458200	3.56507300
C	2.75470000	-1.00389800	-3.45041700
C	2.94820800	-3.38642400	-2.60913600
C	-3.34189000	-1.25295900	0.98267200
C	-2.93931800	-1.27007900	-1.46235400
C	-4.28776100	-0.94327800	-1.65517500
C	-2.04472500	-1.50376400	-2.67717700
C	-5.14974200	-0.77267400	-0.57612300
C	-4.68088600	-0.93254400	0.72540900
C	-2.87617300	-1.48214800	2.41863900
C	-1.94836700	-0.24986800	-3.56752700
C	-2.52074500	-2.72323300	-3.49300700
C	-3.25539900	-2.90007400	2.89858500
C	-3.42626100	-0.42976100	3.40002500
H	1.39687800	-3.82164900	0.50282000
H	-1.37022900	-3.90225100	0.25937900
H	4.97718100	-0.38032400	2.29933900
H	6.23628200	-0.58251400	0.19035200
H	5.09527400	-1.29058200	-1.88043900
H	1.27166800	-0.78458600	2.56513500
H	2.17732900	-3.07159200	2.99876400
H	1.98382000	-2.17103600	4.51233000
H	3.59288400	-2.36920100	3.79616400
H	3.77731100	0.22833900	4.01449500
H	2.09980600	0.38268300	4.52411000
H	2.67246400	1.25525100	3.08529400
H	1.41005300	-1.98064700	-2.10980300
H	4.02793400	-3.42606100	-2.79146300
H	2.44195100	-3.74099600	-3.51396900
H	2.72295000	-4.08790700	-1.79851600

H	3.81687000	-0.96179600	-3.71459600
H	2.42464400	0.01783200	-3.23241600
H	2.21283500	-1.35407200	-4.33603900
H	-4.66976100	-0.83600200	-2.66600700
H	-6.19378000	-0.52748400	-0.74928600
H	-5.36967100	-0.81441400	1.55546400
H	-1.03324600	-1.72758200	-2.32385400
H	-2.55605200	-3.62796600	-2.87637600
H	-1.83936700	-2.90894100	-4.33078300
H	-3.52216500	-2.56334300	-3.90754200
H	-2.92147200	0.02252100	-3.99095100
H	-1.26131900	-0.42728900	-4.40279800
H	-1.58135400	0.61371400	-2.99875300
H	-1.78272000	-1.40759400	2.43674100
H	-4.34298100	-3.03445400	2.89352900
H	-2.89967700	-3.06557500	3.92179500
H	-2.82162100	-3.67808600	2.26184100
H	-4.50438400	-0.54210800	3.55676200
H	-3.24488900	0.59038800	3.04568100
H	-2.94771800	-0.54594800	4.37892700
C	-0.58274100	2.05903800	3.05228200
H	-1.23801300	2.76513300	3.57982600
H	-0.84788900	1.04322900	3.35672700
H	0.44573400	2.24823800	3.38295700
C	-1.67764300	4.90105000	-0.95366500
H	-2.55159500	5.29026500	-1.48287500
H	-1.04043000	5.76009000	-0.71153800

2a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.194361 a.u.

M06 SCF energy in solution: -1698.440746 a.u.

M06 Free energy in solution: -1697.700902 a.u.

C	0.10242900	-4.53828100	-1.46599900
C	0.00510800	-3.44226900	-0.44631200
C	-1.05077000	-2.39955600	-0.32108700
C	-2.11356100	-2.29816000	-1.41575200
H	-2.09993000	-3.22576600	-2.01145900
H	-1.43075100	-2.29041500	0.69379500
C	0.99214000	-3.35933300	-1.73153600
C	-3.58854700	-2.04752900	-1.04112000
C	-3.06613700	-0.92406900	-3.20545900
C	-1.83274200	-1.13980900	-2.34176500
C	-0.72700700	-0.39996100	-2.17919700
H	0.54870600	-3.64762700	0.47355100
H	2.05760300	-3.46247000	-1.55035300
H	0.71847600	-2.74515500	-2.58754700
H	0.58216400	-5.45278900	-1.12987500
H	-0.73198200	-4.69554600	-2.14131200
H	-3.26461600	0.13803600	-3.37828000
H	-2.95775000	-1.38618500	-4.19509400
H	-4.08138500	-2.92697100	-0.61218000
H	-3.65153400	-1.23380900	-0.31057600
C	1.40339900	2.23896200	1.55396000
C	0.07451800	2.33901700	1.79305300
C	0.35941000	0.58867100	0.37973100
N	-0.56033300	1.32595000	1.07442000
N	1.56615100	1.16749300	0.68713300
Rh	0.47569900	-1.07508900	-0.72165700
H	-0.48626500	3.02712600	2.40421400
H	2.23865400	2.81591300	1.91732100
C	2.84055400	0.62804600	0.24985200
C	3.47912500	1.19526600	-0.87738100
C	3.42243700	-0.41294000	1.01442200
C	4.70436500	0.63805900	-1.26665600
C	4.64809700	-0.92714500	0.57161300
C	5.27720800	-0.41636500	-0.56074100
H	5.22325900	1.04362400	-2.12853000
H	5.12685800	-1.72330200	1.13249100
H	6.22988000	-0.82771100	-0.88209300
C	-1.99618000	1.12801600	1.18712200
C	-2.47868700	0.21532100	2.15386400
C	-2.84947400	1.95321300	0.42545400
C	-3.86766200	0.10531200	2.29289800
C	-4.22998700	1.79770100	0.61215600
C	-4.73553500	0.88052900	1.52709000
H	-4.27885800	-0.58649400	3.01999600
H	-4.91674800	2.41515800	0.04221700
H	-5.80925200	0.77979500	1.65773000
C	2.82353700	-0.90429200	2.33186400
H	1.77302200	-0.59780500	2.37006400
C	3.54057900	-0.23262100	3.52378100
H	3.09271000	-0.55564300	4.47016300
H	4.60278400	-0.50098200	3.54289100
H	3.47251600	0.85922700	3.47282100
C	2.85665400	-2.43624400	2.48301100
H	2.31869500	-2.73359600	3.38975000
H	2.38876600	-2.93913500	1.62859100
H	3.87831200	-2.81978500	2.57401700
C	-1.55459300	-0.56357500	3.09075800
H	-0.59969200	-0.71677000	2.57462600
C	-1.27040000	0.25093400	4.37342500
H	-2.20015400	0.44121200	4.92131500
H	-0.59645500	-0.30388500	5.03642100
H	-0.80571200	1.21699400	4.15469500
C	-2.09424500	-1.95284800	3.48099200
H	-2.40806300	-2.54078200	2.61180500
H	-1.31764800	-2.51563700	4.01052100
H	-2.95159800	-1.88010500	4.15875100
C	-2.33570100	3.04548900	-0.50965900
H	-1.27157700	2.86409500	-0.69417600
C	-2.46535800	4.43392600	0.15469600
H	-2.06710200	5.21140800	-0.50687600
H	-3.51512300	4.67205600	0.35982400
H	-1.92242200	4.48884900	1.10421600
C	-3.04461300	3.04911000	-1.87606600
H	-2.56584800	3.77438400	-2.54322900
H	-3.00177900	2.06563000	-2.35189400

H	-4.09779400	3.33725000	-1.78886400
C	2.93112600	2.41989600	-1.60554600
H	1.85479300	2.47684100	-1.41136600
C	3.57525200	3.70869600	-1.04672500
H	4.65940900	3.70218000	-1.20585200
H	3.16470500	4.58904900	-1.55357900
H	3.39730000	3.82568100	0.02731100
C	3.12527100	2.35843100	-3.13170000
H	4.17712700	2.47429500	-3.41500600
H	2.76727300	1.41360800	-3.55294900
H	2.57343600	3.17528300	-3.60873900
C	-0.31433600	0.79424300	-2.98749600
H	0.62922300	0.61612300	-3.51711200
H	-0.17289900	1.68623000	-2.36674100
H	-1.07091300	1.02576500	-3.74856400
C	-4.21270700	-1.61605500	-2.39379800
H	-4.57546500	-2.49568300	-2.93620000
H	-5.07133400	-0.95355500	-2.25143000

TS2a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.189139 a.u.

M06 SCF energy in solution: -1698.433259 a.u.

M06 Free energy in solution: -1697.692738 a.u.

C	-0.89737600	4.39823400	-0.39233400
C	-0.46542500	3.33513600	0.55849000
C	0.76049700	2.58424700	0.57175500
C	1.89795400	2.93605800	-0.37731500
H	1.81738300	4.00385700	-0.64268900
H	1.04412600	2.17397300	1.53891700
C	-1.52593400	3.19108900	-1.04744000
C	3.35773400	2.69204500	0.05510000
C	3.12940000	2.22466000	-2.38120200
C	1.80675000	2.10875100	-1.63666600
C	0.76966500	1.28346500	-1.81535800
H	-1.13083300	3.19555100	1.41064100
H	-2.58714300	3.04284400	-0.85216500
H	-1.20532000	3.00268400	-2.07050900
H	-1.57791800	5.13898200	0.02560900
H	-0.10226200	4.86820300	-0.96892100
H	3.44704500	1.26014600	-2.79046000
H	3.07023400	2.92231300	-3.22625100
H	3.72497700	3.42694800	0.77992500
H	3.44978900	1.69582900	0.50292300
C	-1.25155300	-2.72701600	0.76839200
C	0.08961400	-2.86222200	0.91286000
C	-0.28318600	-0.74408900	0.17830800
N	0.67313900	-1.64956700	0.54967300
N	-1.46152400	-1.43121900	0.32114600
Rh	-0.60660300	1.26484400	-0.35552900
H	0.68494300	-3.69859100	1.24173000
H	-2.06067200	-3.41855300	0.94123900
C	-2.74806400	-0.79765100	0.11037600
C	-3.36266000	-0.89607000	-1.16039800
C	-3.35430300	-0.13285800	1.20552500
C	-4.59121100	-0.24268400	-1.32904500
C	-4.58237300	0.49950100	0.97079600
C	-5.18868300	0.45534500	-0.28268800
H	-5.09389500	-0.29167300	-2.28903300
H	-5.08063900	1.01749200	1.78373600
H	-6.14382700	0.94892400	-0.43851400
C	2.10751100	-1.44508700	0.66416100
C	2.61349400	-0.88296000	1.85821600
C	2.94409500	-1.92253800	-0.36636200
C	4.00406500	-0.75989800	1.97087800
C	4.32694700	-1.77280100	-0.19408200
C	4.85294200	-1.19178600	0.95472900
H	4.43142100	-0.33331400	2.87195700
H	5.00102900	-2.12838800	-0.96648300
H	5.92857800	-1.09027000	1.06788600
C	-2.77161700	-0.17777500	2.61778000
H	-1.70823800	-0.42775600	2.54192900
C	-3.45456100	-1.29631800	3.43615600
H	-3.01797500	-1.35570000	4.43928400
H	-4.52732500	-1.10092000	3.54505100
H	-3.34031700	-2.27552500	2.95960300
C	-2.87161400	1.16237400	3.36836900
H	-2.34719300	1.09094500	4.32728400
H	-2.42283000	1.98422700	2.79875900
H	-3.90854300	1.43720400	3.58858700
C	1.71691300	-0.50200100	3.03597900
H	0.72285800	-0.26277700	2.64135300
C	1.56298600	-1.69507200	4.00622200
H	2.53582900	-1.98184800	4.42131300
H	0.90600300	-1.42723600	4.84185100
H	1.13719400	-2.57398700	3.51231900
C	2.21063600	0.73215700	3.81440300
H	2.42744900	1.58005300	3.15597700
H	1.44773400	1.04521800	4.53582300
H	3.11969900	0.51770300	4.38657900
C	2.41498800	-2.65124900	-1.59978500
H	1.34450500	-2.43658400	-1.68963200
C	2.57202900	-4.17944300	-1.43928000
H	2.16976000	-4.69831800	-2.31668900
H	3.62818300	-4.45434000	-1.34035400
H	2.04721300	-4.55645200	-0.55531400
C	3.09031800	-2.19132000	-2.90513800
H	2.58624800	-2.64411100	-3.76613300
H	3.05191200	-1.10405700	-3.01947100
H	4.14087900	-2.49792100	-2.94989000
C	-2.78584600	-1.75157300	-2.28608300
H	-1.70985800	-1.86171900	-2.11317400
C	-3.40907600	-3.16548700	-2.25061800
H	-4.49222300	-3.11730200	-2.40949800
H	-2.97877600	-3.79005400	-3.04126800
H	-3.23415000	-3.66695400	-1.29294400
C	-2.96981200	-1.13166300	-3.68302500
H	-4.01921600	-1.13293600	-3.99681000

H	-2.60773700	-0.09906000	-3.72461600
H	-2.41390100	-1.71675500	-4.42328200
C	0.49073600	0.41394400	-3.00407300
H	-0.42894600	0.72204500	-3.51800000
H	0.37299500	-0.64113600	-2.73386700
H	1.30596400	0.49173200	-3.73545200
C	4.12128500	2.75309300	-1.29237900
H	4.40019900	3.78901300	-1.51420000
H	5.04783700	2.17266800	-1.26291400

3a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.195327 a.u.

M06 SCF energy in solution: -1698.434962 a.u.

M06 Free energy in solution: -1697.695491 a.u.

C	-0.05943400	-1.71937100	-3.20075000
C	0.55854200	-0.55429700	-2.45089400
C	1.74220600	-0.69751300	-1.68939500
C	2.67673600	-1.89237500	-1.75284700
H	2.63330100	-2.33859800	-2.75939000
H	2.17572900	0.20893500	-1.27040900
C	-0.67500000	-2.49504300	-2.02586200
C	4.16170100	-1.63874700	-1.41380700
C	3.50162600	-3.74964200	-0.32667000
C	2.27952800	-2.92785800	-0.71732500
C	1.05257500	-2.87844600	-0.18511800
H	0.16611900	0.44722500	-2.61298600
H	-1.75291500	-2.32624200	-1.89959100
H	-0.44029600	-3.55868600	-2.00543000
H	-0.80765900	-1.38031200	-3.92389600
H	0.68633300	-2.30841500	-3.74480400
H	3.64995200	-3.73567500	0.76009700
H	3.40582700	-4.80346300	-0.61588300
H	4.71651400	-1.17009900	-2.23327600
H	4.23287000	-0.97951900	-0.53858000
C	-1.93393600	2.26824300	1.31391400
C	-0.66654300	2.73638400	1.44792800
C	-0.53698600	0.74644700	0.35763600
N	0.17321400	1.80130900	0.85547000
N	-1.83644500	1.05304400	0.65217500
Rh	-0.02457100	-1.20472500	-0.50420100
H	-0.28473000	3.63533000	1.90537700
H	-2.88136800	2.68299700	1.61951800
C	-2.96411200	0.21638700	0.29198500
C	-3.40581200	-0.75942000	1.21483500
C	-3.59489600	0.43775800	-0.95174300
C	-4.48674800	-1.56240100	0.82633400
C	-4.67221900	-0.39474500	-1.28051300
C	-5.10694500	-1.38982200	-0.40850000
H	-4.85785700	-2.32400800	1.50392800
H	-5.18578200	-0.25563800	-2.22646800
H	-5.94585000	-2.02229300	-0.68462700
C	1.61322500	1.96068900	0.80779000
C	2.16610700	2.76343300	-0.21397400
C	2.39563700	1.35233400	1.81086000
C	3.55845600	2.91683200	-0.22665000
C	3.78301800	1.54003900	1.74329800
C	4.36036400	2.30764800	0.73534600
H	4.02026100	3.52892300	-0.99490600
H	4.41789800	1.09133800	2.50101400
H	5.43768700	2.44404800	0.70758700
C	-3.19808800	1.57932600	-1.88497100
H	-2.21011300	1.94175800	-1.58111400
C	-4.18747100	2.75645900	-1.74096300
H	-3.88330000	3.59207000	-2.38124600
H	-5.19907400	2.45608600	-2.03647300
H	-4.23702400	3.12121000	-0.70921200
C	-3.09039800	1.14876200	-3.35927900
H	-2.71360500	1.98107300	-3.96391700
H	-2.40930000	0.30001700	-3.48447100
H	-4.06149400	0.86172500	-3.77622900
C	1.31260200	3.49754700	-1.24724100
H	0.29551600	3.09272000	-1.20140800
C	1.22644000	5.00155500	-0.90991000
H	2.21678300	5.46942700	-0.94557000
H	0.58353400	5.51915400	-1.63060600
H	0.81637200	5.17054500	0.09173500
C	1.81524000	3.30080000	-2.69037300
H	1.89867500	2.24020700	-2.95219500
H	1.12031200	3.77136000	-3.39466500
H	2.79652700	3.76047400	-2.84954200
C	1.79458800	0.57633400	2.98036200
H	0.73326200	0.40791200	2.77130500
C	1.88123700	1.40674300	4.27861800
H	1.41365900	0.86653500	5.10949000
H	2.92347500	1.60613700	4.55199200
H	1.37437900	2.37243600	4.17366100
C	2.44267200	-0.80789300	3.17027700
H	1.93560600	-1.34987800	3.97676100
H	2.37585400	-1.40897800	2.25693600
H	3.49956100	-0.72963300	3.44794600
C	-2.81292600	-0.89172300	2.61729800
H	-1.79511100	-0.48397200	2.59836200
C	-3.63017400	-0.05262200	3.62517300
H	-4.66374300	-0.41270200	3.67996800
H	-3.19249000	-0.12671000	4.62696100
H	-3.65994800	1.00608800	3.34793400
C	-2.71637400	-2.34784700	3.10780900
H	-3.70335200	-2.77872300	3.30696500
H	-2.21166400	-2.99441900	2.38219500
H	-2.15521500	-2.38578000	4.04775400
C	0.43123600	-3.81027400	0.81515800
H	-0.27490600	-4.50230300	0.33809000
H	-0.11542900	-3.27697700	1.60554300
H	1.20374500	-4.40986400	1.31502800
C	4.67745500	-3.05279900	-1.06879000
H	5.59530200	-3.03111200	-0.47425500
H	4.90674000	-3.59487700	-1.99375100

TS3a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.161548 a.u.

M06 SCF energy in solution: -1698.412251 a.u.

M06 Free energy in solution: -1697.671633 a.u.

C	2.14437500	-2.04257300	-0.07620700
C	1.23737000	-2.17735300	0.77838000
C	1.29119900	-2.17055600	-2.94617900
C	0.90776100	-0.84560200	-3.01689300
C	-0.46725200	-0.38053400	-2.92077500
C	-1.63110500	-1.15893000	-3.46179300
C	-1.65042600	-1.46591400	-2.00482800
H	-2.38624300	-0.94134600	-1.41489000
H	-1.45826000	-2.49670200	-1.71486200
H	1.67885100	-0.08910500	-3.13816500
H	0.54382700	-2.96215500	-2.97146200
H	-0.62023500	0.68791300	-2.81962600
H	-1.37219300	-1.97764700	-4.13089300
C	2.72598300	-2.58888700	-3.13472400
H	2.77058500	-3.29621000	-3.97375400
H	3.31976500	-1.71421200	-3.43062100
C	3.46166500	-2.30582000	-0.69593700
H	3.94984400	-1.36319000	-0.97421600
H	4.09189400	-2.76966200	0.07534800
H	-2.45112900	-0.55442100	-3.84432700
C	-1.40476000	1.59977100	2.01008700
C	-0.10250800	1.95161600	2.04586600
C	-0.30892300	0.28169900	0.49538000
N	0.56375200	1.15280400	1.12080000
N	-1.53343700	0.59374400	1.05376100
Rh	0.35680300	-1.07678500	-0.87443400
H	0.41599100	2.69472400	2.62924500
H	-2.25824400	1.96717700	2.55662600
C	-2.86539800	0.19021000	0.63094700
C	-3.55227400	1.03474100	-0.27598300
C	-3.47090500	-0.94873000	1.20046800
C	-4.84640100	0.65852300	-0.65717300
C	-4.76671100	-1.27552900	0.77713200
C	-5.44515600	-0.49127500	-0.14969500
H	-5.39947600	1.28316200	-1.35152800
H	-5.25786200	-2.14845400	1.19471200
H	-6.44998600	-0.76296900	-0.46015600
C	1.96351500	1.39840400	0.80256300
C	2.96055200	0.97977900	1.70940400
C	2.26981600	2.16201800	-0.35032200
C	4.29515000	1.25912900	1.38153700
C	3.62098200	2.40006500	-0.62904300
C	4.62746900	1.94143600	0.21734500
H	5.08406200	0.94631800	2.05795800
H	3.89158100	2.97579500	-1.50738700
H	5.66871400	2.14479300	-0.01659200
C	-2.81179700	-1.76924600	2.30134200
H	-1.75340000	-1.50172900	2.32446100
C	-2.97731000	2.35120600	-0.79821500
H	-1.90726600	2.37439400	-0.57202400
C	2.65518200	0.32376900	3.05381900
H	1.61152200	-0.00449700	3.04467000
C	1.19415100	2.82890200	-1.20749400
H	0.29889300	2.19994900	-1.17729800
C	-3.62876500	3.55078300	-0.07542200
H	-3.19496300	4.49209600	-0.43120200
H	-4.70746800	3.58355800	-0.26530000
H	-3.48286000	3.50112200	1.00834600
C	-3.12808200	2.51669800	-2.32283600
H	-2.71378900	1.66467700	-2.87255600
H	-4.17590100	2.62353000	-2.62244900
H	-2.60519100	3.42079900	-2.65410700
C	0.82328000	4.20818400	-0.61529900
H	1.69387900	4.87385500	-0.61507200
H	0.03703300	4.68323100	-1.21390200
H	0.46099500	4.12946000	0.41418600
C	1.58495800	2.99977500	-2.68662200
H	2.36600200	3.75598900	-2.81979200
H	1.94829500	2.06772900	-3.13223900
H	0.71666600	3.33801700	-3.26310600
C	2.81237500	1.34559700	4.20206700
H	2.55064400	0.88492700	5.16134100
H	3.84705000	1.69981300	4.27019900
H	2.17315300	2.22410300	4.06456200
C	3.53105600	-0.91182100	3.33766800
H	3.18838000	-1.41053100	4.25109400
H	3.49155800	-1.63195700	2.51529700
H	4.57978800	-0.63870300	3.49647000
C	-3.41407100	-1.40253600	3.67523200
H	-4.48180200	-1.64604400	3.71565100
H	-2.91164300	-1.95968800	4.47422400
H	-3.30835200	-0.33342900	3.89012200
C	-2.90440100	-3.28658800	2.05760100
H	-3.93870200	-3.64522600	2.08791900
H	-2.48178300	-3.56698400	1.08603000
H	-2.35766200	-3.82680500	2.83864400
C	0.71155600	-2.64007300	2.07921900
H	1.49863000	-3.16439700	2.63358600
H	-0.12620000	-3.32825300	1.93942300
H	0.35920700	-1.80899600	2.69644800
C	3.39388100	-3.24473800	-1.91194400
H	2.86482700	-4.16481300	-1.63486400
H	4.41444500	-3.53311000	-2.18859200

4a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.200047 a.u.

M06 SCF energy in solution: -1698.441522 a.u.

M06 Free energy in solution: -1697.698399 a.u.

C	-2.12795400	-1.30952300	1.96945800
C	-1.17538300	-1.95627700	1.48583400
C	-1.51319000	1.27678000	3.16315000

C	-0.95731600	2.17704700	2.24038800
C	0.38546600	2.07074100	1.80595600
C	1.43006600	1.34741200	2.66269000
C	1.03237800	-0.12112300	2.52854200
H	1.76471300	-0.73809200	2.01244400
H	0.68646800	-0.61438200	3.44049500
H	-1.63190800	2.82977900	1.68898200
H	-0.86440100	0.83469300	3.91658600
H	0.72325600	2.77017100	1.04829500
H	1.41489700	1.70463500	3.70114100
C	-2.97643600	1.26655000	3.51627600
H	-3.12078500	1.85827500	4.43164700
H	-3.56274200	1.75846300	2.72846700
C	-3.47626100	-1.03507900	2.51354300
H	-4.09313900	-0.58324000	1.72405000
H	-3.93175000	-2.00794700	2.74341500
H	2.43158900	1.52362400	2.26398900
C	1.60905700	-0.49562100	-2.42174900
C	0.31794700	-0.41062800	-2.80853600
C	0.37065600	-0.15107600	-0.53826100
N	-0.43009000	-0.19410600	-1.65588100
N	1.64047700	-0.32312200	-1.03691200
Rh	-0.59514200	0.17046500	1.29424700
H	-0.13998400	-0.48105600	-3.78169100
H	2.51238300	-0.65416200	-2.98775100
C	2.92611500	-0.20819700	-0.36096200
C	3.57497500	-1.37836800	0.08992600
C	3.54329700	1.06430300	-0.30465900
C	4.83306400	-1.23302400	0.68984700
C	4.80223600	1.14481700	0.30534500
C	5.43623400	0.01417800	0.81169700
H	5.35344400	-2.11290600	1.05307200
H	5.30121200	2.10583200	0.37045900
H	6.41254400	0.10264000	1.27952000
C	-1.85919400	0.07125700	-1.67838900
C	-2.29617600	1.42065400	-1.66701600
C	-2.75801900	-1.01123300	-1.80718100
C	-3.67886700	1.64846800	-1.67078100
C	-4.12818300	-0.71637600	-1.81934400
C	-4.58654800	0.59391100	-1.72990900
H	-4.05161800	2.66659100	-1.65571700
H	-4.84514000	-1.52526800	-1.91474900
H	-5.65364700	0.79772200	-1.74012400
C	2.94916000	2.31182400	-0.95924400
H	1.86918900	2.16228700	-1.06071400
C	3.52962800	2.50351300	-2.37888100
H	3.32890500	1.64403400	-3.02519300
H	3.09181600	3.38976900	-2.85227100
H	4.61530800	2.64564600	-2.33625500
C	3.16863500	3.60131000	-0.14395900
H	2.86601900	3.49281100	0.90237700
H	4.21803400	3.91473300	-0.15354000
H	2.58965200	4.42089200	-0.58395400
C	3.00623700	-2.77770100	-0.12643400
H	1.93486500	-2.67959300	-0.32345900
C	3.64842100	-3.43368500	-1.36893700
H	4.72999000	-3.54723000	-1.23483300
H	3.22313800	-4.42947900	-1.53847000
H	3.48566200	-2.83968100	-2.27428700
C	3.17690100	-3.69625900	1.09851900
H	4.22576000	-3.96493500	1.26373100
H	2.80738600	-3.22903000	2.01819100
H	2.62887000	-4.63223900	0.94416800
C	-2.29976700	-2.44994200	-2.03154100
H	-1.24895000	-2.52263700	-1.73312000
C	-2.38287300	-2.80657500	-3.53300500
H	-2.01705800	-3.82525600	-3.70371400
H	-3.41828400	-2.75591100	-3.88803900
H	-1.78852400	-2.12641700	-4.15216600
C	-3.09357400	-3.47979300	-1.20644300
H	-2.64159100	-4.47176700	-1.31582400
H	-3.10683300	-3.22172300	-0.14358400
H	-4.13088000	-3.56259200	-1.54811200
C	-1.33167800	2.60186700	-1.78764900
H	-0.39823700	2.33438900	-1.28262400
C	-1.00332300	2.87001500	-3.27494300
H	-1.91258500	3.12885800	-3.82925000
H	-0.30430600	3.70952100	-3.36394800
H	-0.54739200	2.00245000	-3.76028300
C	-1.84882400	3.90235300	-1.14619000
H	-2.66865200	4.34350800	-1.72337100
H	-2.20784900	3.75078800	-0.12321200
H	-1.04475300	4.64542900	-1.11804600
C	-0.44396100	-3.19655800	1.16415000
H	0.49565800	-3.24829300	1.72123300
H	-0.20238800	-3.26107200	0.09948600
H	-1.04758700	-4.07080700	1.43386400
C	-3.52082300	-0.14855000	3.76702000
H	-2.95322200	-0.62724400	4.57532800
H	-4.56059900	-0.08339000	4.10580000

TS4a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.168976 a.u.

M06 SCF energy in solution: -1698.403787 a.u.

M06 Free energy in solution: -1697.659469 a.u.

C	-2.14208300	-2.26625500	-1.33088300
C	-1.98718600	-0.99249100	-1.53874600
C	-0.61378800	-3.54306100	-0.80302200
C	0.46979900	-3.24169600	0.14741500
C	1.66294300	-2.65147400	-0.21279000
C	1.99720200	-2.28579100	-1.65128700
C	0.90976800	-1.30851800	-2.11164200
H	1.28127200	-0.31667500	-2.35404200
H	0.28007900	-1.67270700	-2.92849500
H	0.31112900	-3.53055000	1.18580000
H	-0.25837200	-3.65970200	-1.82722800
H	2.43686500	-2.54564100	0.53779800

H	2.04725800	-3.18578900	-2.28135600
C	-1.54681100	-4.67892200	-0.40873900
H	-0.97856800	-5.61734900	-0.43264500
H	-1.90419400	-4.54224600	0.62035400
C	-3.25480500	-3.27529300	-1.41648500
H	-3.92639800	-3.12158800	-0.56010900
H	-3.84282200	-3.06223000	-2.31811100
H	2.98380900	-1.81888900	-1.68354000
C	1.39109500	2.41048000	1.10437800
C	0.07681800	2.65556300	1.27973200
C	0.25058800	0.66866700	0.16029400
N	-0.61695400	1.60421100	0.68792100
N	1.49492400	1.20007200	0.42699800
Rh	-0.29818900	-1.20156100	-0.44121800
H	-0.43743500	3.47158800	1.75943600
H	2.26476300	2.96787500	1.39901600
C	2.80951800	0.62293900	0.21556800
C	3.49837800	0.91721200	-0.98147000
C	3.40363900	-0.08705100	1.28444100
C	4.79007100	0.39212500	-1.12365200
C	4.69681700	-0.58680000	1.08184200
C	5.37734400	-0.36469900	-0.11273600
H	5.35092300	0.59070300	-2.03092000
H	5.18777900	-1.13835800	1.87750600
H	6.38102700	-0.75861700	-0.24535900
C	-2.06704800	1.62285000	0.68663800
C	-2.77514300	0.67600500	1.46326400
C	-2.71576100	2.66703500	-0.01106300
C	-4.16995400	0.77990800	1.49303400
C	-4.11491300	2.72774000	0.07423600
C	-4.83640600	1.79450000	0.80795200
H	-4.74796900	0.07026500	2.07386600
H	-4.64361500	3.51980600	-0.44675800
H	-5.91953700	1.86006600	0.85699200
C	2.74401200	-0.22472000	2.65883400
H	1.67927300	0.00804200	2.55464800
C	3.35506300	0.80128000	3.64056400
H	3.26375400	1.82779600	3.27209800
H	2.85131300	0.74595300	4.61211400
H	4.42017600	0.59992700	3.80108700
C	2.84281900	-1.63517300	3.27004600
H	2.38408900	-2.39785500	2.63305100
H	3.87995400	-1.93225800	3.45800600
H	2.32403600	-1.65319900	4.23484500
C	2.92779200	1.84859500	-2.05121300
H	1.83652000	1.85420000	-1.94979300
C	3.41976800	3.29493800	-1.81686900
H	4.51170200	3.35132800	-1.89071500
H	2.99522700	3.96796700	-2.57033200
H	3.13133400	3.67079900	-0.82995500
C	3.25912300	1.41443500	-3.49140800
H	4.32420300	1.53249400	-3.71827700
H	2.98947900	0.37054500	-3.68300500
H	2.70940100	2.04150600	-4.20150600
C	-1.98666400	3.73986500	-0.82510200
H	-0.92445100	3.48185000	-0.87159100
C	-2.10669800	5.12236200	-0.14777600
H	-1.52998000	5.86923700	-0.70439700
H	-3.14915300	5.45892700	-0.12090900
H	-1.74068300	5.11356100	0.88476400
C	-2.48701200	3.82725700	-2.28124600
H	-1.91176200	4.58532000	-2.82420500
H	-2.37166500	2.87601200	-2.80844200
H	-3.54179600	4.11729900	-2.33621900
C	-2.06453400	-0.38059600	2.30962800
H	-1.18439400	-0.73628500	1.74545700
C	-1.53909600	0.23210300	3.62607700
H	-2.37383500	0.60364400	4.23163000
H	-1.00621800	-0.52350500	4.21474800
H	-0.85580700	1.06788700	3.44747700
C	-2.91950100	-1.62181900	2.61185300
H	-3.73818900	-1.39627400	3.30366400
H	-3.35136900	-2.05162900	1.70188900
H	-2.29945400	-2.38678700	3.09243900
C	-2.72837400	0.03046100	-2.32776100
H	-2.04134600	0.58930600	-2.97297700
H	-3.23121400	0.75129800	-1.67933400
H	-3.48214100	-0.44583400	-2.96737500
C	-2.71379600	-4.70411400	-1.39260200
H	-3.48495800	-5.42232700	-1.09963700
H	-2.35320400	-4.99573400	-2.38689400

TS5a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.192324 a.u.

M06 SCF energy in solution: -1698.433704 a.u.

M06 Free energy in solution: -1697.692484 a.u.

C	0.28184800	-1.30663500	-3.35817800
C	0.98527500	-1.23361900	-2.01727800
C	0.66444900	-2.15392600	-0.98509400
C	-0.14889000	-3.41775800	-1.20948900
H	0.13590500	-3.86872900	-2.17516000
H	1.30977400	-2.15763900	-0.10969400
C	-1.13923900	-0.83159900	-3.02362200
C	-0.03359900	-4.52341800	-0.13765000
C	-2.40204800	-4.35548600	-0.75277000
C	-1.63808500	-3.11652000	-1.20305900
C	-2.09347200	-1.86554400	-1.39764800
H	1.88084000	-0.62831000	-1.91420500
H	-1.29051700	0.24699600	-3.17033000
H	-1.92501200	-1.36696600	-3.55139400
H	0.75458500	-0.64809700	-4.09503100
H	0.28534600	-2.32060500	-3.77536700
H	-3.03280700	-4.13057600	0.11660700
H	-3.07345300	-4.73432400	-1.53367800
H	0.89693000	-5.09574000	-0.21185700
H	-0.07557900	-4.07354000	0.86353200
C	0.26637300	2.45003000	1.97769700

C	1.56605100	2.07999100	1.85334800
C	0.36404200	0.77050100	0.44047000
N	1.61383700	1.05175900	0.91637300
N	-0.44932500	1.64106500	1.10871700
Rh	-0.64214800	-0.44061400	-0.92358200
H	2.45840400	2.44945000	2.33287300
H	-0.20791000	3.19750300	2.59409800
C	-1.88061700	1.68200400	0.89645400
C	-2.71078700	0.91682600	1.74907800
C	-2.39247600	2.54452300	-0.10437600
C	-4.09348100	1.01063500	1.54804400
C	-3.78443700	2.58643000	-0.25982000
C	-4.62468600	1.83014800	0.55449000
H	-4.76373000	0.44220600	2.18548300
H	-4.21770700	3.23767600	-1.01208000
H	-5.70132200	1.89039100	0.42239500
C	2.86351800	0.44358300	0.50197200
C	3.56220700	1.02108300	-0.57987600
C	3.36265200	-0.65004200	1.24250800
C	4.77944500	0.43051800	-0.94449200
C	4.58479600	-1.19631000	0.82972400
C	5.28163100	-0.66985700	-0.25529200
H	5.34723300	0.84698100	-1.77057900
H	5.00276200	-2.03837200	1.37134400
H	6.22888400	-1.10954600	-0.55419000
C	-1.50255600	3.47970000	-0.92108800
H	-0.46661800	3.13925800	-0.82225400
C	-1.57635400	4.91361400	-0.35186100
H	-0.90927900	5.57981700	-0.91002800
H	-2.59348600	5.31444600	-0.42664200
H	-1.28184400	4.94635300	0.70276600
C	-1.84042100	3.47936800	-2.42309500
H	-1.12300500	4.10487600	-2.96520100
H	-1.79793100	2.47036200	-2.84835500
H	-2.83823500	3.88509900	-2.62173500
C	3.08268800	2.28077300	-1.29950500
H	2.05002000	2.47772200	-0.99401200
C	3.93181600	3.49782700	-0.87355400
H	4.98047500	3.36821800	-1.16398200
H	3.56032500	4.40993500	-1.35406000
H	3.90393000	3.65049000	0.21096300
C	3.08014000	2.13568400	-2.83301400
H	2.46209400	1.29214500	-3.16001100
H	2.67819600	3.04538100	-3.29274400
H	4.08875300	1.98805200	-3.23365600
C	2.66435600	-1.18226000	2.49349200
H	1.61381400	-0.87301800	2.45370200
C	3.28705500	-0.55853800	3.76241400
H	2.76791000	-0.91686500	4.65847300
H	4.34415100	-0.83301600	3.85197000
H	3.22686000	0.53474300	3.75270800
C	2.68519100	-2.71821300	2.60193000
H	2.07447200	-3.03668100	3.45377200
H	2.28857500	-3.20144400	1.70277100
H	3.69645300	-3.10395500	2.77022200
C	-2.16403800	0.05657000	2.88498700
H	-1.07138000	0.05883000	2.82070800
C	-2.54547200	0.65424300	4.25558700
H	-3.63175300	0.66530000	4.39866000
H	-2.10831500	0.05759700	5.06377900
H	-2.18536500	1.68364600	4.36179100
C	-2.62150900	-1.41043900	2.77470200
H	-3.70919900	-1.50564500	2.86786300
H	-2.32143100	-1.84623400	1.81533000
H	-2.17077300	-2.00394500	3.57805300
C	-3.53567900	-1.43895400	-1.41884800
H	-3.92461900	-1.36245500	-2.44314500
H	-3.69183400	-0.46470700	-0.94125700
H	-4.15611600	-2.16907200	-0.88539900
C	-1.29117800	-5.37855500	-0.39235500
H	-1.55749500	-6.00555400	0.46333300
H	-1.11194700	-6.04885800	-1.24118600

5a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.266137 a.u.

M06 SCF energy in solution: -1698.51288 a.u.

M06 Free energy in solution: -1697.766795 a.u.

C	-1.34814500	-2.72415000	-2.09055200
C	-0.90349400	-1.28609800	-1.87183100
C	0.39362700	-0.85597900	-2.25456900
C	1.44191800	-1.90136100	-2.57537800
H	1.09822100	-2.59799300	-3.35594000
H	0.56320100	0.17350800	-2.56537600
C	2.84018500	-1.35751500	-2.93947000
C	3.13817300	-2.59432800	-0.87976900
C	1.64674400	-2.62702800	-1.22094000
C	0.67358400	-3.35095400	-0.55366100
H	-1.69945300	-0.54919700	-1.86921300
H	-2.43351600	-2.78806700	-1.97165900
H	-1.13869400	-2.99288700	-3.13582300
H	3.36826000	-1.78124900	-0.17676000
H	3.48202700	-3.52644000	-0.42179000
H	2.99480900	-1.29905000	-4.02098300
H	2.96405400	-0.34675300	-2.53118100
C	-1.55502900	2.53211900	1.22403000
C	-0.24544300	2.83174600	1.40153900
C	-0.35161300	0.77555700	0.42453600
N	0.47751200	1.75501800	0.90432500
N	-1.60981700	1.28036100	0.61879600
Rh	0.34979100	-1.06170100	-0.15487000
H	0.23735000	3.69579600	1.82980100
H	-2.44999800	3.08109800	1.46921100
C	3.81519800	-2.31463700	-2.23680200
H	4.82141100	-1.89898200	-2.12903300
H	3.90398500	-3.24856700	-2.80598500
C	1.02856200	-4.16583100	0.67687500
H	1.95033300	-3.83600600	1.15957700

H	0.22237100	-4.13033800	1.41832300
H	1.15510400	-5.22228500	0.39919800
C	1.92230400	1.67065000	0.91792600
C	2.53920000	0.94641300	1.95985400
C	2.65319500	2.33958200	-0.08626900
C	3.93597900	0.84737300	1.93827600
C	4.04845500	2.21801700	-0.04825000
C	4.68304900	1.47063000	0.94097000
H	4.44787700	0.29536000	2.72006900
H	4.64774700	2.72211900	-0.79992200
H	5.76642000	1.39114900	0.94754800
C	-2.86913800	0.64731200	0.27840100
C	-3.54278000	1.07819800	-0.88649200
C	-3.40296100	-0.31921700	1.15438800
C	-4.77134500	0.47212600	-1.17809500
C	-4.63283800	-0.89341400	0.80624800
C	-5.30827300	-0.50914900	-0.34839400
H	-5.31946100	0.77856200	-2.06344000
H	-5.07555900	-1.63943000	1.45919100
H	-6.26384300	-0.96335500	-0.59448800
C	-2.74034900	-0.70501300	2.47421000
H	-1.75198600	-0.23600200	2.51132100
C	-3.01465000	2.19286100	-1.79002500
H	-1.97124600	2.38806700	-1.51881700
C	1.72968600	0.29158900	3.07688800
H	0.74196700	0.76383600	3.09988200
C	1.98865400	3.22112400	-1.14093400
H	0.91382700	3.01008000	-1.13104300
C	-3.80644300	3.49849500	-1.56077400
H	-3.39901900	4.30628900	-2.17897500
H	-4.86118200	3.36954400	-1.82833000
H	-3.76850500	3.82121900	-0.51465900
C	-3.03107800	1.81890000	-3.28505700
H	-2.47222800	0.89796500	-3.48362700
H	-4.05003300	1.67965800	-3.66186100
H	-2.57591000	2.62342800	-3.87316400
C	-3.55111400	-0.16327100	3.67019800
H	-4.55389900	-0.60365300	3.70300600
H	-3.04863200	-0.40486000	4.61377900
H	-3.66713200	0.92473900	3.61633000
C	-2.52661600	-2.22498900	2.59916000
H	-1.93186400	-2.60984300	1.76276100
H	-2.00098400	-2.45837100	3.53241300
H	-3.47606800	-2.77092700	2.61497700
C	2.35466500	0.49304400	4.47098100
H	1.67445500	0.11825300	5.24335800
H	3.30167500	-0.04565200	4.58203100
H	2.54373300	1.55250600	4.67054000
C	1.51540300	-1.20651100	2.80430900
H	0.96926400	-1.37957500	1.85070100
H	2.46577800	-1.74450400	2.72588700
H	0.90999000	-1.67596800	3.58726700
C	2.17311700	4.71364900	-0.79045900
H	3.23344000	4.99034900	-0.79615100
H	1.65674200	5.34453700	-1.52243600
H	1.77489300	4.95140600	0.20201100
C	2.49327400	2.94126300	-2.56837900
H	3.55165000	3.19719800	-2.68783400
H	2.37079500	1.88809700	-2.84219100
H	1.93079200	3.54676000	-3.28756900
C	-0.68428300	-3.73672700	-1.13421500
H	-1.35880800	-3.90379200	-0.28669300
H	-0.58486500	-4.71577000	-1.62777700

6a ($X = CH_2$)

B3LYP SCF energy in gas phase: -1699.16119 a.u.

M06 SCF energy in solution: -1698.417206 a.u.

M06 Free energy in solution: -1697.683825 a.u.

C	-1.41259800	-0.17372100	1.62668500
H	-1.51655100	-0.92215000	2.41659800
C	-0.95178100	1.12264500	1.99159400
H	-1.20894700	1.98879300	1.38590500
C	-0.36313800	1.38091600	3.32968200
C	-0.82896200	0.74417000	4.60606100
H	-0.76488500	1.34837700	5.50579800
H	-1.69960200	0.09638300	4.55951400
C	0.46039900	0.21768200	4.03810800
H	0.43682200	-0.81207200	3.67349000
H	1.39376700	0.50792900	4.50903500
C	1.53191300	-0.75409000	-2.57976000
C	1.32428200	0.58125800	-2.66628200
C	0.88570000	-0.03088800	-0.52420700
N	1.25197000	-1.12352700	-1.26829900
N	0.91921600	1.01814100	-1.40821700
H	0.10937500	2.35335700	3.43474900
C	-2.35828800	-0.41431300	0.47755700
H	-2.14980400	-1.39413800	0.03518700
H	-2.20162300	0.33332900	-0.30641700
C	-4.82232300	-0.72309500	-0.17835400
H	-4.67676100	-0.02507600	-1.01532100
H	-4.58612200	-1.72250200	-0.57204700
C	-6.21564400	-0.68106500	0.26543200
C	-7.36091300	-0.64112000	0.65281700
Rh	0.70893600	0.01426900	1.44201700
H	1.85937100	-1.47149500	-3.31473800
H	1.43373900	1.26364700	-3.49334500
C	0.67289200	2.41797900	-1.10907000
C	-0.53072100	3.00996300	-1.55532800
C	1.67761100	3.15638000	-0.44726300
C	-0.73001300	4.36498100	-1.25943800
C	1.41684100	4.50591200	-0.17546400
C	0.22351500	5.10444200	-0.56594500
H	-1.64320500	4.85146900	-1.58590700
H	2.17019800	5.10081500	0.33202900
H	0.04470600	6.15371400	-0.34925900
C	1.45301500	-2.46593200	-0.75547100
C	0.49007800	-3.46154600	-1.02712000

C	2.64357400	-2.73596400	-0.04632200
C	0.73008200	-4.74182100	-0.51111200
C	2.81949800	-4.02940600	0.45976100
C	1.87014600	-5.02224600	0.23635600
H	0.01258400	-5.53359100	-0.69904200
H	3.71877500	-4.26829000	1.01858100
H	2.02791800	-6.02222300	0.62991600
C	-1.57278500	2.26895700	-2.39196600
H	-1.39198700	1.19260800	-2.29240100
C	3.04567700	2.58377100	-0.08645500
H	3.04483000	1.51459500	-0.32019000
C	-0.74420400	-3.21298000	-1.89056600
H	-0.91896400	-2.13170700	-1.92988900
C	3.72429700	-1.68062800	0.17118100
H	3.54084200	-0.85477700	-0.52384700
C	-1.42862600	2.62994700	-3.88741500
H	-2.15905500	2.07431200	-4.48606000
H	-1.60514500	3.69937100	-4.04744100
H	-0.43075100	2.39948600	-4.27441500
C	-3.01838200	2.54257900	-1.93323700
H	-3.71031900	1.88592400	-2.47197800
H	-3.15088700	2.37174800	-0.85984400
H	-3.32528700	3.57217300	-2.14562400
C	-0.50879200	-3.70392400	-3.33623400
H	-0.32516800	-4.78406900	-3.35429600
H	-1.38927700	-3.50101700	-3.95607400
H	0.35194400	-3.21478400	-3.80402900
C	-2.01671500	-3.86922300	-1.32071200
H	-2.17219400	-3.61692900	-0.26643200
H	-2.89329300	-3.53569500	-1.88705900
H	-1.98225500	-4.96114600	-1.39865300
C	4.15342200	3.23376100	-0.94191300
H	4.23209400	4.30852000	-0.74448500
H	5.12543400	2.78086900	-0.71560500
H	3.95953000	3.10531900	-2.01225200
C	3.35611900	2.72704600	1.41542300
H	3.40108100	3.77736200	1.72262300
H	2.58908100	2.23322700	2.02572700
H	4.32694300	2.27602700	1.65033200
C	5.14212500	-2.20513400	-0.12964400
H	5.86571200	-1.38472400	-0.07122200
H	5.45988400	-2.97239300	0.58407400
H	5.19812700	-2.63620300	-1.13420400
C	3.65898400	-1.10954800	1.59724800
H	2.66227400	-0.66234500	1.81957300
H	3.80851100	-1.88705400	2.35425000
H	4.40034000	-0.31921200	1.75207400
C	-8.74898900	-0.59697200	1.10807100
H	-9.17793800	-1.60388500	1.17572900
H	-9.37425900	-0.01509000	0.42036200
H	-8.82826300	-0.13508300	2.09956700
C	-3.82692000	-0.37788600	0.95094500
H	-4.06428400	0.61600200	1.35011300
H	-3.96974600	-1.08743100	1.77583000

TS6a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.150491 a.u.

M06 SCF energy in solution: -1698.403552 a.u.

M06 Free energy in solution: -1697.671495 a.u.

C	-1.48227800	-0.09615100	1.69973000
H	-1.59416000	-0.85368300	2.47753500
C	-1.02193700	1.19862500	2.08537900
H	-1.25041100	2.08087100	1.49200800
C	-0.19952500	1.33875600	3.25865100
C	-0.23601400	0.47921600	4.48158700
H	0.06747600	0.97663000	5.40200400
H	-1.16161500	-0.07786300	4.62511300
C	0.83747600	-0.24616900	3.71187900
H	0.66300000	-1.31002200	3.53117500
H	1.85712000	0.00937600	3.99361000
C	1.43741000	-0.81351800	-2.60207800
C	1.39110000	0.53785700	-2.68955500
C	0.84464000	-0.02334800	-0.55214000
N	1.09057100	-1.14807100	-1.29703200
N	1.02567900	1.00935800	-1.43335900
H	0.38462200	2.25306200	3.33607100
C	-2.43576700	-0.27603700	0.54715000
H	-2.27237800	-1.25650300	0.08981400
H	-2.24157100	0.47521200	-0.22635200
C	-4.90831900	-0.37116900	-0.13626600
H	-4.70539400	0.37062000	-0.92269500
H	-4.73863100	-1.35515900	-0.59665700
C	-6.29964900	-0.26118900	0.30166500
C	-7.44379800	-0.16699500	0.68291700
Rh	0.65828000	0.12147000	1.51224200
H	1.69259900	-1.56268900	-3.33358700
H	1.59128000	1.20411600	-3.51333700
C	0.96844800	2.41768200	-1.09619700
C	-0.17408800	3.16529500	-1.45101700
C	2.08716200	2.99542700	-0.45838300
C	-0.19082700	4.52036900	-1.09274200
C	2.00755800	4.34990800	-0.11272100
C	0.87791800	5.10461600	-0.41877600
H	-1.05127700	5.12898900	-1.35117100
H	2.84614900	4.82590500	0.38587700
H	0.83904800	6.15624500	-0.14946400
C	1.11650900	-2.50945100	-0.79252700
C	0.04904700	-3.38108700	-1.10903000
C	2.24470400	-2.93330600	-0.05535200
C	0.11387100	-4.68614300	-0.60541900
C	2.24667400	-4.24926200	0.42703200
C	1.19040600	-5.11487900	0.16603000
H	-0.68928600	-5.38130800	-0.82543100
H	3.09909400	-4.60629100	0.99654800
H	1.21463500	-6.13229000	0.54570100
C	-1.33496500	2.57531400	-2.24856500
H	-1.27016800	1.48311600	-2.18456700

C	3.35590400	2.20266400	-0.15371900
H	3.32612900	1.27705900	-0.73760600
C	-1.11340400	-2.98377200	-2.01724100
H	-1.17924000	-1.88988100	-2.02751500
C	3.48788800	-2.06983600	0.15248100
H	3.26248300	-1.04982400	-0.17445100
C	-1.22266000	2.96264900	-3.73956500
H	-2.03951200	2.51198200	-4.31423200
H	-1.28116000	4.04965400	-3.86497900
H	-0.27663000	2.62960600	-4.17938800
C	-2.71407300	2.99032500	-1.70188600
H	-3.50434100	2.44706200	-2.23179400
H	-2.81380300	2.77739200	-0.63186100
H	-2.90692600	4.05855700	-1.84759600
C	-0.86150500	-3.45502900	-3.46753500
H	-0.78497400	-4.54728300	-3.51109800
H	-1.68962700	-3.14901600	-4.11667600
H	0.06211300	-3.04306200	-3.88585500
C	-2.47195700	-3.53110300	-1.53651700
H	-2.65035500	-3.32560700	-0.47606800
H	-3.28224200	-3.07538100	-2.11606900
H	-2.54757300	-4.61420900	-1.68012800
C	4.63774300	2.94967500	-0.57138100
H	4.80692800	3.84878700	0.03041400
H	5.50992800	2.29994800	-0.43961800
H	4.59529900	3.25170100	-1.62278200
C	3.42507400	1.80646800	1.33139700
H	3.44222900	2.68651100	1.98447700
H	2.53292800	1.21688100	1.63023300
H	4.31140200	1.19951600	1.54281200
C	4.64997300	-2.58072700	-0.72580500
H	5.52728900	-1.93323100	-0.61513200
H	4.94468800	-3.59680300	-0.44094100
H	4.37214100	-2.59890800	-1.78510500
C	3.91621700	-1.99281200	1.62992000
H	3.10865100	-1.60733700	2.26491800
H	4.20468500	-2.97249500	2.02468800
H	4.78177200	-1.33003800	1.73994100
C	-8.83078100	-0.05635500	1.13003900
H	-9.32275600	-1.03618500	1.14730800
H	-9.41120300	0.59513900	0.46584100
H	-8.89075900	0.36321800	2.14147600
C	-3.90239300	-0.17215400	1.01869800
H	-4.07565800	0.80814500	1.47993300
H	-4.09907200	-0.92150600	1.79567600

7a (X = CH_2)

B3LYP SCF energy in gas phase: -1699.158757 a.u.

M06 SCF energy in solution: -1698.406284 a.u.

M06 Free energy in solution: -1697.675222 a.u.

C	1.57210900	-0.38559100	-1.78959600
H	1.75354500	-0.99522900	-2.67241900
C	0.95381900	0.88479000	-1.96990900
H	1.09017800	1.67389200	-1.23494500
C	-0.04442800	1.02646100	-2.97221500
C	-0.12213100	0.11074000	-4.18509700
H	-0.85601700	0.48609500	-4.90386300
H	0.83893000	0.04102100	-4.70765900
C	-0.56521600	-1.18376000	-3.48535300
H	0.10908800	-2.03508900	-3.62243900
H	-1.58956100	-1.47672700	-3.73640700
C	-1.71403300	-0.35652400	2.65725800
C	-1.48820800	0.97952100	2.59743700
C	-0.89416200	0.11325700	0.57757900
N	-1.33894100	-0.86877900	1.42055300
N	-0.98427500	1.25250900	1.32715100
H	-0.64104800	1.93648200	-2.94916900
C	2.50957300	-0.68436800	-0.65330600
H	2.38598300	-1.73455400	-0.36114200
H	2.26233700	-0.07503600	0.22284800
C	4.96928000	-0.85389100	0.05079800
H	4.73883400	-0.27784900	0.95880400
H	4.80908400	-1.91008700	0.31220200
C	6.36466300	-0.64199800	-0.33214900
C	7.51206600	-0.46162000	-0.67013800
Rh	-0.59063900	-0.48644000	-1.50931300
H	-2.10656400	-0.97600700	3.44769600
H	-1.63994800	1.75726100	3.32889200
C	-0.66466300	2.59590800	0.88242200
C	0.59585800	3.13961300	1.21479900
C	-1.64956600	3.33053000	0.18718600
C	0.86906200	4.44440800	0.78267300
C	-1.31651800	4.62895500	-0.22074700
C	-0.07030100	5.17910100	0.06459600
H	1.82704300	4.89503400	1.02027100
H	-2.05038500	5.22401500	-0.75492500
H	0.16344900	6.18950500	-0.25842600
C	-1.48771600	-2.23700100	0.97254300
C	-0.53760000	-3.20956900	1.36103100
C	-2.60029800	-2.54405600	0.15300800
C	-0.70112100	-4.50217000	0.84796300
C	-2.69466600	-3.84992200	-0.34894800
C	-1.75251500	-4.81645300	-0.01106500
H	0.00625900	-5.27740500	1.12265000
H	-3.52990100	-4.11955500	-0.98737100
H	-1.84844900	-5.82559600	-0.40111200
C	1.61925500	2.39415900	2.06950600
H	1.36337700	1.32854900	2.05498100
C	-3.06320700	2.80436900	-0.05040800
H	-3.06097000	1.72580100	0.13434900
C	0.58753200	-2.90731600	2.34738600
H	0.77774700	-1.82805700	2.31943300
C	-3.70399300	-1.52706500	-0.14142300
H	-3.60496100	-0.70486100	0.57424500
C	1.54916300	2.86876300	3.53750700
H	2.26201100	2.31015500	4.15446700
H	1.79809500	3.93321900	3.61454400

H	0.55088600	2.72935200	3.96524800
C	3.06036400	2.53152900	1.54310100
H	3.73026900	1.88063300	2.11572200
H	3.14064500	2.25741700	0.48558800
H	3.43981100	3.55305200	1.65039100
C	0.15990400	-3.27546700	3.78620000
H	-0.04199500	-4.34958000	3.86693400
H	0.95743700	-3.02763100	4.49529900
H	-0.74504100	-2.74464600	4.09839800
C	1.90848600	-3.62113900	2.00539700
H	2.20246200	-3.46548800	0.96242900
H	2.71086600	-3.24166100	2.64701800
H	1.84559400	-4.70120500	2.17691600
C	-4.04737900	3.44376600	0.95333400
H	-4.10261600	4.52908600	0.81284700
H	-5.05502600	3.03522400	0.81561200
H	-3.74481300	3.25747200	1.98953200
C	-3.55312000	3.01761700	-1.49467000
H	-3.65293600	4.07933700	-1.74371000
H	-2.87266800	2.56449200	-2.22430800
H	-4.54181900	2.56346300	-1.62606700
C	-5.11445700	-2.11934200	0.05090300
H	-5.86659500	-1.32820900	-0.03873700
H	-5.34972900	-2.88085900	-0.70012100
H	-5.21954700	-2.57678800	1.03970500
C	-3.56591600	-0.92982300	-1.55075100
H	-2.63858800	-0.31717400	-1.66057600
H	-3.55572700	-1.70175700	-2.32588800
H	-4.37845000	-0.22749800	-1.76901600
C	8.90281700	-0.25105600	-1.06649100
H	9.47431300	-1.18573000	-1.02061900
H	9.39818900	0.47433500	-0.41014700
H	8.97039500	0.12917500	-2.09286100
C	3.98109200	-0.45608900	-1.06745900
H	4.13545600	0.59771600	-1.32951200
H	4.20931900	-1.03940600	-1.96783400

TS1a (X = O)

B3LYP SCF energy in gas phase: -1735.034916 a.u.

M06 SCF energy in solution: -1734.296548 a.u.

M06 Free energy in solution: -1733.58199 a.u.

C	3.24935300	3.38868900	-1.23832000
C	2.43320400	2.13100600	-0.93229000
C	0.97881700	2.07963100	-1.25857800
C	0.09149200	3.19839200	-0.90840500
H	0.60898600	3.95209000	-0.31328300
H	0.78927600	1.62302200	-2.23970600
C	3.02211500	2.96081700	0.18318300
C	-0.89415600	3.87123000	-1.83885800
C	-2.07966300	4.17546100	0.15293000
C	-1.14391200	3.07047200	0.56881600
C	-0.73798200	2.31134400	1.55177100
H	2.94777000	1.19821700	-1.13637000
H	3.85186400	2.52161100	0.72854600
H	2.36173200	3.56318800	0.80272500
H	4.23225400	3.25452700	-1.68034100
H	2.71514800	4.26460500	-1.59812700
H	-3.07908300	3.73500200	0.01142100
H	-2.15218900	4.95941200	0.91341000
H	-0.37401200	4.46665900	-2.59677500
H	-1.54108000	3.13908500	-2.34623900
O	-1.63298200	4.78880100	-1.04879700
Rh	-0.41264700	1.15432500	-0.05653500
C	-0.03722600	-0.88569700	0.12107300
N	1.05233400	-1.69462900	0.31407100
C	0.67129900	-3.02321800	0.43473700
C	2.45344900	-1.31936800	0.29372300
N	-1.09826700	-1.75954500	0.11812100
C	-0.67973800	-3.06490100	0.30718800
C	-2.48322600	-1.39565000	-0.12021800
C	3.06522600	-0.88733600	1.48817300
C	3.16787300	-1.50297700	-0.90969900
C	4.43841000	-0.61391900	1.44219300
C	2.30499600	-0.78414600	2.80756900
C	5.16880200	-0.77248100	0.26691700
C	4.53923800	-1.21459400	-0.89320200
C	2.52771900	-2.03337300	-2.19196500
C	2.70428700	0.45092100	3.63450900
C	2.48685200	-2.07185200	3.64010700
C	2.80236700	-1.12873200	-3.40901800
C	2.99064400	-3.47749700	-2.47940900
C	-3.34496900	-1.22632000	0.98606600
C	-2.92686800	-1.29018600	-1.45611100
C	-4.27316700	-0.96336400	-1.66341500
C	-2.02568800	-1.55096700	-2.66052900
C	-5.14137200	-0.77015400	-0.59319800
C	-4.68135600	-0.90714300	0.71413400
C	-2.88871300	-1.42960500	2.42903300
C	-1.92718200	-0.31935500	-3.58137700
C	-2.49649100	-2.79062600	-3.44872200
C	-3.26903900	-2.83942900	2.93148300
C	-3.44754200	-0.36118700	3.38797900
H	1.39440000	-3.80842700	0.58804400
H	-1.37103500	-3.89231700	0.32347800
H	4.94752300	-0.28590900	2.34249400
H	6.23476400	-0.56304300	0.25930200
H	5.12253500	-1.34934800	-1.79894000
H	1.23983600	-0.68565000	2.57445900
H	2.13741700	-2.95775900	3.09882300
H	1.92291600	-2.00546800	4.57765800
H	3.54185800	-2.22876400	3.89183100
H	3.72783100	0.37824200	4.01757100
H	2.04529600	0.54479000	4.50488600
H	2.63019100	1.36982300	3.04255200
H	1.44228000	-2.05931000	-2.05074500
H	4.07261100	-3.51992400	-2.64713100
H	2.49667200	-3.86592300	-3.37707000

H	2.75798300	-4.15085500	-1.64728600
H	3.86773100	-1.09467400	-3.66118500
H	2.46815500	-0.09998000	-3.23423400
H	2.27238100	-1.51281200	-4.28769600
H	-4.64853700	-0.87388500	-2.67840600
H	-6.18340000	-0.52484000	-0.77760500
H	-5.37509800	-0.77151100	1.53728000
H	-1.01545500	-1.76451400	-2.29715400
H	-2.53451300	-3.68006000	-2.81039000
H	-1.81093500	-2.99643100	-4.27833800
H	-3.49593900	-2.64128200	-3.87176300
H	-2.89791600	-0.06043200	-4.01819400
H	-1.23410000	-0.51548700	-4.40740300
H	-1.56695000	0.55974900	-3.03230600
H	-1.79540200	-1.35265400	2.45357900
H	-4.35629200	-2.97574900	2.92051700
H	-2.92091600	-2.98600700	3.96016700
H	-2.82918100	-3.62802300	2.31219000
H	-4.52614700	-0.47386400	3.54080500
H	-3.26800100	0.65304000	3.01588400
H	-2.97431700	-0.45783200	4.37156500
C	-0.63699900	2.16897000	3.02142900
H	-1.30128100	2.88755600	3.51954500
H	-0.89626100	1.16173000	3.35757000
H	0.38801300	2.37744100	3.35131300

TS4a (X = O)

B3LYP SCF energy in gas phase: -1735.055647 a.u.

M06 SCF energy in solution: -1734.309466 a.u.

M06 Free energy in solution: -1733.588611 a.u.

C	-2.09851700	-2.26766800	-1.35506000
C	-1.98290200	-0.99520700	-1.57194800
C	-0.56411300	-3.53191100	-0.85252200
C	0.49791800	-3.24578400	0.11728800
C	1.68390200	-2.62433600	-0.22377100
C	2.02815500	-2.25205800	-1.65852600
C	0.92910400	-1.29155500	-2.12499000
H	1.28406800	-0.29085900	-2.35481100
H	0.31031900	-1.66067400	-2.94773200
H	0.32933700	-3.54510500	1.15122800
H	-0.21406300	-3.64732400	-1.87742000
H	2.44811300	-2.51238200	0.53566900
H	2.09771200	-3.15008100	-2.28918900
C	-1.53791700	-4.64171700	-0.48631000
H	-1.04486300	-5.61326700	-0.58767000
H	-1.89087500	-4.53342800	0.55326700
C	-3.16211700	-3.33411700	-1.39601800
H	-3.82490600	-3.20903600	-0.52281500
H	-3.76417700	-3.21967500	-2.30330200
H	3.00716500	-1.76932800	-1.68019400
C	1.35617700	2.41311600	1.12355400
C	0.03819400	2.63946900	1.29738800
C	0.24159200	0.66398400	0.16491100
N	-0.63993200	1.58319800	0.69648200
N	1.47759300	1.20902000	0.43826300
Rh	-0.28600200	-1.21304200	-0.45696300
O	-2.60724900	-4.62755100	-1.40359800
H	-0.48791400	3.44486900	1.78209500
H	2.22165700	2.97993900	1.42427200
C	2.80019200	0.65092600	0.22357300
C	3.48525600	0.96193500	-0.97145400
C	3.40286600	-0.05844000	1.28815200
C	4.78345000	0.45389200	-1.11673700
C	4.70209000	-0.54086900	1.08231400
C	5.37987200	-0.30237300	-0.11073400
H	5.34192800	0.66541700	-2.02250000
H	5.19985200	-1.09165800	1.87426100
H	6.38831000	-0.68301400	-0.24582000
C	-2.09046700	1.58036600	0.69181900
C	-2.78582000	0.61435300	1.45677300
C	-2.75356700	2.62186900	0.00352700
C	-4.18232900	0.69403700	1.48099300
C	-4.15406700	2.65754200	0.08308900
C	-4.86288700	1.70401300	0.80284500
H	-4.75097600	-0.03062900	2.05232900
H	-4.69393400	3.44686700	-0.43048100
H	-5.94716200	1.75059700	0.84751300
C	2.74460900	-0.21322600	2.66142800
H	1.67637100	0.00370400	2.55776100
C	3.33973000	0.81656700	3.64905400
H	3.23389300	1.84366700	3.28623800
H	2.83619500	0.74858300	4.61988200
H	4.40751400	0.62975900	3.80922000
C	2.86500400	-1.62492000	3.26608500
H	2.42016800	-2.39248200	2.62495400
H	3.90642500	-1.90608000	3.45466500
H	2.34481700	-1.65603300	4.22973300
C	2.90311200	1.89301100	-2.03529600
H	1.81165800	1.88311400	-1.93529300
C	3.37482800	3.34434500	-1.78989800
H	4.46597100	3.41611700	-1.86134600
H	2.94247600	4.01665600	-2.53950400
H	3.07961100	3.70955600	-0.80096900
C	3.24217900	1.47401900	-3.47819800
H	4.30565700	1.60898600	-3.70285000
H	2.98793900	0.42775900	-3.67808300
H	2.68447500	2.09838600	-4.18439000
C	-2.03986400	3.71957400	-0.79096200
H	-0.97347600	3.47971700	-0.83933600
C	-2.18400100	5.08791200	-0.08957800
H	-1.61615300	5.85322200	-0.62996600
H	-3.23162700	5.40781700	-0.06211300
H	-1.82315800	5.06658800	0.94458900
C	-2.53831400	3.82563600	-2.24647700
H	-1.97321200	4.60180300	-2.77417400
H	-2.40756700	2.88616000	-2.79088400
H	-3.59706100	4.10113400	-2.29904700

C	-2.06102400	-0.43759100	2.29717700
H	-1.18110300	-0.78555900	1.72669800
C	-1.53144900	0.17667400	3.61138000
H	-2.36552900	0.53975300	4.22284900
H	-0.98916400	-0.57616800	4.19490400
H	-0.85602000	1.01829500	3.43110900
C	-2.90407100	-1.68546900	2.60541800
H	-3.71703300	-1.46612000	3.30586000
H	-3.34390000	-2.11774400	1.70044800
H	-2.27455000	-2.44713900	3.07875300
C	-2.72439500	0.02842300	-2.35767100
H	-2.03267200	0.61626200	-2.97053600
H	-3.25835700	0.72275200	-1.70495400
H	-3.45019200	-0.44846300	-3.02771700

1b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.081217 a.u.

M06 SCF energy in solution: -1734.339335 a.u.

M06 Free energy in solution: -1733.62387 a.u.

C	-2.56579900	-1.37785400	-3.66944200
C	-2.09180700	-0.82563200	-2.37942000
C	-0.67302900	-0.37433900	-2.19754200
C	0.38402400	-1.23606100	-2.57435500
H	0.05649600	-2.22621500	-2.89518800
H	-0.52782900	0.70351700	-2.21824800
C	1.76936500	-0.87212200	-3.05153500
C	2.97122800	-2.46283000	-1.40214300
C	1.68021700	-2.70862100	-0.71934200
C	0.64985300	-3.31830300	-0.29343400
H	-2.82764500	-0.33693100	-1.74659300
H	-1.86528200	-1.47871200	-4.49841600
H	3.52236800	-1.67930800	-0.87026800
H	3.58207300	-3.37442500	-1.36796200
H	1.70562500	-0.63751900	-4.12628100
H	2.14037500	0.02826400	-2.55189900
Rh	0.23638400	-1.27826500	-0.44680300
C	-0.08515200	0.54405400	0.51724700
N	-1.21137200	1.06130900	1.10181600
C	-0.88698900	2.08499200	1.98483400
C	-2.59177200	0.69277800	0.84862600
N	0.93766100	1.29293600	1.03951200
C	0.45826700	2.23424000	1.94033400
C	2.34621200	1.18021100	0.71127200
C	-3.13084000	-0.44084600	1.49429400
C	-3.36234500	1.54383900	0.02614900
C	-4.47929400	-0.73315400	1.25432700
C	-2.32714900	-1.27927800	2.48612600
C	-5.25992300	0.07550900	0.43218000
C	-4.70852400	1.20444500	-0.16606200
C	-2.81000000	2.81591700	-0.61788300
C	-2.68834200	-2.77451000	2.45435400
C	-2.48891500	-0.72171400	3.91769600
C	-3.10297400	2.89804200	-2.12902000
C	-3.35439700	4.07119000	0.09732800
C	3.15070900	0.30371000	1.47064100
C	2.86385700	2.01649900	-0.30224700
C	4.23247800	1.90899200	-0.58279200
C	2.01822900	3.07477700	-1.01091300
C	5.04613200	1.02764800	0.12454000
C	4.51233600	0.24323800	1.14479300
C	2.60848800	-0.48425400	2.66200200
C	2.26966000	3.15575100	-2.52795400
C	2.24911900	4.46041300	-0.36745600
C	2.88328900	0.27993000	3.97628300
C	3.16391300	-1.91673500	2.75832000
H	-1.64308000	2.60400700	2.55154200
H	1.11689400	2.91382500	2.45648300
H	-4.93049000	-1.59865100	1.72682300
H	-6.30520600	-0.16972600	0.26761500
H	-5.33327900	1.83610500	-0.78987300
H	-1.26638800	-1.19794600	2.21895100
H	-2.16492600	0.32188100	3.98935200
H	-1.89397200	-1.30904300	4.62643400
H	-3.53671900	-0.77026100	4.23525400
H	-3.68516200	-2.96454400	2.86686100
H	-1.97834900	-3.33875600	3.06967400
H	-2.66250300	-3.17618900	1.43624200
H	-1.72086000	2.81669200	-0.50099400
H	-4.44353000	4.13840300	-0.00239300
H	-2.92081800	4.97800300	-0.33885200
H	-3.12075800	4.06576500	1.16740300
H	-4.17577300	2.97957200	-2.33358300
H	-2.72709100	2.02170700	-2.66774300
H	-2.62388500	3.78723400	-2.55341400
H	4.67106600	2.53610000	-1.35232600
H	6.10614500	0.96708800	-0.10567000
H	5.16726600	-0.41431000	1.70709700
H	0.96211600	2.81799100	-0.87106400
H	2.01748400	4.45858400	0.70271100
H	1.61679600	5.21508900	-0.84845800
H	3.29317100	4.77295000	-0.48094100
H	3.28256000	3.50268100	-2.75859700
H	1.57487400	3.87217400	-2.97979300
H	2.12557700	2.18930800	-3.02135900
H	1.52105700	-0.56507900	2.54843800
H	3.96084700	0.38783300	4.14454100
H	2.46094200	-0.26274600	4.82943100
H	2.44539600	1.28352500	3.96454900
H	4.23558200	-1.92737800	2.98431400
H	3.00480700	-2.47823200	1.83230600
H	2.66059000	-2.45319700	3.57030900
C	-0.16159400	-4.50981500	0.03872800
H	0.43834900	-5.42291000	-0.05029700
H	-0.56262900	-4.45394400	1.05462400
H	-1.01157500	-4.58185300	-0.64923200
C	2.75964300	-2.03816800	-2.87774400
H	3.73311800	-1.76461800	-3.29847900

H	2.39832400	-2.90253600	-3.44891200
O	-2.30857000	-2.23094300	-2.54802900
H	-3.61394000	-1.27514900	-3.94773800

TS1b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.051929 a.u.

M06 SCF energy in solution: -1734.302369 a.u.

M06 Free energy in solution: -1733.587152 a.u.

C	3.26938800	3.28649400	-0.91745000
C	2.45359900	2.05986900	-0.77823000
C	1.06425500	1.94782700	-1.32746000
C	0.16049500	3.10297900	-1.16777700
H	0.67563300	3.88897700	-0.60928800
H	1.03811000	1.43285300	-2.29496100
C	-0.74711400	3.67150500	-2.23855500
C	-2.03529500	4.19529300	-0.16698600
C	-1.08595000	3.11979600	0.28511800
C	-0.67452200	2.42816400	1.32067900
H	2.98924900	1.11887100	-0.68972800
H	4.35559200	3.20813800	-0.92552800
H	2.86003900	4.15930100	-1.42639500
H	-3.02819200	3.73680400	-0.25656400
H	-2.11715500	4.98523500	0.58824000
H	-0.14524000	4.09984800	-3.05057300
H	-1.37847800	2.88885800	-2.67568200
Rh	-0.40392100	1.12463200	-0.16983700
C	-0.04202200	-0.88843200	0.16212300
N	1.04608200	-1.69310700	0.37705200
C	0.65794600	-3.00611400	0.60404200
C	2.44656400	-1.32845500	0.28927700
N	-1.10968000	-1.74803000	0.25573500
C	-0.69658300	-3.04197900	0.52288700
C	-2.49633800	-1.37768900	0.04278500
C	3.09064000	-0.79904000	1.42685400
C	3.12496500	-1.60095100	-0.91846900
C	4.45896800	-0.52069100	1.31536600
C	2.36694200	-0.58046900	2.75232100
C	5.15442200	-0.76853000	0.13435000
C	4.49391400	-1.30459300	-0.96743300
C	2.44820700	-2.22438800	-2.13788000
C	2.82058200	0.70018800	3.47735100
C	2.53587500	-1.80989300	3.67142700
C	2.64982700	-1.38435800	-3.41401700
C	2.93710400	-3.67110900	-2.36050600
C	-3.30857300	-1.10409500	1.16530800
C	-2.99051300	-1.36419400	-1.27959400
C	-4.33702300	-1.02252300	-1.45936900
C	-2.14556200	-1.75368300	-2.48964000
C	-5.15653400	-0.72636600	-0.37414800
C	-4.64792100	-0.77466500	0.92140500
C	-2.79739200	-1.21149300	2.60017300
C	-2.11575600	-0.64615000	-3.56006600
C	-2.63311400	-3.08804300	-3.09173700
C	-3.17987100	-2.57505400	3.21610700
C	-3.29829000	-0.06676900	3.50084500
H	1.37928200	-3.78564400	0.79085700
H	-1.39451500	-3.85814600	0.61992900
H	4.98993700	-0.10898800	2.16674900
H	6.21706500	-0.55028600	0.07613000
H	5.05018300	-1.50379600	-1.87835200
H	1.29881800	-0.47054800	2.53599800
H	2.15265900	-2.72401700	3.20489000
H	1.99564600	-1.66021500	4.61327500
H	3.59243500	-1.97457000	3.91181300
H	3.83940600	0.60874400	3.86990300
H	2.16726800	0.89035800	4.33629300
H	2.79144000	1.57090100	2.81376100
H	1.37064600	-2.26860400	-1.94987200
H	4.01204000	-3.69836600	-2.57108700
H	2.41724700	-4.12327800	-3.21255200
H	2.75604200	-4.29916800	-1.48137000
H	3.70347400	-1.33652400	-3.70943800
H	2.29379700	-0.35635500	-3.28143700
H	2.09659000	-1.82947000	-4.24851200
H	-4.75209300	-1.00367000	-2.46261400
H	-6.19991800	-0.47126300	-0.53659700
H	-5.30493000	-0.55971100	1.75765100
H	-1.11427000	-1.90648400	-2.15601300
H	-2.61252400	-3.89353800	-2.34948400
H	-1.99464800	-3.38393100	-3.93180500
H	-3.65994200	-3.00569200	-3.46495700
H	-3.10814600	-0.46510200	-3.98714500
H	-1.45067200	-0.93203200	-4.38275900
H	-1.75618100	0.30184700	-3.14155000
H	-1.70299900	-1.15468900	2.57600700
H	-4.26873900	-2.69096100	3.25879100
H	-2.79129000	-2.65599200	4.23751000
H	-2.77881000	-3.41300000	2.63635900
H	-4.37278300	-0.14319800	3.69909100
H	-3.11010400	0.91462000	3.05285500
H	-2.79110300	-0.10638400	4.47134800
C	-0.49507100	2.42780500	2.78805600
H	-1.14808300	3.18136700	3.24874000
H	-0.71046900	1.45452300	3.23623600
H	0.54199200	2.69143700	3.03022700
O	2.63820200	2.95222900	0.32681400
C	-1.58152100	4.75733800	-1.53737400
H	-2.43783500	5.07637200	-2.13759200
H	-0.95184500	5.64105000	-1.38081700

2b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.096258 a.u.

M06 SCF energy in solution: -1734.341975 a.u.

M06 Free energy in solution: -1733.621219 a.u.

C	0.24335500	-4.01205300	-1.98355000
C	-0.28617400	-3.61744000	-0.67171600

C	-1.12183500	-2.37549700	-0.50524000
C	-2.04219400	-2.08248400	-1.70308300
H	-2.19431700	-3.02822200	-2.25230000
H	-1.62186200	-2.34437700	0.46342800
C	-3.44564300	-1.47649600	-1.51247100
C	-2.43866400	-0.69916500	-3.67120600
C	-1.40927500	-1.07077100	-2.61915100
C	-0.25601600	-0.48460400	-2.26422900
H	-0.22459500	-4.33937000	0.13944500
H	0.61655400	-5.02470000	-2.11586700
H	-0.08902100	-3.50371300	-2.88351800
H	-2.34809300	0.33924600	-4.00275600
H	-2.34466800	-1.32450900	-4.56843100
H	-4.17692500	-2.19354100	-1.12346100
H	-3.39588900	-0.63370400	-0.81818000
C	1.23987200	2.10240900	1.81806700
C	-0.10101600	2.17604200	1.98956400
C	0.28064500	0.50144300	0.51126000
N	-0.68233200	1.19309100	1.18847100
N	1.46155000	1.07896300	0.90717500
Rh	0.56536500	-1.16072400	-0.56882100
H	-0.70450200	2.83119800	2.59644700
H	2.04569700	2.67351600	2.24952700
C	2.75353200	0.62616100	0.42560100
C	3.48937700	1.46197600	-0.44664900
C	3.24125600	-0.63121100	0.87326500
C	4.72650200	0.98499100	-0.89933900
C	4.47590100	-1.05593000	0.36490200
C	5.20844700	-0.26112800	-0.51259200
H	5.32099100	1.60005900	-1.56673000
H	4.87995800	-2.01320200	0.67237000
H	6.16731000	-0.61039700	-0.88451100
C	-2.12539200	1.03580000	1.15402700
C	-2.73144100	0.11868100	2.04128300
C	-2.86620700	1.90870600	0.33034900
C	-4.13048100	0.06207800	2.04351100
C	-4.26330600	1.80932400	0.38326100
C	-4.88943200	0.89384300	1.22306000
H	-4.63587600	-0.63080400	2.70775800
H	-4.86766200	2.46663300	-0.23396800
H	-5.97381300	0.83572800	1.24925900
C	2.53301900	-1.45662000	1.95463400
H	1.44327500	-1.38059200	1.80313400
C	2.82715500	-0.86861700	3.35352400
H	2.30580000	-1.44424300	4.12634000
H	3.90158900	-0.91422400	3.56432400
H	2.50962000	0.17495200	3.43741200
C	2.87958600	-2.95537300	1.92914100
H	2.23689000	-3.48802600	2.63869400
H	2.73476700	-3.39543600	0.93708800
H	3.91367800	-3.13807900	2.24021100
C	-1.92689100	-0.72108000	3.03306200
H	-0.91674300	-0.84944800	2.62713000
C	-1.79626400	0.01606700	4.38496900
H	-2.78312600	0.18195500	4.83153800
H	-1.20287400	-0.57852800	5.08895000
H	-1.30998800	0.99053700	4.27534000
C	-2.51043300	-2.12724100	3.26668100
H	-2.70022400	-2.66004400	2.32857300
H	-1.81170200	-2.72404600	3.86317800
H	-3.45347700	-2.09129700	3.82247000
C	-2.21876100	2.98010900	-0.54478500
H	-1.14115300	2.78833300	-0.58182700
C	-2.42226400	4.38181400	0.06945000
H	-1.92503700	5.14217400	-0.54324500
H	-3.48653400	4.63724900	0.12220900
H	-2.01549900	4.44680000	1.08458900
C	-2.73207800	2.95186400	-1.99596500
H	-2.18224800	3.68149600	-2.60096400
H	-2.59838800	1.96391300	-2.44532100
H	-3.79400000	3.21303800	-2.05990800
C	3.03004800	2.86182600	-0.85132800
H	1.95944400	2.94775800	-0.63467500
C	3.76885100	3.93352500	-0.01808800
H	4.84592000	3.90509800	-0.21792200
H	3.40512500	4.93400000	-0.27676900
H	3.63273600	3.79250300	1.05950500
C	3.21967300	3.15413800	-2.35249000
H	4.27834900	3.22006800	-2.62472000
H	2.75707100	2.38829000	-2.98125100
H	2.76408700	4.11904300	-2.59984300
C	0.46388600	0.61982500	-2.97813900
H	1.50185400	0.34455000	-3.20399400
H	0.49084000	1.53870900	-2.37958500
H	-0.02625400	0.84987000	-3.93318700
O	1.11460300	-3.21483300	-1.13975700
C	-3.80117200	-0.98437800	-2.94478900
H	-4.35865900	-1.75687700	-3.48441300
H	-4.43819700	-0.09566400	-2.91488200

TS2b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.091623 a.u.

M06 SCF energy in solution: -1734.336446 a.u.

M06 Free energy in solution: -1733.618106 a.u.

C	0.03815900	-3.84048900	-2.12405100
C	-0.61455000	-3.33720500	-0.90570300
C	-1.38745700	-2.11461500	-0.85800100
C	-2.12584000	-1.67164100	-2.12587400
H	-2.17597500	-2.52605800	-2.81995000
H	-1.93072500	-1.97427500	0.07513300
C	-3.56339500	-1.12364300	-2.01161300
C	-2.34677200	0.03938600	-3.85915200
C	-1.41631600	-0.52837300	-2.79977000
C	-0.26846200	-0.05824500	-2.29785600
H	-0.39728500	-3.87214100	0.01452900
H	0.38179900	-4.87552600	-2.10509700
H	-0.37131600	-3.54789000	-3.09100500

H	-2.26348200	1.12691500	-3.94560900
H	-2.12536200	-0.37128000	-4.85259800
H	-4.31023000	-1.90317200	-1.82558600
H	-3.61858500	-0.40066400	-1.19091400
C	1.32847500	1.80427700	2.07028800
C	-0.00450400	1.86515900	2.29958900
C	0.30137200	0.43481300	0.56566900
N	-0.62613700	1.02497400	1.37562700
N	1.50336300	0.93417900	1.00208100
Rh	0.46888100	-1.08778700	-0.74257900
H	-0.57491200	2.42055400	3.02632200
H	2.15639000	2.29158400	2.55868800
C	2.76760500	0.52226100	0.42203300
C	3.49701400	1.44418500	-0.36641500
C	3.23764500	-0.79095900	0.69119200
C	4.68779700	0.98957100	-0.94595000
C	4.42698500	-1.18714400	0.06365400
C	5.13819100	-0.31329000	-0.75299500
H	5.27191500	1.66792900	-1.55868000
H	4.81234600	-2.18562200	0.23374600
H	6.06004600	-0.64271900	-1.22348600
C	-2.06508300	0.84230100	1.37821400
C	-2.61264200	-0.19541100	2.16493000
C	-2.86029600	1.78091600	0.68879500
C	-4.00837600	-0.30881800	2.19403800
C	-4.25083400	1.62223900	0.76554700
C	-4.81966700	0.58502300	1.49911300
H	-4.46876900	-1.09335100	2.78573700
H	-4.89645500	2.32686700	0.25127000
H	-5.90013100	0.48242700	1.54429900
C	2.58417900	-1.70633200	1.73339100
H	1.49729600	-1.54076100	1.71797900
C	3.07584600	-1.32385500	3.14825700
H	2.60108300	-1.96201900	3.90193700
H	4.16054600	-1.45945400	3.22473200
H	2.84722200	-0.28223300	3.39453200
C	2.81344400	-3.20730600	1.48245300
H	2.20766900	-3.78986000	2.18573600
H	2.53993000	-3.49958000	0.46339700
H	3.85652000	-3.49474700	1.65294500
C	-1.75287800	-1.10496700	3.04269200
H	-0.72662100	-1.07765800	2.65995100
C	-1.72054300	-0.57279400	4.49278500
H	-2.72460800	-0.57962500	4.93172100
H	-1.07464000	-1.20057800	5.11707500
H	-1.34215800	0.45338800	4.54133400
C	-2.20403300	-2.57774900	3.03797300
H	-2.27342400	-2.98726400	2.02389300
H	-1.48857900	-3.18656900	3.60178800
H	-3.18113600	-2.70993800	3.51427900
C	-2.26963600	2.97789700	-0.05330100
H	-1.20099500	2.79089000	-0.20356300
C	-2.40565900	4.26094700	0.79531200
H	-1.95344100	5.11220500	0.27415400
H	-3.45934600	4.49987800	0.97840600
H	-1.91419500	4.16192000	1.76920400
C	-2.89192300	3.19032200	-1.44469700
H	-2.36627900	3.99661600	-1.96815500
H	-2.82270300	2.28480900	-2.05376900
H	-3.94655800	3.48032800	-1.38348200
C	3.08717800	2.90667300	-0.53300000
H	2.02141000	2.99353300	-0.29316900
C	3.87075600	3.79471900	0.46110300
H	4.94353600	3.76702400	0.23940200
H	3.53791100	4.83578200	0.38604000
H	3.74445800	3.47283100	1.50000600
C	3.28631000	3.44628000	-1.96262700
H	4.34713600	3.52764500	-2.22287400
H	2.80289500	2.81607800	-2.71396300
H	2.86074600	4.45275800	-2.03767800
C	0.53251600	1.10829500	-2.78599100
H	1.56504700	0.81952500	-3.01838400
H	0.57369100	1.91328000	-2.04262700
H	0.09488600	1.51586100	-3.70688600
O	1.01771800	-2.94122800	-1.61045300
C	-3.76743000	-0.41717600	-3.37902600
H	-4.19928200	-1.11679400	-4.10231900
H	-4.46232500	0.42381500	-3.29872500

3b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.108002 a.u.

M06 SCF energy in solution: -1734.356158 a.u.

M06 Free energy in solution: -1733.637835 a.u.

C	0.03580500	-3.61293100	1.60763000
C	0.83199500	-2.82576200	0.57743000
C	1.72940500	-1.81117900	0.92353600
C	2.23360500	-1.53392600	2.31676300
H	1.96802100	-2.36667300	2.98333100
H	2.26682300	-1.31474300	0.11970600
C	3.73748700	-1.22957800	2.48976000
C	2.46548000	0.33953600	3.91585000
C	1.58116400	-0.27255600	2.83518700
C	0.45292400	0.16287000	2.27258300
H	0.69321700	-3.06371300	-0.47617300
H	-0.39949800	-4.51867300	1.16614700
H	0.62996100	-3.90787400	2.48249400
C	-1.47861300	1.49415100	-2.23774400
C	-0.15961400	1.57593300	-2.53375300
C	-0.33682200	0.35999600	-0.62327700
N	0.53067800	0.87984200	-1.54262000
N	-1.57284500	0.75744500	-1.06470100
Rh	-0.40108800	-1.04813500	0.90443800
H	0.35815500	2.06212700	-3.34457100
H	-2.34582400	1.88611500	-2.74340400
C	-2.80166300	0.40650500	-0.37585300
C	-3.47595400	1.40082600	0.37626400
C	-3.30638500	-0.91164200	-0.52422700

C	-4.63793800	1.01139700	1.05270500
C	-4.46673800	-1.23798100	0.19132200
C	-5.11770300	-0.29418500	0.97886700
H	-5.18094800	1.74223700	1.64249700
H	-4.87507900	-2.23946000	0.11771500
H	-6.01707200	-0.57102600	1.52122000
C	1.97874600	0.79021400	-1.55205600
C	2.58935500	-0.26343800	-2.26924300
C	2.71669200	1.81277900	-0.92049900
C	3.98959300	-0.30160300	-2.28358900
C	4.11443100	1.71971500	-0.96921500
C	4.74507100	0.67142500	-1.63305900
H	4.49704900	-1.09628000	-2.82028400
H	4.71645600	2.48794300	-0.49457100
H	5.82984900	0.62216400	-1.66115000
C	-2.71710100	-1.91509600	-1.51811500
H	-1.64837200	-1.69757600	-1.63913100
C	-3.37701500	-1.72846600	-2.90334000
H	-2.94434900	-2.42741400	-3.62793700
H	-4.45366800	-1.92400600	-2.84657300
H	-3.23870300	-0.71283700	-3.28880300
C	-2.83766100	-3.38028600	-1.06077800
H	-2.26342100	-4.02429800	-1.73647500
H	-2.46528000	-3.51659500	-0.04035600
H	-3.87383600	-3.73314700	-1.09443500
C	1.78742000	-1.29207300	-3.06591000
H	0.77127200	-1.32202500	-2.65531200
C	1.67736500	-0.86488300	-4.54654500
H	2.66972400	-0.81092900	-5.00815100
H	1.08156900	-1.59141600	-5.11043000
H	1.20391400	0.11583800	-4.65606100
C	2.36381100	-2.71849100	-2.98002000
H	2.53896200	-3.03520400	-1.94592400
H	1.66949600	-3.42831000	-3.44302500
H	3.31423200	-2.80753500	-3.51663000
C	2.05756900	3.03037700	-0.27730100
H	0.99486800	2.80752700	-0.13524000
C	2.15431500	4.25202400	-1.21701100
H	1.64977800	5.11679800	-0.77156500
H	3.19968900	4.52763300	-1.39592700
H	1.69123400	4.05470900	-2.18997000
C	2.63899500	3.36861400	1.10656100
H	2.06890400	4.18598400	1.56188800
H	2.59483400	2.50444400	1.77588800
H	3.68164900	3.69859000	1.04511200
C	-3.04493300	2.86710100	0.39341400
H	-1.98833900	2.91754800	0.10587800
C	-3.85650100	3.67195900	-0.64826900
H	-4.92192700	3.66763700	-0.39249000
H	-3.51905100	4.71402200	-0.67039200
H	-3.76103100	3.26454600	-1.65972600
C	-3.18484000	3.54119200	1.77170400
H	-4.23430300	3.67531400	2.05419900
H	-2.69427600	2.97200900	2.56598900
H	-2.73377900	4.53880700	1.73967600
C	-0.38527300	1.34722700	2.62911200
H	-1.42882800	1.06620700	2.81784300
H	-0.37752800	2.11226300	1.84494300
H	-0.00544100	1.79798900	3.55629300
O	-0.96344500	-2.66182000	1.93160300
C	3.76972900	-0.51017600	3.85788100
H	4.07264000	-0.55476700	1.69110800
H	4.36651400	-2.12499400	2.46303000
H	3.76365800	-1.25427600	4.66228700
H	4.67021200	0.09657000	3.98854800
H	1.99824200	0.29353800	4.90674100
H	2.66410900	1.39730600	3.71029400

4b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.080993 a.u.

M06 SCF energy in solution: -1734.3276 a.u.

M06 Free energy in solution: -1733.612521 a.u.

C	-1.85833600	0.22827200	1.93787000
C	-1.04665500	-0.62382100	2.46559400
C	-1.25007300	3.40505100	2.24168700
C	-0.65574800	3.71192100	1.07865300
C	0.78804100	3.60843500	0.77049000
C	1.81089200	3.01481600	1.63786100
H	-1.27401400	4.01020400	0.23384300
H	-0.64685500	3.13297100	3.10918000
H	1.14756700	4.27284000	-0.01192700
H	1.54001400	2.63053600	2.61863300
C	-2.73927200	3.41329100	2.44378600
H	-2.98569300	4.14040500	3.23055700
H	-3.22843500	3.76437600	1.52656100
C	-3.18488100	0.89747900	1.84579700
H	-3.35486400	1.26173900	0.82641100
H	-3.96138900	0.14576400	2.04087200
H	2.85009400	3.31528200	1.52809000
C	1.34121500	-1.83301600	-1.98969900
C	0.02085400	-1.87285800	-2.27917000
C	0.27055700	-0.54452200	-0.45779200
N	-0.63316200	-1.08290700	-1.33541600
N	1.49095700	-1.00859900	-0.87824600
Rh	-0.04610400	0.52366300	1.15437100
H	-0.52153100	-2.37693900	-3.06227800
H	2.18902700	-2.29999800	-2.46414200
C	2.79014100	-0.64340900	-0.34191900
C	3.53398600	0.34775300	-1.02055100
C	3.29030800	-1.33907700	0.78068800
C	4.79725800	0.66628600	-0.50598900
C	4.55651600	-0.96901400	1.25229100
C	5.29951200	0.02629300	0.62300400
H	5.40045300	1.41886800	-1.00390300
H	4.97597000	-1.47864800	2.11277900
H	6.28291900	0.28903100	1.00289200
C	-2.06305500	-0.84861600	-1.39906900

C	-2.93418900	-1.81756900	-0.85878900
C	-2.52500200	0.29296200	-2.09031100
C	-4.31063900	-1.59627400	-1.00277900
C	-3.91145000	0.46167600	-2.19792700
C	-4.79610000	-0.46932400	-1.65888800
H	-5.01170100	-2.32281300	-0.60500600
H	-4.30511500	1.32368700	-2.72649900
H	-5.86742600	-0.32227200	-1.76353300
C	2.55049600	-2.51737500	1.41019000
H	1.47980400	-2.38117600	1.22588500
C	3.05690600	1.01562500	-2.30902000
H	1.98564600	0.81954400	-2.42193600
C	-2.43723600	-3.09896000	-0.19302900
H	-1.38481900	-2.95418200	0.07522900
C	-1.57963500	1.27675000	-2.77638400
H	-0.59759600	1.19336100	-2.29881200
C	3.77696700	0.40567500	-3.53181600
H	3.40475100	0.85666500	-4.45861600
H	4.85663300	0.58596500	-3.47998900
H	3.62653600	-0.67697100	-3.59951700
C	3.23696800	2.54471600	-2.29966100
H	2.74887500	2.99058800	-1.42883100
H	4.29318100	2.83540500	-2.28799000
H	2.79467700	2.97666600	-3.20447100
C	-1.41142900	0.91305600	-4.26799000
H	-2.37052800	0.97902500	-4.79429700
H	-0.71170300	1.60251800	-4.75417600
H	-1.02780700	-0.10416200	-4.39834700
C	-2.02516400	2.74331400	-2.63625800
H	-2.93499600	2.95546200	-3.20810700
H	-2.21698800	3.00598100	-1.59058800
H	-1.24352700	3.40798200	-3.02094100
C	-2.51296400	-4.29114900	-1.17187000
H	-2.13157000	-5.20117500	-0.69502100
H	-3.54846800	-4.47974600	-1.47717100
H	-1.92572000	-4.11577100	-2.07912700
C	-3.20097200	-3.43438000	1.10172700
H	-2.72900600	-4.28683900	1.60298000
H	-3.20846100	-2.58873100	1.79645100
H	-4.24017900	-3.71677700	0.90212500
C	2.97959000	-3.83971100	0.73618200
H	4.05132600	-4.01913800	0.87881400
H	2.43510400	-4.68553000	1.17169300
H	2.78205900	-3.83153600	-0.34091100
C	2.74380200	-2.61456000	2.93366300
H	3.76846900	-2.89426000	3.20099100
H	2.51083300	-1.66771900	3.43314500
H	2.08694400	-3.38985400	3.34269200
C	-0.81199300	-1.77250700	3.37432100
H	-1.66220300	-1.91473800	4.05215300
H	0.09346700	-1.63736100	3.97184100
H	-0.68555400	-2.69465000	2.79510400
O	1.31552700	2.22548600	0.52057900
C	-3.35505600	2.05759700	2.86186500
H	-4.42954800	2.22101700	3.00468500
H	-2.95772000	1.74796400	3.83630400

TS3b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.053211 a.u.

M06 SCF energy in solution: -1734.304275 a.u.

M06 Free energy in solution: -1733.587798 a.u.

C	2.16621700	-1.76464600	0.37905800
C	1.34960100	-1.74403900	1.32569500
C	0.97061100	-3.40624000	-1.82379100
C	0.92062600	-2.19857100	-2.50279000
C	-0.25071100	-1.50104900	-2.91243200
C	-1.62785600	-1.97217700	-2.66149700
H	1.86472500	-1.74706400	-2.80364000
H	0.05542500	-3.93521600	-1.56946100
H	-0.13292700	-0.54589900	-3.41190300
H	-1.74219200	-3.05202000	-2.50803100
C	2.28548900	-4.14643300	-1.70729300
H	2.08125100	-5.22182400	-1.67238700
H	2.83881100	-3.96542600	-2.63839600
C	3.39263000	-2.28598700	-0.26420500
H	3.64673900	-1.73978300	-1.17959400
H	4.22995500	-2.13220500	0.42912800
H	-2.37681200	-1.60724200	-3.36954000
C	-1.34340300	2.22264800	1.37154600
C	-0.04010800	2.56460900	1.26673300
C	-0.27067600	0.48159600	0.37772900
N	0.61492700	1.49768800	0.65802400
N	-1.48537400	0.95644300	0.81332800
Rh	0.19823400	-1.30586300	-0.46381800
H	0.48472900	3.46195700	1.55040200
H	-2.18983100	2.75678700	1.77208900
C	-2.82602300	0.42543400	0.58743700
C	-3.55559900	0.94513500	-0.50618700
C	-3.39094400	-0.47567200	1.50858500
C	-4.86681100	0.49034600	-0.68208300
C	-4.70708700	-0.89955400	1.27749100
C	-5.43726100	-0.43138700	0.19140900
H	-5.45509500	0.87218200	-1.51095700
H	-5.17107500	-1.59345600	1.97142600
H	-6.45821300	-0.76850400	0.03603100
C	2.00936200	1.61627500	0.25747600
C	3.01481200	1.55381600	1.24599200
C	2.30058500	1.91562000	-1.09440500
C	4.34331500	1.72545500	0.83246100
C	3.64754900	2.06564900	-1.44741500
C	4.66206500	1.96212800	-0.49949100
H	5.13831100	1.68276300	1.57012600
H	3.90718200	2.29388700	-2.47556100
H	5.69886400	2.09226300	-0.79671000
C	-2.67097200	-0.94516400	2.76601800
H	-1.62676000	-0.63140800	2.69142500
C	-3.00812600	2.01100000	-1.45367500

H	-1.93890000	2.13304600	-1.25818200
C	2.72464100	1.37657700	2.73441900
H	1.68551800	1.05065900	2.84305900
C	1.21634500	2.18981500	-2.13498200
H	0.31666900	1.64008800	-1.84522200
C	-3.68578300	3.37372000	-1.19446500
H	-3.26042800	4.14369300	-1.84833100
H	-4.76224200	3.32263600	-1.39285000
H	-3.55613400	3.70241400	-0.15771800
C	-3.15057600	1.61986800	-2.93614500
H	-2.67231400	0.65643400	-3.13274300
H	-4.19934200	1.54592600	-3.24303400
H	-2.68001800	2.37879900	-3.57208600
C	0.86279200	3.69400100	-2.15394400
H	1.73533300	4.29456500	-2.43528700
H	0.06773500	3.89197300	-2.88240900
H	0.51692000	4.04241300	-1.17552500
C	1.59342100	1.72616300	-3.55391600
H	2.37945200	2.34679000	-3.99719500
H	1.94892800	0.68902000	-3.56588000
H	0.72234900	1.80375000	-4.21496300
C	2.87389600	2.71795800	3.48588900
H	2.62932700	2.59049100	4.54645700
H	3.90264400	3.08960800	3.42058900
H	2.21764600	3.49527600	3.08071100
C	3.62049100	0.31083400	3.39558600
H	3.28291200	0.12074000	4.42052700
H	3.59967900	-0.63391800	2.84390900
H	4.66327800	0.63987800	3.45789600
C	-3.26522800	-0.27078200	4.02065800
H	-4.31610600	-0.54826000	4.15972000
H	-2.71612800	-0.57756600	4.91849700
H	-3.21708800	0.82160200	3.95027200
C	-2.68841100	-2.47847200	2.90960800
H	-3.70540900	-2.86278200	3.04116500
H	-2.26045400	-2.96721100	2.02662500
H	-2.11468200	-2.78509900	3.79204800
C	0.87476500	-1.82501000	2.72012600
H	1.70199000	-2.14563700	3.36398400
H	0.05905500	-2.54474600	2.82370000
H	0.51778300	-0.85845500	3.08743300
O	-1.61556000	-1.21025100	-1.47025100
C	3.23325400	-3.79753200	-0.53078400
H	4.21353200	-4.22982400	-0.76148000
H	2.88113300	-4.27478300	0.38974200

5b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.088446 a.u.

M06 SCF energy in solution: -1734.336801 a.u.

M06 Free energy in solution: -1733.620452 a.u.

C	2.34854000	-2.17646900	-0.04348500
C	1.47454400	-2.22916500	0.82857700
C	1.20906000	-2.15340400	-2.80822900
C	0.57349600	-0.95340300	-3.12177100
C	-0.70055000	-0.59441800	-2.58571500
C	-1.64832800	-1.67926400	-2.07920900
H	1.15680000	-0.17769700	-3.61708500
H	0.60748900	-3.00340200	-2.49086700
H	-1.10734000	0.37756400	-2.84330100
H	-1.78266000	-2.48985100	-2.81190000
C	2.62883600	-2.44952200	-3.20526500
H	2.61525400	-3.09395700	-4.09616300
H	3.14040600	-1.52286900	-3.49858700
C	3.59351500	-2.35125000	-0.81690100
H	4.04072100	-1.37278600	-1.03756300
H	4.30136100	-2.86769800	-0.15443800
H	-2.62746300	-1.25571000	-1.83356700
C	-1.54522600	1.72497400	1.87342100
C	-0.25463800	2.11691800	1.96826200
C	-0.34736600	0.39580200	0.47798300
N	0.47043300	1.29811500	1.10835400
N	-1.60189300	0.68485100	0.94505200
Rh	0.52585100	-0.91935800	-0.84768700
H	0.21444000	2.88956300	2.55532200
H	-2.43453600	2.08384800	2.36538200
C	-2.89479800	0.20667200	0.47112100
C	-3.56724500	0.97980400	-0.50533800
C	-3.47932200	-0.92680200	1.06969100
C	-4.83285900	0.54070300	-0.91577300
C	-4.74504600	-1.31820200	0.61400300
C	-5.41306700	-0.60201200	-0.37333800
H	-5.37724100	1.10821400	-1.66350800
H	-5.22021800	-2.19076700	1.04983300
H	-6.39525700	-0.92354700	-0.70783600
C	1.88182000	1.45360200	0.81050100
C	2.84064000	1.03867700	1.76248500
C	2.24509800	2.08101600	-0.41028800
C	4.19132100	1.18371800	1.42115500
C	3.61420600	2.17467800	-0.70137600
C	4.57665900	1.72131500	0.19627900
H	4.95411600	0.87448300	2.12811700
H	3.93214800	2.64332400	-1.62613900
H	5.63136000	1.81786100	-0.04578900
C	-2.83465700	-1.67838800	2.22688600
H	-1.78066600	-1.39181400	2.26475800
C	-3.01997900	2.29178300	-1.06836100
H	-1.94425000	2.33124600	-0.86753800
C	2.46861300	0.52187000	3.15030900
H	1.41410600	0.22637800	3.13167500
C	1.22894800	2.79512500	-1.30473200
H	0.27786800	2.25815400	-1.24623200
C	-3.67148100	3.50125700	-0.36101600
H	-3.26158400	4.43947900	-0.75206100
H	-4.75417000	3.51049900	-0.52921700
H	-3.50302800	3.48563500	0.72012900
C	-3.20981900	2.42919100	-2.59206800
H	-2.84699500	1.55239700	-3.13822100

H	-4.26219500	2.56909800	-2.86040700
H	-2.66792500	3.30868900	-2.95723300
C	0.99142300	4.22906300	-0.77649000
H	1.92078300	4.80915100	-0.80267900
H	0.25305700	4.74611800	-1.39983300
H	0.62180300	4.23046500	0.25360000
C	1.63087100	2.85451800	-2.78879500
H	2.47379300	3.53292800	-2.95901900
H	1.90923100	1.87141500	-3.18319600
H	0.79273200	3.23450700	-3.38260800
C	2.62223200	1.64571400	4.20012700
H	2.31493100	1.28715500	5.18869400
H	3.66621200	1.97145900	4.26955300
H	2.01904100	2.52704700	3.95812000
C	3.29114000	-0.70654200	3.58331400
H	2.88983100	-1.11109500	4.51890700
H	3.26833300	-1.49653400	2.82739700
H	4.33900300	-0.44850400	3.77083900
C	-3.47941400	-1.25837600	3.56568300
H	-4.54495300	-1.51354800	3.58629200
H	-2.99445000	-1.77381800	4.40272100
H	-3.39314500	-0.17945500	3.73772300
C	-2.89532200	-3.20641800	2.04887700
H	-3.92212900	-3.58366300	2.10263900
H	-2.47122700	-3.50795400	1.08579200
H	-2.33510200	-3.70076300	2.85102000
C	0.71355800	-2.66265900	2.00747700
H	1.30626500	-3.37993200	2.58689700
H	-0.21272300	-3.14978600	1.69273500
H	0.45467400	-1.82389900	2.65955400
O	-0.99896700	-2.16898900	-0.91028700
C	3.44009200	-3.16821700	-2.11289500
H	2.97694000	-4.13453800	-1.87858900
H	4.44228000	-3.38215700	-2.50040500

TS4b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.060513 a.u.

M06 SCF energy in solution: -1734.29859 a.u.

M06 Free energy in solution: -1733.580428 a.u.

C	-2.07544700	-2.23620600	-1.35242200
C	-1.77753400	-0.99875100	-1.56534000
C	-0.66321500	-3.59881700	-0.59539800
C	0.27425000	-3.34326300	0.50299700
C	1.52282600	-2.78092500	0.33448700
C	2.03962900	-2.38247700	-1.03578200
H	-0.04568100	-3.63061300	1.50406900
H	-0.17849000	-3.66816300	-1.56871600
H	2.18430700	-2.70192700	1.19010300
H	2.18757900	-3.27065900	-1.67335600
C	-1.69137300	-4.69084100	-0.35853600
H	-1.16969200	-5.65648200	-0.33677100
H	-2.16999800	-4.56086300	0.62112100
C	-3.21038300	-3.19726200	-1.54112800
H	-3.95353700	-3.01964200	-0.75098500
H	-3.70056900	-2.95851900	-2.49361100
H	3.00528700	-1.87704500	-0.93465500
C	1.37538100	2.50498300	0.97108900
C	0.06472200	2.72823200	1.19958000
C	0.25112800	0.66770000	0.24586700
N	-0.62919000	1.61451800	0.73008100
N	1.48400500	1.24372100	0.39581900
Rh	-0.27267300	-1.23199200	-0.20712700
H	-0.44473100	3.56653100	1.64349700
H	2.24344200	3.11596300	1.15479400
C	2.79131600	0.71733200	0.04621700
C	3.23702900	0.85958700	-1.28440900
C	3.60598000	0.20175200	1.07980600
C	4.53176600	0.41099500	-1.57557700
C	4.89048800	-0.23103800	0.72423400
C	5.34717400	-0.13574100	-0.58790900
H	4.91067400	0.50265000	-2.58825000
H	5.54851200	-0.63294000	1.48796900
H	6.34896300	-0.47357300	-0.83797200
C	-2.08082600	1.59857000	0.74064800
C	-2.76588800	0.59397200	1.46593200
C	-2.76898300	2.63985100	0.07203700
C	-4.16258100	0.64911900	1.49993300
C	-4.16996000	2.64696500	0.15863800
C	-4.86226100	1.66831400	0.85754500
H	-4.71731600	-0.10438100	2.04617900
H	-4.72419800	3.43778800	-0.33647700
H	-5.94673600	1.69731300	0.90797700
C	3.18196800	0.18556300	2.55012900
H	2.09143700	0.28636500	2.59337400
C	3.80094400	1.38414400	3.30496500
H	3.52693100	2.34391900	2.85732000
H	3.46651200	1.39219100	4.34853100
H	4.89474700	1.31873500	3.30206400
C	3.55210400	-1.11316100	3.29191000
H	3.15618000	-2.00551100	2.79760900
H	4.63619600	-1.23846100	3.38315900
H	3.14498700	-1.08580000	4.30861000
C	2.40851800	1.54661100	-2.36669500
H	1.37109100	1.59045300	-2.02197400
C	2.89864500	2.99721800	-2.56815200
H	3.93665400	3.01654600	-2.91933100
H	2.28218400	3.50737200	-3.31716100
H	2.85135500	3.57636800	-1.63874300
C	2.40240000	0.78079400	-3.70186000
H	3.39587800	0.74712700	-4.16290500
H	2.04462900	-0.24251200	-3.55965200
H	1.73759500	1.28542100	-4.41262300
C	-2.09655700	3.77118800	-0.71506300
H	-1.02753900	3.55701700	-0.79946200
C	-2.25408900	5.12043600	0.02071700
H	-1.70675600	5.90775600	-0.50887400
H	-3.30684400	5.42048100	0.06794500

H	-1.88280500	5.08420900	1.05085700
C	-2.63440200	3.90445900	-2.15492000
H	-2.09544100	4.70461600	-2.67384900
H	-2.49925500	2.98391900	-2.72975700
H	-3.69835400	4.16271000	-2.17529100
C	-2.03039400	-0.49761700	2.23906600
H	-1.20202400	-0.89016300	1.59345500
C	-1.34535600	0.05785000	3.50415000
H	-2.10623100	0.42785900	4.20106400
H	-0.77696900	-0.72930200	4.01182200
H	-0.66461100	0.88330500	3.28030800
C	-2.88928300	-1.71907400	2.59488500
H	-3.64109200	-1.47221000	3.35205800
H	-3.40458100	-2.12776800	1.71992500
H	-2.25436800	-2.50366500	3.02017300
C	-2.19042400	0.10442200	-2.46958800
H	-1.31503700	0.51200800	-2.98727700
H	-2.66360100	0.91498000	-1.91174200
H	-2.89733800	-0.26016400	-3.22495700
O	1.08094100	-1.51821900	-1.62730400
C	-2.72714300	-4.64603800	-1.48040500
H	-3.55570600	-5.33741100	-1.30189700
H	-2.25762300	-4.93118100	-2.42972100

TS5b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.090019 a.u.

M06 SCF energy in solution: -1734.333946 a.u.

M06 Free energy in solution: -1733.616859 a.u.

C	0.55634900	1.62327200	-3.37508100
C	-0.46254000	0.70749800	-2.72152200
C	-1.30873900	1.22657600	-1.71650800
C	-1.51210000	2.71866300	-1.51238500
H	-1.65606200	3.18701700	-2.50180400
H	-2.09577500	0.58307300	-1.33275100
C	-2.69488500	3.16964900	-0.63034500
C	-0.77927100	4.64000900	-0.12388100
C	-0.32917900	3.36376900	-0.82428900
C	0.85862000	2.75449900	-0.72174300
H	-0.62053000	-0.29613800	-3.10961400
H	1.06131000	1.14545000	-4.22144000
H	0.13554500	2.57906300	-3.71468900
C	0.73751700	-2.61548300	1.61088000
C	-0.61617000	-2.68301100	1.52234900
C	0.03377100	-0.86768100	0.33124000
N	-1.03720100	-1.60991100	0.74054600
N	1.11264800	-1.50109500	0.87969400
Rh	0.64733800	0.63781600	-0.91267400
H	-1.32068700	-3.37976200	1.94781700
H	1.45191100	-3.23987800	2.12406400
C	2.44325300	-0.95159300	0.71711000
C	2.95568600	-0.12515900	1.74788400
C	3.19285000	-1.30242700	-0.43490900
C	4.24385000	0.39253100	1.56918900
C	4.46994300	-0.73809100	-0.55764600
C	4.98704800	0.09995200	0.42668900
H	4.67593800	1.02463200	2.33887200
H	5.07501000	-0.97365500	-1.42655400
H	5.98428400	0.51489400	0.31105900
C	-2.44059200	-1.31327600	0.52907300
C	-3.08042100	-1.82078100	-0.62245800
C	-3.11791100	-0.57782400	1.52413100
C	-4.43973500	-1.52280700	-0.78085900
C	-4.47700900	-0.31163800	1.30837800
C	-5.12894400	-0.76951200	0.16743900
H	-4.96984300	-1.89147000	-1.65260200
H	-5.03415700	0.25023300	2.05177700
H	-6.18358800	-0.55323400	0.02274100
C	2.70723100	-2.33546000	-1.44976100
H	1.61977000	-2.42348300	-1.35400800
C	3.31419500	-3.71814200	-1.12281200
H	2.94389500	-4.47130900	-1.82714300
H	4.40714200	-3.69378200	-1.19802100
H	3.05604500	-4.04691500	-0.11000800
C	3.00669800	-1.94191300	-2.90732900
H	2.53219000	-2.65761700	-3.58771900
H	2.62931800	-0.93993800	-3.13697000
H	4.08017000	-1.95623000	-3.12480800
C	-2.36012800	-2.71475500	-1.63045300
H	-1.28645400	-2.50366200	-1.56195000
C	-2.56331000	-4.20370400	-1.27296200
H	-3.62534400	-4.47093000	-1.31224100
H	-2.02711700	-4.84396700	-1.98249100
H	-2.19734800	-4.43518900	-0.26722500
C	-2.78613000	-2.46050600	-3.08842600
H	-2.72726600	-1.39976800	-3.35648500
H	-2.13600700	-3.02223200	-3.76815100
H	-3.81147000	-2.79488800	-3.27932200
C	-2.45971500	-0.13984900	2.83202700
H	-1.38558800	-0.33875500	2.76201100
C	-3.00546700	-0.97260300	4.01196600
H	-2.49538100	-0.69610500	4.94148800
H	-4.07831500	-0.80231800	4.15532500
H	-2.85962500	-2.04654900	3.85116400
C	-2.61733500	1.36587400	3.11168000
H	-2.11878700	1.62488300	4.05249400
H	-2.16875700	1.96830700	2.31524700
H	-3.66841300	1.65880600	3.20814600
C	2.19651000	0.14499500	3.04502500
H	1.17656500	-0.23534500	2.93146600
C	2.84787300	-0.62225300	4.21585600
H	3.87106700	-0.27478100	4.39706400
H	2.27357200	-0.46959000	5.13620900
H	2.89339400	-1.69924600	4.01920000
C	2.08193000	1.64551400	3.37140500
H	3.06237200	2.10801000	3.52869500
H	1.57302500	2.18973200	2.56915100
H	1.50511100	1.78225500	4.29264900

C	2.16411700	3.24663500	-0.19519800
H	2.67693300	3.86750700	-0.93735300
H	2.83999100	2.43232900	0.08294600
H	1.98186300	3.84892400	0.70432200
O	1.52801000	1.83404300	-2.33377600
C	-2.32708400	4.62794300	-0.28374900
H	-3.65982400	3.08369600	-1.14077000
H	-2.73902400	2.55291700	0.27479300
H	-0.48272200	4.63267500	0.93196800
H	-0.32723700	5.53546000	-0.56901500
H	-2.84021900	4.99009600	0.61160600
H	-2.61795700	5.28630700	-1.11032100

6b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.155385 a.u.

M06 SCF energy in solution: -1734.397319 a.u.

M06 Free energy in solution: -1733.677563 a.u.

C	1.18043000	1.01570900	-3.11236000
C	-0.07456900	1.00307100	-2.27199800
C	-0.12082600	1.90574200	-1.17063800
C	0.76133100	3.14741800	-1.10045300
H	0.43101400	3.77555700	-1.95168500
H	-1.08867900	2.03791800	-0.69102400
C	0.60325200	4.02880900	0.15629100
C	2.91386700	4.26708800	-0.61011000
C	2.27615800	3.01914300	-1.21348300
C	2.95166200	1.96097900	-1.67029200
H	-0.97384900	0.54566600	-2.67419200
H	1.23336600	0.17110700	-3.80273300
H	1.37217300	1.94826400	-3.65682300
C	-1.01043700	-2.43661400	1.95870200
C	-2.20119200	-1.85390100	1.66253400
C	-0.62842000	-0.77151400	0.45457800
N	-1.95953200	-0.83223300	0.73814700
N	-0.06306500	-1.75533200	1.20799300
Rh	0.77932500	0.05404400	-0.63920100
H	-3.19690300	-2.05878900	2.02175100
H	-0.75905700	-3.25027400	2.62106200
C	1.36657700	-1.93304500	1.05380300
C	2.23940800	-1.22137900	1.91811300
C	1.83517100	-2.81784700	0.04490100
C	3.61559600	-1.38700700	1.71257100
C	3.22338000	-2.93264500	-0.10714100
C	4.10121900	-2.22532700	0.71149000
H	4.31536600	-0.86401100	2.35679000
H	3.62190300	-3.59963600	-0.86479800
H	5.17317300	-2.34139300	0.57847000
C	-3.00244800	0.01771100	0.19809600
C	-3.58050300	-0.32410100	-1.04469900
C	-3.42962200	1.12162400	0.96526500
C	-4.59135300	0.51440100	-1.53036500
C	-4.44950700	1.91920100	0.42860400
C	-5.01777500	1.62622400	-0.80717300
H	-5.06000500	0.29007900	-2.48253700
H	-4.80801600	2.77586100	0.99053200
H	-5.80699000	2.25851900	-1.20390400
C	0.89860400	-3.69351300	-0.78364000
H	-0.12442100	-3.33381900	-0.63661100
C	0.95215200	-5.15192300	-0.27828100
H	0.24621200	-5.77354900	-0.83979800
H	1.95287000	-5.57968300	-0.40616300
H	0.69328700	-5.22093500	0.78417900
C	1.19350800	-3.62413500	-2.29303800
H	0.45471600	-4.21664900	-2.84360800
H	1.14860000	-2.59256900	-2.66018600
H	2.18195400	-4.02769500	-2.53817300
C	-3.19472600	-1.59287700	-1.80407700
H	-2.16549600	-1.85106100	-1.53109400
C	-4.10164600	-2.76964000	-1.37922800
H	-5.14929900	-2.55948700	-1.62274900
H	-3.81024400	-3.68618900	-1.90488700
H	-4.04094600	-2.96455300	-0.30348800
C	-3.23111300	-1.43250500	-3.33477700
H	-2.65080600	-0.56729500	-3.67448500
H	-2.81473500	-2.32719400	-3.81014400
H	-4.25294200	-1.31584700	-3.71177700
C	-2.87739200	1.42706000	2.35621900
H	-1.96108600	0.84363500	2.49655000
C	-3.88117800	0.98634400	3.44355600
H	-3.46855200	1.16935700	4.44209800
H	-4.82008800	1.54513300	3.35954600
H	-4.12296500	-0.07948100	3.36750300
C	-2.50288900	2.90862600	2.54259000
H	-2.03515700	3.05395400	3.52271900
H	-1.79734400	3.24530200	1.77671600
H	-3.38094300	3.56217900	2.50374300
C	1.73617300	-0.37337300	3.08234200
H	0.64958900	-0.28017900	2.99111400
C	2.02885700	-1.07676700	4.42503700
H	3.10658300	-1.18396500	4.59157400
H	1.61802800	-0.49201100	5.25529600
H	1.58417400	-2.07743200	4.46234400
C	2.31985400	1.05140800	3.06834100
H	3.40707300	1.04896000	3.20484700
H	2.09789400	1.56086900	2.12398200
H	1.88890200	1.63976600	3.88586300
C	4.43207700	1.75984500	-1.73976000
H	4.76525700	1.65896400	-2.78048200
H	4.71867900	0.83807600	-1.21809800
H	4.96831400	2.59686100	-1.28724400
O	2.25977400	0.80662800	-2.13081500
C	1.73152300	5.06345000	0.00180600
H	-0.38949100	4.48609400	0.22308600
H	0.75587900	3.41868400	1.05607800
H	3.63897900	3.98721300	0.16377900
H	3.46285200	4.85787600	-1.35262500
H	1.99820900	5.54777800	0.94522400

H	1.41213700	5.85354200	-0.68792300

7b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.161571 a.u.

M06 SCF energy in solution: -1734.419843 a.u.

M06 Free energy in solution: -1733.699085 a.u.

C	-1.33988500	-2.85789700	-1.81758600
C	-0.98301300	-1.38384300	-1.72896500
C	0.22664900	-0.88436600	-2.28470200
C	1.29443400	-1.88927600	-2.65840200
H	0.94266500	-2.60428500	-3.41899200
H	0.28019200	0.13158000	-2.67218300
C	2.65422700	-1.30080800	-3.09104400
C	3.11264700	-2.55143500	-1.06332500
C	1.60023200	-2.59049700	-1.31049400
C	0.70955000	-3.37586000	-0.59875100
H	-1.84749000	-0.72827400	-1.69736400
H	-2.36962200	-3.01740200	-1.49304500
H	-1.25236800	-3.20997500	-2.85451100
H	3.39118800	-1.75435100	-0.35949000
H	3.49494800	-3.49184500	-0.65501000
H	2.74541100	-1.22279700	-4.17849800
H	2.77029000	-0.29309500	-2.67326000
C	-1.56559400	2.49673200	1.33497000
C	-0.25746900	2.80000800	1.51963900
C	-0.35305300	0.78457800	0.46014900
N	0.47051600	1.74951200	0.97617000
N	-1.61371700	1.26910600	0.68066700
Rh	0.41087000	-0.99775600	-0.18681000
H	0.22051800	3.65065500	1.97924100
H	-2.46434500	3.02922500	1.60237100
O	-0.55958200	-3.71820200	-0.97009400
C	3.69226400	-2.24099600	-2.45945500
H	4.69376000	-1.80315100	-2.41169200
H	3.76459700	-3.16698800	-3.04347500
C	1.11385200	-4.23319100	0.57460400
H	2.05160000	-3.90573100	1.02431800
H	0.32787900	-4.22702200	1.33506900
H	1.23424800	-5.27089900	0.23778500
C	1.91529900	1.66619000	0.96423200
C	2.54959000	0.90555300	1.97026200
C	2.62918600	2.36601300	-0.03154000
C	3.94563900	0.80356700	1.91775500
C	4.02436800	2.24079900	-0.02337800
C	4.67522400	1.45896400	0.92814100
H	4.47093700	0.22482700	2.67075600
H	4.61068900	2.76839100	-0.76921200
H	5.75831200	1.37713000	0.91167800
C	-2.87018000	0.65273300	0.30251600
C	-3.53605800	1.14696900	-0.84106700
C	-3.40576800	-0.36528800	1.11714400
C	-4.76719100	0.56487000	-1.16930200
C	-4.63792600	-0.91227100	0.73428800
C	-5.31162000	-0.45712000	-0.39560400
H	-5.30913500	0.92174000	-2.03959000
H	-5.08211700	-1.69616400	1.34009500
H	-6.26924200	-0.89172300	-0.66777100
C	-2.73461100	-0.85016600	2.39884000
H	-1.74976600	-0.37776500	2.46880600
C	-2.98981500	2.28998700	-1.69597300
H	-1.96562900	2.50258900	-1.37131600
C	1.76009200	0.21991900	3.08358900
H	0.77511100	0.69507600	3.14119800
C	1.94735000	3.27839400	-1.04780900
H	0.86943000	3.08992500	-1.00392400
C	-3.81730200	3.57576200	-1.48671700
H	-3.39474000	4.40150400	-2.07002800
H	-4.85508900	3.43445500	-1.80863700
H	-3.83664100	3.87966200	-0.43425400
C	-2.92288400	1.92964400	-3.19309900
H	-2.32580200	1.02740700	-3.36733000
H	-3.91788600	1.75865300	-3.61781400
H	-2.46602100	2.75179600	-3.75505500
C	-3.54272700	-0.41619200	3.63940600
H	-4.54133500	-0.86713800	3.64182900
H	-3.03234700	-0.73081900	4.55685000
H	-3.66847400	0.67152400	3.67636400
C	-2.50842200	-2.37432300	2.39268300
H	-1.92547700	-2.68744500	1.51905200
H	-1.96822100	-2.67871400	3.29690100
H	-3.45509200	-2.92561200	2.37987100
C	2.41544100	0.37646200	4.46942700
H	1.74887300	-0.01714300	5.24424800
H	3.36076000	-0.17133500	4.54427800
H	2.61577300	1.42828200	4.69641000
C	1.53276100	-1.26814300	2.76885800
H	0.94978800	-1.40665000	1.83137600
H	2.47848100	-1.80530800	2.64304900
H	0.95138500	-1.76154000	3.55547900
C	2.17478300	4.76065900	-0.68067900
H	3.23941200	5.01762000	-0.71838100
H	1.64645000	5.41340400	-1.38434600
H	1.81502900	4.98890600	0.32873000
C	2.39653000	3.00596200	-2.49530200
H	3.45923900	3.22585300	-2.64414900
H	2.22680300	1.96210900	-2.78032700
H	1.83340100	3.64260300	-3.18660300

TS6b (X = CH_2)

B3LYP SCF energy in gas phase: -464.6315469 a.u.

M06 SCF energy in solution: -464.4180599 a.u.

M06 Free energy in solution: -464.2358679 a.u.

C	2.16776800	-1.50450400	-0.11519600
C	1.24630300	-1.60927600	0.92755000
C	-0.09558100	-1.32848000	0.71299600
C	-0.67910400	-0.88350500	-0.58984600

H	-0.17370300	-1.27540800	-1.47441300
H	-0.76608400	-1.31586900	1.56927700
C	-2.21138600	-0.90852100	-0.66844200
C	-1.56432000	1.26576900	0.27812900
C	-0.32248100	0.54055600	-0.21490200
C	0.97783300	1.03869000	-0.30315300
H	1.60641300	-1.63866700	1.95437200
H	3.23092600	-1.53074500	0.10517900
H	1.90944900	-1.82296600	-1.11543200
H	-1.43872800	1.76078400	1.24855600
H	-1.83012100	2.05660400	-0.43922900
H	-2.51367400	-0.64792400	-1.69006800
H	-2.63553600	-1.89316400	-0.44077900
C	1.34675700	2.37628200	0.31078200
H	2.09869100	2.87430800	-0.30875300
H	1.79249700	2.21829800	1.30331400
H	0.48570800	3.04099100	0.42918000
O	1.93881200	0.34607000	-0.80894000
C	-2.67503100	0.18653700	0.31843700
H	-2.76095400	-0.22532100	1.33085500
H	-3.65991900	0.58922100	0.06132800

TS7b (X = CH_2)

B3LYP SCF energy in gas phase: -464.6659335 a.u.

M06 SCF energy in solution: -464.4632351 a.u.

M06 Free energy in solution: -464.2818181 a.u.

C	-3.27575400	-0.66352200	-0.27103100
C	-2.15663700	-0.00288000	-0.57013900
C	-0.79521700	-0.62338600	-0.49991500
C	-0.12042900	-0.89595600	0.81052500
H	-0.64386100	-0.56630900	1.70341700
H	-0.60965500	-1.34357800	-1.29787900
C	0.88393700	-2.03656000	0.89197100
C	1.78276700	-0.35388500	-0.66863200
C	0.46148900	0.18182900	-0.10774400
C	0.28621500	1.62359800	0.24560700
H	-2.22323500	1.02503200	-0.91938500
H	-4.25268600	-0.19931100	-0.37471000
H	-3.25966000	-1.68882100	0.09328800
H	1.91489500	-0.15411500	-1.73938100
H	2.61903700	0.12856300	-0.14738300
H	1.47827500	-1.92255300	1.80778200
H	0.40978800	-3.02473200	0.93539900
C	1.32028000	2.61348500	-0.26832000
H	0.98341600	3.62859000	-0.04937000
H	1.48166200	2.49673000	-1.34669500
H	2.28943700	2.44654900	0.21863500
O	-0.66328800	2.00547900	0.91470000
C	1.77688500	-1.87205500	-0.36066400
H	1.35087500	-2.42780900	-1.20311900
H	2.78680000	-2.26606900	-0.20813800

8b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.065037 a.u.

M06 SCF energy in solution: -1734.321614 a.u.

M06 Free energy in solution: -1733.611124 a.u.

C	1.38992000	0.10531100	1.65203700
H	1.50470000	0.82216200	2.46793100
C	0.91038500	-1.20011300	1.96368400
H	1.15176000	-2.04791900	1.32680300
C	0.38032400	-1.51599900	3.32623900
C	0.50013600	-0.59517900	4.46292600
H	0.31261100	-0.97573600	5.46407700
H	1.14570900	0.27704700	4.40804900
C	-1.43878600	0.81553200	-2.57960100
C	-1.28927900	-0.52745100	-2.66669700
C	-0.85983900	0.05958800	-0.51631700
N	-1.16388500	1.16951000	-1.26259600
N	-0.92505200	-0.98465100	-1.40292500
H	0.08567300	-2.54301800	3.52327200
C	2.34289800	0.37171600	0.51398100
H	2.15943300	1.37468300	0.11548300
H	2.16955300	-0.33719000	-0.30202700
C	4.81848800	0.61754400	-0.12791400
H	4.65618700	-0.05761900	-0.98052400
H	4.61427000	1.63183800	-0.50048200
C	6.20729000	0.52393100	0.32211900
C	7.34806200	0.44164700	0.71603400
Rh	-0.72220600	0.00682900	1.45180900
H	-1.72259800	1.54808000	-3.31763800
H	-1.41489900	-1.20251700	-3.49758800
C	-0.74959000	-2.39456300	-1.10192700
C	0.43266100	-3.03967100	-1.53049100
C	-1.79790100	-3.08637700	-0.45703600
C	0.56278400	-4.40446800	-1.24085500
C	-1.60566000	-4.44855400	-0.19092400
C	-0.43661000	-5.10146000	-0.56831300
H	1.45679800	-4.93209900	-1.55669100
H	-2.39363400	-5.00966100	0.30184900
H	-0.31238100	-6.15972800	-0.35709700
C	-1.31663500	2.51544200	-0.74181700
C	-0.31735400	3.47801900	-1.00461900
C	-2.49670200	2.82327800	-0.03035600
C	-0.50714500	4.75933800	-0.47114400
C	-2.62097000	4.11573000	0.49412000
C	-1.63366300	5.07322400	0.28391700
H	0.23936400	5.52575600	-0.65104300
H	-3.51012000	4.38161800	1.05697000
H	-1.75122700	6.07278400	0.69228500
C	1.52483000	-2.34231500	-2.34027200
H	1.38008100	-1.25963400	-2.25208100
C	-3.14220300	-2.44925300	-0.11503600
H	-3.06780800	-1.37158000	-0.29067500
C	0.90112400	3.19737300	-1.88092200
H	1.04082200	2.11147800	-1.93141300
C	-3.62500900	1.81424200	0.16639300

H	-3.46109000	0.97861600	-0.52177600
C	1.41152100	-2.70657700	-3.83722900
H	2.17785500	-2.18021500	-4.41712700
H	1.55440800	-3.78236700	-3.98783200
H	0.43346000	-2.44284700	-4.25284600
C	2.94465500	-2.66433900	-1.83471400
H	3.67838400	-2.04809000	-2.36594700
H	3.05380400	-2.47509300	-0.76156900
H	3.21447000	-3.71012000	-2.01595600
C	0.66861900	3.70910600	-3.32014300
H	0.52228900	4.79505500	-3.32625900
H	1.53563800	3.48191600	-3.95048400
H	-0.21302700	3.25528500	-3.78438300
C	2.19934900	3.80972000	-1.32005900
H	2.35484200	3.55288400	-0.26694400
H	3.05992400	3.44748800	-1.89318700
H	2.20064500	4.90217800	-1.39777100
C	-4.24849600	-2.98726600	-1.04720500
H	-4.39381500	-4.06468100	-0.91107800
H	-5.20238500	-2.49164700	-0.83380500
H	-4.00398200	-2.81465300	-2.10095800
C	-3.52653400	-2.64501500	1.36363200
H	-3.66209000	-3.70259000	1.61393000
H	-2.75953700	-2.23776600	2.03347500
H	-4.47332900	-2.13722600	1.57962400
C	-5.01012200	2.39997100	-0.17254800
H	-5.77148200	1.61378600	-0.12387200
H	-5.30839400	3.18775100	0.52709700
H	-5.02359000	2.82355500	-1.18183800
C	-3.62027900	1.24775900	1.59567700
H	-2.65459200	0.75500500	1.84968200
H	-3.75161300	2.03364300	2.34707000
H	-4.40158800	0.49386700	1.73512200
C	8.73109200	0.34711000	1.17892200
H	9.33610500	-0.26610800	0.50042300
H	8.78717700	-0.10719300	2.17549400
H	9.19911800	1.33694800	1.23859500
O	-0.70907000	-0.52978100	3.66331300
C	3.80842300	0.27699000	0.98949100
H	4.01310500	-0.73377300	1.36392100
H	3.97068600	0.96076900	1.83229500

TS8b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.056692 a.u.

M06 SCF energy in solution: -1734.310005 a.u.

M06 Free energy in solution: -1733.601392 a.u.

C	-1.40797600	-0.16982700	1.66791600
H	-1.52112700	-0.87893400	2.48957300
C	-0.93929000	1.14684800	1.98713800
H	-1.11668600	1.98668700	1.31910700
C	-0.32231000	1.43413800	3.25538600
C	-0.24525900	0.45750000	4.35152000
H	0.05367600	0.85453400	5.32324800
H	-1.06461900	-0.26149400	4.44528300
C	1.46603400	-0.70876000	-2.60701000
C	1.28139300	0.63197400	-2.66124000
C	0.84807300	-0.02121800	-0.52778300
N	1.18805300	-1.10045000	-1.30189500
N	0.89466300	1.04527900	-1.38905400
H	0.19610700	2.38054400	3.37906700
C	-2.36199300	-0.43281800	0.53341200
H	-2.17645900	-1.43551900	0.13504900
H	-2.19256000	0.27613600	-0.28326900
C	-4.83671800	-0.69852900	-0.10013200
H	-4.67947800	-0.02827100	-0.95747200
H	-4.62678700	-1.71420000	-0.46564400
C	-6.22478400	-0.60970800	0.35239200
C	-7.36501100	-0.53158700	0.74874700
Rh	0.70627300	-0.06398400	1.47128200
H	1.77713700	-1.41405700	-3.36052800
H	1.39564100	1.33151100	-3.47335700
C	0.67782800	2.43995500	-1.04991000
C	-0.52959600	3.05886800	-1.44712900
C	1.70931100	3.14624700	-0.39317800
C	-0.70465800	4.40718000	-1.10769700
C	1.47234200	4.49085800	-0.07709800
C	0.27665200	5.11458300	-0.41903000
H	-1.61909200	4.91425300	-1.39752300
H	2.24669000	5.06269700	0.42498200
H	0.11770700	6.15969100	-0.16908300
C	1.36855900	-2.44900600	-0.79906300
C	0.38190400	-3.42552300	-1.06074500
C	2.55755400	-2.74158100	-0.09536300
C	0.59309700	-4.70538900	-0.53279700
C	2.70235000	-4.03396000	0.42522400
C	1.72780300	-5.00450100	0.21686200
H	-0.14266800	-5.48241300	-0.71107600
H	3.59776900	-4.28871300	0.98324000
H	1.86133500	-6.00324100	0.62229800
C	-1.59966200	2.35239700	-2.27829800
H	-1.42358100	1.27233800	-2.21854500
C	3.08178200	2.54674700	-0.09709000
H	3.04227200	1.47420300	-0.30998400
C	-0.84323000	-3.15613800	-1.93123800
H	-1.01165900	-2.07324100	-1.95431600
C	3.67777600	-1.72057000	0.08953100
H	3.49411500	-0.88362900	-0.59215400
C	-1.49067700	2.75954100	-3.76454200
H	-2.23792000	2.22564600	-4.36216600
H	-1.66591900	3.83418000	-3.88707600
H	-0.50314800	2.53667000	-4.18147800
C	-3.03054600	2.61972500	-1.77225400
H	-3.74278600	1.99377400	-2.32098500
H	-3.13942200	2.40303000	-0.70417700
H	-3.33181800	3.66044500	-1.93151300
C	-0.59507200	-3.62415800	-3.38269200
H	-0.41673800	-4.70481900	-3.41563400

H	-1.46811600	-3.40683000	-4.00820200
H	0.27273000	-3.13237800	-3.83392000
C	-2.12569600	-3.81708700	-1.38994700
H	-2.28752000	-3.59716700	-0.32935100
H	-2.99500600	-3.45884500	-1.95226700
H	-2.10044300	-4.90639300	-1.50110700
C	4.14808200	3.15735900	-1.03159800
H	4.25924300	4.23348400	-0.85829200
H	5.12270800	2.68789300	-0.85646000
H	3.88683300	3.01493700	-2.08581800
C	3.49197300	2.70666200	1.37893000
H	3.58832900	3.75970500	1.66440100
H	2.76211600	2.24012400	2.05123600
H	4.46455400	2.23359700	1.55484900
C	5.06202100	-2.29265100	-0.27632100
H	5.81619000	-1.49891200	-0.24077700
H	5.38111200	-3.07800400	0.41679300
H	5.06104900	-2.71519300	-1.28617300
C	3.69181100	-1.15958200	1.52062600
H	2.74018600	-0.64647500	1.77790600
H	3.81618200	-1.94778200	2.27036800
H	4.48565100	-0.41780700	1.65545600
C	-8.74737400	-0.44288000	1.21461300
H	-9.35788300	0.16240800	0.53395800
H	-8.80352400	0.01704800	2.20857200
H	-9.20877500	-1.43533100	1.28149500
O	0.86737200	0.00455900	3.59638200
C	-3.82735800	-0.34477100	1.01406600
H	-4.03821000	0.66650000	1.38363800
H	-3.98246600	-1.02542300	1.86045200

9b (X = CH_2)

B3LYP SCF energy in gas phase: -1735.077238 a.u.

M06 SCF energy in solution: -1734.327385 a.u.

M06 Free energy in solution: -1733.618252 a.u.

C	1.56286100	0.25195100	1.67246800
H	1.68415900	0.90855300	2.53296600
C	0.86590400	-0.97424900	1.86582600
H	0.98300600	-1.78811900	1.15434200
C	-0.17986500	-1.03597500	2.82447000
C	-0.27461900	-0.03052700	3.97289000
H	-1.12062900	-0.28409500	4.62780400
H	0.63777800	-0.02830600	4.59133700
C	-1.62191600	0.53057300	-2.66155900
C	-1.59859300	-0.82374200	-2.58379000
C	-0.93571900	-0.03433800	-0.56558300
N	-1.20432700	0.99679000	-1.42131800
N	-1.17186300	-1.15929400	-1.29884100
H	-0.82369800	-1.91275200	2.81468300
C	2.56482500	0.45338600	0.57409800
H	2.53930800	1.50379300	0.26158600
H	2.31430000	-0.15516800	-0.30198300
C	5.05454400	0.37581800	-0.02693100
H	4.80047400	-0.20452000	-0.92617900
H	5.00952400	1.43350200	-0.32487100
C	6.40669400	0.04030500	0.41656500
C	7.51757800	-0.24202400	0.80322200
Rh	-0.58701600	0.52518700	1.39727700
H	-1.89658200	1.19036500	-3.46855000
H	-1.84810000	-1.57917800	-3.31159000
C	-1.05170800	-2.52950400	-0.83724500
C	0.13320900	-3.24050400	-1.13223900
C	-2.14408000	-3.11371000	-0.16161300
C	0.21719600	-4.56334200	-0.67889900
C	-1.99884100	-4.43989300	0.26812500
C	-0.83065300	-5.15499700	0.02196100
H	1.11089300	-5.14285500	-0.88597200
H	-2.81930500	-4.92457800	0.78792200
H	-0.74259900	-6.18304800	0.36134900
C	-1.08955300	2.35921600	-0.94482000
C	-0.01588900	3.17146400	-1.38034800
C	-2.05532900	2.80503900	-0.00738800
C	0.12015300	4.42287100	-0.76928300
C	-1.83729300	4.05395100	0.59699700
C	-0.75516500	4.84607900	0.23118100
H	0.93092700	5.07723500	-1.07149900
H	-2.54177800	4.41999500	1.33676300
H	-0.60753000	5.81227000	0.70443300
C	1.26671000	-2.64982400	-1.96960100
H	1.15304600	-1.55945000	-1.97564400
C	-3.47788700	-2.39819900	0.03888000
H	-3.33804600	-1.33848300	-0.19769400
C	0.91270100	2.75942500	-2.52042000
H	0.90917300	1.66461700	-2.58207800
C	-3.36069000	2.04606300	0.25543700
H	-3.45511300	1.26872300	-0.51055100
C	1.16867600	-3.13366900	-3.43306600
H	1.96374500	-2.68389000	-4.03822700
H	1.27532600	-4.22265400	-3.49126800
H	0.20801800	-2.86958600	-3.88733500
C	2.66503200	-2.96625300	-1.40583200
H	3.42833900	-2.42657900	-1.97717000
H	2.76264300	-2.67812300	-0.35324700
H	2.90466800	-4.03213200	-1.48019800
C	0.38018600	3.31235600	-3.86274500
H	0.38996600	4.40808500	-3.85778100
H	1.00952800	2.97257200	-4.69254400
H	-0.64830600	2.99588600	-4.06547700
C	2.37301500	3.20703100	-2.32799400
H	2.77473100	2.90085800	-1.35738300
H	2.99958600	2.76425900	-3.10941900
H	2.48203300	4.29390000	-2.40819900
C	-4.53503400	-2.95218400	-0.94081200
H	-4.72991100	-4.01370900	-0.75174700
H	-5.48142700	-2.41144700	-0.82796000
H	-4.21005900	-2.85391400	-1.98234600
C	-3.98917600	-2.47941400	1.48928300

H	-4.21340700	-3.50870300	1.78824900
H	-3.25887100	-2.07518800	2.19915000
H	-4.91592800	-1.90430900	1.59327100
C	-4.59018500	2.96599800	0.10970600
H	-5.50768600	2.37022800	0.16510700
H	-4.63840800	3.71709700	0.90485300
H	-4.58291800	3.49022400	-0.85123800
C	-3.36994400	1.35114900	1.62537800
H	-2.64943100	0.49975600	1.67218300
H	-3.12780500	2.03012600	2.44719100
H	-4.34142800	0.88401700	1.82482200
C	8.86557900	-0.57586600	1.25799900
H	9.31573100	-1.35410700	0.63028400
H	8.85639500	-0.94533000	2.29043000
H	9.52358800	0.30057900	1.22492400
O	-0.47795800	1.19371300	3.29436200
C	3.99232900	0.11241200	1.06319700
H	4.03980000	-0.94048400	1.36641000
H	4.23465300	0.70726800	1.95176400

TS1b (X = O)

B3LYP SCF energy in the gas: -1770.933897 a.u.

M06 SCF energy in solution: -1770.203747 a.u.

M06 Free energy in solution: -1769.513277 a.u.

C	3.28978400	3.24937100	-0.97749700
C	2.47257900	2.02378200	-0.83364200
C	1.07333000	1.92161400	-1.35854900
C	0.19016100	3.08397100	-1.18628200
H	0.70362000	3.87469600	-0.63526600
H	1.01714800	1.38778800	-2.31419600
C	-0.74705600	3.66541200	-2.22048600
C	-1.98779500	4.19793600	-0.30664100
C	-1.08636000	3.12269700	0.24284100
C	-0.70321900	2.46745300	1.30765000
H	3.00466400	1.07936000	-0.76162600
H	4.37525800	3.16605400	-1.00292300
H	2.87601300	4.12745000	-1.47350100
H	-2.99613400	3.77095400	-0.42105200
H	-2.05184500	5.06077900	0.36395900
H	-0.18873100	4.17363600	-3.01414000
H	-1.38579900	2.89334300	-2.67672000
O	-1.50177600	4.66724700	-1.55822100
Rh	-0.39638400	1.13691500	-0.16325000
C	-0.04732600	-0.88339600	0.16790200
N	1.03610700	-1.69069700	0.39334200
C	0.64112600	-3.00038300	0.62291500
C	2.43851200	-1.32956500	0.31772800
N	-1.11937000	-1.73723800	0.25700600
C	-0.71352100	-3.03102700	0.53223800
C	-2.50360400	-1.36094000	0.03534200
C	3.06840800	-0.78156600	1.45441700
C	3.13136600	-1.62293900	-0.87691100
C	4.43814600	-0.50574900	1.35503200
C	2.32917500	-0.54344500	2.76795900
C	5.14823900	-0.77442100	0.18739000
C	4.50127200	-1.32896100	-0.91339000
C	2.46912400	-2.26406700	-2.09535300
C	2.77397800	0.74794100	3.47919500
C	2.48743900	-1.75965200	3.70636100
C	2.68945900	-1.44458800	-3.38187100
C	2.95794200	-3.71493200	-2.28918000
C	-3.32107200	-1.08279500	1.15310300
C	-2.98951400	-1.34694800	-1.29011600
C	-4.33307000	-0.99821800	-1.47817600
C	-2.13972800	-1.74304300	-2.49460300
C	-5.15739200	-0.69627500	-0.39820900
C	-4.65707700	-0.74631500	0.90054100
C	-2.82031700	-1.19464000	2.59145400
C	-2.10009700	-0.63871100	-3.56806200
C	-2.62975900	-3.07698400	-3.09579600
C	-3.21159600	-2.55826600	3.20191600
C	-3.32441100	-0.05090600	3.49166300
H	1.35764700	-3.78221300	0.81860000
H	-1.41528200	-3.84405600	0.62810300
H	4.95887500	-0.08008000	2.20582700
H	6.21173900	-0.55808700	0.13901000
H	5.06871800	-1.54426000	-1.81365600
H	1.26364300	-0.43689500	2.53767600
H	2.11056400	-2.68055100	3.24796400
H	1.93560800	-1.59723000	4.63930800
H	3.54102200	-1.92018200	3.96197100
H	3.78807800	0.66297700	3.88504700
H	2.11072600	0.95056100	4.32764100
H	2.75282200	1.60847600	2.80211900
H	1.38895000	-2.30307600	-1.92129500
H	4.03557100	-3.74728300	-2.48457200
H	2.44883900	-4.17908700	-3.14120800
H	2.76400400	-4.32927200	-1.40311300
H	3.74681500	-1.40429500	-3.66471200
H	2.33496100	-0.41340000	-3.27056900
H	2.14548800	-1.90109200	-4.21621700
H	-4.74203300	-0.97789400	-2.48383800
H	-6.19818900	-0.43523300	-0.56733200
H	-5.31821700	-0.52745400	1.73246100
H	-1.11076900	-1.89947800	-2.15523300
H	-2.61635600	-3.88075800	-2.35152300
H	-1.98823500	-3.37751200	-3.93184400
H	-3.65424100	-2.99116900	-3.47449600
H	-3.08875800	-0.45707600	-4.00322400
H	-1.42940300	-0.92814400	-4.38491500
H	-1.74292500	0.31035300	-3.14968300
H	-1.72550000	-1.14131100	2.57582300
H	-4.30108400	-2.67049400	3.23667100
H	-2.83049100	-2.64252100	4.22583600
H	-2.80944100	-3.39653400	2.62345800
H	-4.39994000	-0.12632600	3.68428100
H	-3.13358700	0.93141300	3.04667100

H	-2.82238200	-0.09297700	4.46472200
C	-0.54291900	2.49262200	2.77620400
H	-1.19600000	3.25876000	3.21497700
H	-0.77077600	1.52869400	3.23786200
H	0.49334700	2.75274900	3.02548300
O	2.67638400	2.90748900	0.27355700

TS4b (X = O)

B3LYP SCF energy in gas phase: -1770.946106 a.u.

M06 SCF energy in solution: -1770.203279 a.u.

M06 Free energy in solution: -1769.508403 a.u.

C	-2.03056500	-2.23423400	-1.38379300
C	-1.77335800	-0.99289600	-1.60239900
C	-0.61547800	-3.58642500	-0.65179100
C	0.30081100	-3.34873000	0.46051200
C	1.54076600	-2.75534800	0.30836800
C	2.06125300	-2.34698900	-1.05819500
H	-0.02563600	-3.64917200	1.45579200
H	-0.13600200	-3.65284300	-1.62697400
H	2.19482200	-2.67343700	1.16918600
H	2.22350500	-3.23069700	-1.69790900
C	-1.68179400	-4.64808200	-0.44654800
H	-1.22852600	-5.64238400	-0.50877300
H	-2.16008600	-4.54182600	0.54211100
C	-3.12574500	-3.25290900	-1.52538900
H	-3.86358600	-3.10103800	-0.71881400
H	-3.63148100	-3.11125300	-2.48605100
H	3.01852100	-1.82773500	-0.95084100
C	1.34351100	2.50345400	0.99936200
C	0.02953000	2.71006600	1.22520900
C	0.24266800	0.66152700	0.25338800
N	-0.65001600	1.59312300	0.74255700
N	1.46814100	1.24909800	0.41273200
Rh	-0.26338800	-1.24332900	-0.22170500
O	-2.62542500	-4.56704700	-1.49023100
H	-0.49053700	3.53823400	1.67573400
H	2.20407200	3.12237100	1.19165600
C	2.78201900	0.74160500	0.05834400
C	3.22669000	0.90355900	-1.27041300
C	3.60120100	0.22270600	1.08675000
C	4.52574200	0.47023800	-1.56590900
C	4.88968000	-0.19431200	0.72677800
C	5.34570400	-0.08032500	-0.58415600
H	4.90421300	0.57665600	-2.57725700
H	5.55132100	-0.59833300	1.48622500
H	6.35051000	-0.40633500	-0.83766300
C	-2.10134600	1.55838000	0.74810900
C	-2.77547900	0.53399600	1.45625800
C	-2.80112800	2.59970800	0.09172600
C	-4.17296500	0.56887700	1.48458500
C	-4.20257200	2.58572200	0.17232300
C	-4.88410300	1.58743300	0.85367700
H	-4.71975000	-0.19954500	2.01775500
H	-4.76574000	3.37605400	-0.31336900
H	-5.96904100	1.60046500	0.89966700
C	3.17760900	0.18835700	2.55682000
H	2.08615600	0.27825300	2.60118300
C	3.78475300	1.38631400	3.32226800
H	3.50216700	2.34716300	2.88229200
H	3.44949200	1.38252000	4.36556300
H	4.87909100	1.33129800	3.31968800
C	3.56088400	-1.11323200	3.28695900
H	3.17497900	-2.00574100	2.78476700
H	4.64613800	-1.22805200	3.37768500
H	3.15310200	-1.09930600	4.30362100
C	2.39254100	1.59498400	-2.34555400
H	1.35418500	1.62404200	-2.00177000
C	2.86810400	3.05294900	-2.52821000
H	3.90663300	3.08719400	-2.87652600
H	2.24817000	3.56584700	-3.27240900
H	2.81279400	3.62012200	-1.59189500
C	2.39634700	0.84577200	-3.69014700
H	3.39051900	0.82928300	-4.15051000
H	2.05026400	-0.18344900	-3.56211100
H	1.72672100	1.35168300	-4.39539900
C	-2.14187900	3.75268200	-0.67498000
H	-1.06990200	3.55417100	-0.76017900
C	-2.31965600	5.08714300	0.08307900
H	-1.77996000	5.89011700	-0.43050900
H	-3.37633000	5.37293800	0.13023900
H	-1.95289900	5.03834500	1.11432900
C	-2.67783900	3.90389900	-2.11377200
H	-2.15029300	4.72209900	-2.61592200
H	-2.52609800	2.99692800	-2.70583100
H	-3.74567200	4.14549200	-2.13289300
C	-2.02867200	-0.55827300	2.21770100
H	-1.20137200	-0.94397100	1.56346700
C	-1.33717700	-0.00939700	3.48204800
H	-2.09622800	0.34868700	4.18709000
H	-0.76048800	-0.79735600	3.97883600
H	-0.66375300	0.82269300	3.26176500
C	-2.87737200	-1.78710100	2.57242700
H	-3.62604100	-1.54726300	3.33488300
H	-3.39629100	-2.19638600	1.70001600
H	-2.23561300	-2.56940200	2.99152000
C	-2.18723600	0.11749100	-2.49490200
H	-1.30935500	0.54530000	-2.99114200
H	-2.68034300	0.91135300	-1.93033600
H	-2.87574600	-0.24497300	-3.26748700
O	1.09071200	-1.49373000	-1.64801700

1c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.608279 a.u.

M06 SCF energy in solution: -2612.560365 a.u.

M06 Free energy in solution: -2611.649737 a.u.

C	2.88037300	2.44018900	-0.83618700

C	2.30138100	1.09804300	-0.52231600
C	0.95691600	0.68958400	-1.03646700
C	-0.14313800	1.56794700	-0.89029700
H	0.06506500	2.45463900	-0.29042100
H	0.97800600	-0.00237500	-1.87432800
C	-1.30147400	1.69685200	-1.84863800
C	-3.10708400	1.45781700	-0.01534100
C	-2.02796300	1.10106800	0.92986300
C	-1.28007200	1.18956500	1.96681500
H	3.01550300	0.30008800	-0.34703400
H	2.25285900	3.10788500	-1.43024300
H	-3.55366200	0.54439900	-0.42270800
H	-3.88630400	2.02255900	0.50565600
H	-0.99520300	2.34921500	-2.67715300
H	-1.56171400	0.73282200	-2.29144300
Rh	-0.40929700	-0.01653000	0.51250400
C	0.04734100	-1.99183700	-0.04608100
N	1.18253200	-2.75554200	-0.13233400
C	0.87299400	-4.10812400	-0.17784500
C	2.56253800	-2.31788000	-0.21734100
N	-0.97130600	-2.91368400	-0.06942300
C	-0.47776800	-4.20645500	-0.14205600
C	-2.39686700	-2.63633100	-0.04106100
C	3.27723700	-2.07807200	0.97439000
C	3.16014400	-2.25479500	-1.49588500
C	4.62912900	-1.72994700	0.85121500
C	2.65820900	-2.24026700	2.35986200
C	5.24071400	-1.63483100	-0.39568500
C	4.51377200	-1.89960500	-1.55329800
C	2.41510300	-2.60113100	-2.78492700
C	2.99177500	-1.06604900	3.29859000
C	3.08839500	-3.58235500	2.98965500
C	2.62822900	-1.56070300	-3.90199100
C	2.81810000	-4.00453500	-3.28764000
C	-3.05449200	-2.61501000	1.20751300
C	-3.07710900	-2.49528800	-1.27174200
C	-4.46014000	-2.27827000	-1.21486200
C	-2.37946700	-2.65735800	-2.62192800
C	-5.13320700	-2.22457300	0.00392800
C	-4.43861800	-2.39741100	1.19800700
C	-2.33304900	-2.88995800	2.52595500
C	-2.92245000	-1.72116400	-3.71728400
C	-2.47436200	-4.12262000	-3.10550100
C	-2.51564000	-4.36664600	2.94088500
C	-2.77677200	-1.95984300	3.66995700
H	1.64203500	-4.86171800	-0.23071000
H	-1.12993300	-5.06441700	-0.16110900
H	5.21328100	-1.53780100	1.74532000
H	6.28818600	-1.35717600	-0.46607200
H	5.00784800	-1.83418700	-2.51724200
H	1.56878400	-2.26337500	2.24666600
H	2.80272700	-4.43410000	2.36256100
H	2.61914300	-3.71257000	3.97154900
H	4.17491600	-3.61999500	3.12836600
H	4.05884800	-1.02777700	3.54302100
H	2.45261300	-1.18367200	4.24560500
H	2.71061300	-0.10341300	2.85847900
H	1.34194800	-2.62617900	-2.56526600
H	3.88691800	-4.04212700	-3.52630000
H	2.26092500	-4.25909900	-4.19620700
H	2.61719500	-4.77977500	-2.54066400
H	3.66368600	-1.54970200	-4.25824800
H	2.38123700	-0.54562400	-3.57264700
H	1.99299500	-1.80273300	-4.76112700
H	-5.01914800	-2.16475600	-2.13759100
H	-6.20756800	-2.06353700	0.02186300
H	-4.98118000	-2.37494000	2.13735000
H	-1.31773900	-2.42117800	-2.48417500
H	-2.02592700	-4.82425100	-2.39529600
H	-1.95796300	-4.23973900	-4.06497300
H	-3.52088300	-4.41468200	-3.24893000
H	-3.92987800	-2.01184400	-4.03577000
H	-2.28124500	-1.78463000	-4.60344400
H	-2.96453700	-0.67416400	-3.40373900
H	-1.26085800	-2.72159700	2.36959700
H	-3.57418300	-4.59432000	3.11049200
H	-1.97347500	-4.57188800	3.87085500
H	-2.14503100	-5.05651700	2.17534500
H	-3.81212500	-2.14923500	3.97320800
H	-2.69083800	-0.90518800	3.39196500
H	-2.14844400	-2.13214700	4.55082900
C	-2.56782600	2.31833800	-1.20468100
O	2.33565600	2.14017400	0.45767700
C	-2.28331400	3.74717900	-0.70213900
O	-2.42747900	4.12643200	0.43924300
O	-1.84286700	4.52270000	-1.70506800
C	-3.68196400	2.38684300	-2.26737900
O	-3.67926600	1.76775800	-3.30793700
O	-4.67704700	3.18914600	-1.86273500
C	-5.79630000	3.31762500	-2.76748300
H	-6.49165100	3.99321600	-2.27110400
H	-5.46231300	3.73382500	-3.72048300
H	-6.25660800	2.34192800	-2.93861000
C	-1.58183500	5.90321800	-1.36785900
H	-1.24840400	6.36833000	-2.29474800
H	-2.49460000	6.37808300	-1.00144200
H	-0.80682100	5.96516300	-0.60045100
C	4.34617700	2.67828600	-0.94591200
C	4.86406900	3.25052200	-2.11532200
C	5.21847500	2.32952800	0.09350400
C	6.23686400	3.45716800	-2.25190600
H	4.19068600	3.53812200	-2.92011200
C	6.59010000	2.54354300	-0.04226800
H	4.81178100	1.91354900	1.01003000
C	7.10332400	3.10318500	-1.21526000
H	6.62817000	3.90233000	-3.16232700
H	7.25964400	2.28300100	0.77306600
H	8.17159400	3.27215600	-1.31690600

C	-0.92828800	1.78874100	3.23166600
C	-0.05843100	1.14636100	4.13124400
C	-1.47192200	3.04642700	3.56856000
C	0.25783300	1.74434700	5.34749600
H	0.35842100	0.17999200	3.86710100
C	-1.14639600	3.63814600	4.78593100
H	-2.12375600	3.54802400	2.86085500
C	-0.28520800	2.98997400	5.67653100
H	0.92680300	1.24225200	6.04038500
H	-1.56392700	4.60784000	5.04088400
H	-0.03693000	3.45514900	6.62624000

TS1c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.580936 a.u.

M06 SCF energy in solution: -2612.528186 a.u.

M06 Free energy in solution: -2611.618888 a.u.

C	2.38891000	2.85999500	-0.25864700
C	1.91305200	1.44948900	-0.38389200
C	0.56753200	1.11148000	-0.94719600
C	-0.57576400	1.93967900	-0.52590900
H	-0.24823100	2.67432200	0.21350800
H	0.61590200	0.84118300	-2.00688200
C	-1.63005400	2.48402600	-1.46613400
C	-3.00513900	2.03442500	0.56018900
C	-1.73906800	1.27318600	0.81967700
C	-1.08436300	0.60928000	1.75321600
H	2.68112400	0.69120300	-0.50834400
H	1.69008300	3.63710800	-0.57671100
H	-3.77409400	1.31684000	0.24880500
H	-3.35766400	2.53676900	1.46380900
H	-1.20392100	3.26445200	-2.10700400
H	-2.04058600	1.71206200	-2.12234200
Rh	-0.60456000	-0.29300600	-0.00466400
C	0.23411000	-2.17836300	-0.32882700
N	1.48099700	-2.73153800	-0.46614000
C	1.40430800	-4.10920400	-0.61700400
C	2.75131800	-2.04090200	-0.57516400
N	-0.61221100	-3.25986800	-0.41362900
C	0.08865100	-4.44078900	-0.59013300
C	-2.06149900	-3.18236800	-0.43045200
C	3.50059800	-1.79566500	0.59294700
C	3.22942800	-1.73348200	-1.86875100
C	4.76121500	-1.20472000	0.43376400
C	3.01657400	-2.18355000	1.98643100
C	5.25275000	-0.87404200	-0.82571500
C	4.49366200	-1.13771800	-1.96253300
C	2.45929500	-2.07213400	-3.14387300
C	3.21849700	-1.05199600	3.01162200
C	3.70535100	-3.48109600	2.46032400
C	2.38068400	-0.89009300	-4.12898700
C	3.07182200	-3.30724800	-3.83834700
C	-2.77870700	-3.44864600	0.75705900
C	-2.69905900	-2.90158200	-1.65881700
C	-4.09814100	-2.83251600	-1.65794600
C	-1.94296600	-2.72313100	-2.97286300
C	-4.82996300	-3.05944200	-0.49639000
C	-4.17592200	-3.37420200	0.69205200
C	-2.09810900	-3.87106200	2.05703900
C	-2.18646100	-1.33544000	-3.59540600
C	-2.29624500	-3.84565600	-3.97036000
C	-2.12932000	-5.40782500	2.20991100
C	-2.71314100	-3.20590700	3.30228200
H	2.28778900	-4.71623200	-0.73505800
H	-0.40723900	-5.39312000	-0.68958000
H	5.36831800	-1.00466800	1.31048500
H	6.23006500	-0.41050500	-0.92188200
H	4.89365200	-0.88674100	-2.93984200
H	1.94123400	-2.38181900	1.92813300
H	3.51696500	-4.31507200	1.77483900
H	3.33776600	-3.76925500	3.45189500
H	4.79082800	-3.34674100	2.53075500
H	4.28058600	-0.86077000	3.20216800
H	2.76517700	-1.32925400	3.96909100
H	2.75737900	-0.11748700	2.67585400
H	1.43146500	-2.32612600	-2.86571300
H	4.10516000	-3.11170800	-4.14641500
H	2.49704300	-3.56824000	-4.73426600
H	3.08171400	-4.18042100	-3.17716100
H	3.36316800	-0.62857700	-4.53619100
H	1.96819300	0.00774900	-3.65549300
H	1.73789100	-1.15212700	-4.97675600
H	-4.62040200	-2.61387000	-2.58439600
H	-5.91492000	-3.00879500	-0.52013400
H	-4.76180000	-3.57301500	1.58319300
H	-0.87090600	-2.80165800	-2.76798900
H	-2.08770900	-4.83536900	-3.54938100
H	-1.70859000	-3.73605100	-4.88875200
H	-3.35562900	-3.81807200	-4.24810600
H	-3.23868000	-1.18602800	-3.86102500
H	-1.59360100	-1.21885000	-4.50984900
H	-1.90400900	-0.53649300	-2.89919400
H	-1.04680000	-3.56462400	2.00451000
H	-3.16171200	-5.77133800	2.26552900
H	-1.61447600	-5.71137300	3.12845300
H	-1.64400400	-5.91412000	1.36888200
H	-3.72950000	-3.56546300	3.49582300
H	-2.75120000	-2.11625400	3.20659500
H	-2.11452200	-3.44760300	4.18737100
O	1.93595000	2.11358400	0.88344900
C	-2.76406600	3.06229500	-0.58369000
C	-2.30384600	4.39749600	0.02586500
O	-1.95151000	4.54454600	1.17759500
O	-2.28749900	5.36630300	-0.89979900
C	-4.04770800	3.25989900	-1.39869300
O	-4.22846600	2.82728500	-2.51433000
O	-4.96205800	3.92785400	-0.67853300
C	-6.23136500	4.15782900	-1.32768900

H	-6.83407900	4.69963600	-0.59980300
H	-6.08790800	4.75215200	-2.23287600
H	-6.70005000	3.20633200	-1.58930600
C	-1.87003000	6.67237300	-0.44467700
H	-1.93002800	7.31570900	-1.32159700
H	-2.53874400	7.02587000	0.34315400
H	-0.84794200	6.63145500	-0.06094200
C	3.82599600	3.24438800	-0.32939800
C	4.77118500	2.69325500	0.54486900
C	4.24060500	4.17314900	-1.29343000
C	6.11346800	3.06057300	0.44662100
H	4.44295600	1.99587100	1.30880700
C	5.58434200	4.53262700	-1.39545700
H	3.50949300	4.61823000	-1.96529700
C	6.52460800	3.97613100	-0.52525000
H	6.83929000	2.63975900	1.13736800
H	5.89522800	5.25290600	-2.14690300
H	7.56993400	4.26264800	-0.59759200
C	-0.77333000	0.58577400	3.15156900
C	-0.31288000	-0.57644000	3.80296300
C	-0.94030100	1.77667100	3.89871300
C	-0.04695700	-0.55550800	5.16761400
H	-0.17081900	-1.48329900	3.22443200
C	-0.67678900	1.78574900	5.26382500
H	-1.26560000	2.67975400	3.39025700
C	-0.23169400	0.62221100	5.90054400
H	0.30195600	-1.45519100	5.66632100
H	-0.80914300	2.70132800	5.83254000
H	-0.02393700	0.63400900	6.96663300

2c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.620895 a.u.

M06 SCF energy in solution: -2612.560285 a.u.

M06 Free energy in solution: -2611.643248 a.u.

C	1.00816700	3.41615600	-0.02488400
C	0.68545700	2.58098300	1.15097500
C	0.88568100	1.08421100	1.14968000
C	2.08421600	0.64493300	0.29083200
H	2.73312700	1.52763300	0.18044700
H	0.86614100	0.66229000	2.15333700
C	3.04544300	-0.50228100	0.65166000
C	2.85272300	-0.26245200	-1.83253100
C	1.63309600	0.23212900	-1.07887400
C	0.32294200	0.20111500	-1.37302000
H	0.50908300	3.09715900	2.09280500
H	1.51318100	2.92936500	-0.85469100
H	2.63460600	-1.11635700	-2.47754400
H	3.29878600	0.51756600	-2.45729400
H	3.69267300	-0.29763300	1.50975900
H	2.51767000	-1.43946100	0.83828700
C	-3.56383700	-2.12058600	1.23305000
C	-2.51560200	-2.75623700	1.80439900
C	-1.67588300	-0.95348400	0.71350700
N	-1.36443000	-2.03640700	1.48881100
N	-3.04042900	-1.02235000	0.56505500
Rh	-0.89308200	0.79633600	0.11441600
H	-2.46900500	-3.64961900	2.40496800
H	-4.61851300	-2.34165800	1.23599300
C	-3.82323700	-0.04085900	-0.16047100
C	-4.48368700	-0.43896100	-1.34356400
C	-3.93228200	1.27265200	0.37091000
C	-5.22237100	0.53697100	-2.02609700
C	-4.66679100	2.20451200	-0.37360100
C	-5.29914500	1.84456200	-1.56118800
H	-5.74243500	0.26518300	-2.93862100
H	-4.76575800	3.22070300	-0.01130800
H	-5.87011200	2.58490200	-2.11410400
C	-0.07728900	-2.47479500	2.00044800
C	0.35649600	-1.98450600	3.25330200
C	0.60905000	-3.48557000	1.29477200
C	1.55680700	-2.49962700	3.75846100
C	1.80097500	-3.96378000	1.85517300
C	2.27495200	-3.47119900	3.06634600
H	1.92951800	-2.14785700	4.71481900
H	2.37266500	-4.72135000	1.33211600
H	3.20517400	-3.85258900	3.47703200
C	-3.39872300	1.65285600	1.75890900
H	-2.39753100	1.20111600	1.90112900
C	-4.30216800	1.06052700	2.86457300
H	-3.91110300	1.31875400	3.85498400
H	-5.31392800	1.47375400	2.78224700
H	-4.37496300	-0.02861300	2.80307800
C	-3.23297500	3.16536200	1.97813100
H	-2.73634500	3.33984500	2.93905500
H	-2.63254600	3.63143200	1.19152100
H	-4.20244700	3.67304300	2.02511700
C	-0.47142100	-1.01268300	4.09586600
H	-1.11288100	-0.43515500	3.42007100
C	-1.39394600	-1.78523300	5.06620100
H	-0.80228300	-2.39729700	5.75619400
H	-1.99205800	-1.08666800	5.66265100
H	-2.08368000	-2.44929500	4.53662000
C	0.37821000	-0.00705300	4.89629800
H	1.11644000	0.50777200	4.27211200
H	-0.27286600	0.74896900	5.34916300
H	0.91960000	-0.49259400	5.71517900
C	0.06649200	-4.11503000	0.01267600
H	-0.68930500	-3.44165900	-0.40658000
C	-0.62196800	-5.46346400	0.32024900
H	-1.03102000	-5.90075900	-0.59776000
H	0.09413300	-6.17704500	0.74328800
H	-1.44423000	-5.35466900	1.03513400
C	1.14582800	-4.31865300	-1.06545900
H	0.67820600	-4.66507800	-1.99426500
H	1.69185200	-3.39420300	-1.26987100
H	1.88272300	-5.07266600	-0.77154000
C	-4.48454100	-1.87545300	-1.86277100

H	-3.69207800	-2.42900600	-1.34871500
C	-5.83087100	-2.56314000	-1.54322000
H	-6.65557100	-2.06550700	-2.06590900
H	-5.80949800	-3.60871600	-1.86978100
H	-6.06807100	-2.54734100	-0.47356100
C	-4.19289700	-1.96763700	-3.37085600
H	-5.00060300	-1.53298400	-3.97029900
H	-3.26202000	-1.46071700	-3.63330700
H	-4.10428700	-3.01961300	-3.66435300
C	3.86441700	-0.63633900	-0.67954000
O	-0.37641100	2.94874400	0.12756900
C	5.01181900	0.38684000	-0.63703500
O	4.97815400	1.49291700	-1.13472300
O	6.03952000	-0.07451900	0.09402900
C	4.43851600	-2.03927100	-0.87510300
O	4.21676800	-2.99967100	-0.16979400
O	5.20349500	-2.07787700	-1.98127700
C	5.81241600	-3.34778100	-2.28378800
H	6.39405700	-3.18222400	-3.19022400
H	6.45902500	-3.66314900	-1.46138300
H	5.04554100	-4.10827100	-2.45141400
C	7.16367600	0.81754900	0.23663600
H	7.89147900	0.27207000	0.83651200
H	7.57647100	1.06467300	-0.74410400
H	6.85710800	1.73700600	0.74136100
C	1.21724900	4.88765400	0.06029000
C	2.30689600	5.44497300	-0.62144900
C	0.37694400	5.71697700	0.81592700
C	2.56287500	6.81396900	-0.53661300
H	2.95852000	4.80633800	-1.21336500
C	0.62983200	7.08561900	0.89044400
H	-0.48366800	5.29537600	1.32770800
C	1.72471000	7.63608300	0.21821500
H	3.41153600	7.23702400	-1.06599400
H	-0.02921700	7.72461000	1.47123000
H	1.91936700	8.70290100	0.27887200
C	-0.27773200	-0.12163100	-2.68175500
C	-0.90614200	0.89381100	-3.43083200
C	-0.16156900	-1.40211800	-3.25580800
C	-1.37010700	0.64511000	-4.72233200
H	-0.99537100	1.89031400	-3.00558000
C	-0.61296500	-1.64387700	-4.55302200
H	0.30874100	-2.19850800	-2.68860200
C	-1.21349600	-0.62097600	-5.29241800
H	-1.83672400	1.44477200	-5.29075100
H	-0.49371900	-2.63194100	-4.98939900
H	-1.55853600	-0.81020300	-6.30488200

TS2c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.614475 a.u.

M06 SCF energy in solution: -2612.557375 a.u.

M06 Free energy in solution: -2611.642751 a.u.

C	0.36486400	3.45388500	-0.23002900
C	0.25127000	2.58309400	0.96307200
C	0.79417700	1.24629800	1.03515500
C	2.03852900	0.96015200	0.19052400
H	2.50544900	1.92898600	-0.04077400
H	0.76621700	0.79997500	2.02607100
C	3.19009800	0.06787600	0.68789800
C	2.97929200	-0.07440400	-1.80199600
C	1.68273600	0.30928800	-1.11336400
C	0.40330700	0.06412900	-1.42478700
H	-0.35596700	2.97128800	1.77624000
H	1.16619400	3.18667300	-0.92058700
H	2.91402200	-1.03302300	-2.32123400
H	3.29215900	0.67695600	-2.53368500
H	3.78357300	0.50799000	1.49493800
H	2.83731100	-0.91039500	1.02091500
C	-3.22687400	-2.50174900	1.32959100
C	-2.11522600	-2.91493300	1.98028300
C	-1.51619100	-1.11682900	0.72586600
N	-1.07565100	-2.06314700	1.61225300
N	-2.85027400	-1.40817900	0.56312000
Rh	-0.94340700	0.66930300	-0.05433500
H	-1.95686300	-3.72867500	2.66885300
H	-4.23698800	-2.87677700	1.33749900
C	-3.75775400	-0.61427500	-0.24291100
C	-4.25859100	-1.15920200	-1.44681900
C	-4.16053100	0.65603400	0.24484200
C	-5.12295600	-0.35692400	-2.20270000
C	-5.01316200	1.41454500	-0.56768200
C	-5.48059600	0.91996400	-1.78213000
H	-5.52306700	-0.74053200	-3.13522600
H	-5.33445400	2.39576800	-0.23740900
H	-6.14560200	1.52504500	-2.39168000
C	0.23863200	-2.22424600	2.20769500
C	0.51393900	-1.55784400	3.42407700
C	1.12963200	-3.14989500	1.62575600
C	1.76136300	-1.79565500	4.01509900
C	2.36045900	-3.34783900	2.26614500
C	2.67810500	-2.67181000	3.43973800
H	2.01400200	-1.30220800	4.94804100
H	3.08436300	-4.03009200	1.83619800
H	3.64098200	-2.83751000	3.91392100
C	-3.81769600	1.14397000	1.65588400
H	-2.82888100	0.75305000	1.93427600
C	-4.83063500	0.57080400	2.67306200
H	-4.58015700	0.89936200	3.68812400
H	-5.84247400	0.92321200	2.44291800
H	-4.84444400	-0.52347800	2.66568200
C	-3.74851500	2.67492700	1.78483200
H	-3.35516500	2.94338400	2.77193500
H	-3.10183300	3.11449700	1.01912100
H	-4.73799300	3.13703500	1.70268300
C	-0.52049600	-0.69518100	4.14933100
H	-1.25634800	-0.35188400	3.41319500
C	-1.27641600	-1.53546200	5.20347100

H	-0.58495200	-1.91344500	5.96492700
H	-2.03424500	-0.92517800	5.70799800
H	-1.78224300	-2.39577700	4.75479500
C	0.07331700	0.55553900	4.82573700
H	0.66954500	1.16372700	4.13669500
H	-0.73509100	1.18238700	5.21812400
H	0.71500300	0.29531000	5.67396700
C	0.76548700	-3.98548200	0.40023300
H	-0.08221100	-3.50556900	-0.10132600
C	0.31840100	-5.40114700	0.82746400
H	0.03210200	-5.99156800	-0.05037300
H	1.13201500	-5.92869800	1.33803400
H	-0.53872600	-5.37391200	1.50845100
C	1.90799400	-4.08590300	-0.62561200
H	1.55822400	-4.61950400	-1.51698500
H	2.26422900	-3.09734700	-0.92716900
H	2.76834400	-4.63692700	-0.23285100
C	-3.96424700	-2.58726500	-1.89999800
H	-3.07486100	-2.94021900	-1.36661500
C	-5.14269000	-3.51942700	-1.53781300
H	-6.05101500	-3.21873200	-2.07219500
H	-4.91129500	-4.55183500	-1.82247300
H	-5.37555300	-3.50906600	-0.46778200
C	-3.66596600	-2.69219000	-3.40526600
H	-4.55866300	-2.50126800	-4.01144100
H	-2.88731800	-1.99172300	-3.71239100
H	-3.32743600	-3.70643900	-3.64391900
O	-0.84524600	2.73467900	-0.51265800
C	4.02800200	-0.11323800	-0.62383100
C	4.98870400	1.08213500	-0.73763800
O	4.76052800	2.09895400	-1.35877100
O	6.08691400	0.89056700	0.01048800
C	4.82583200	-1.41775900	-0.62573400
O	4.76650200	-2.28358000	0.22039700
O	5.58576700	-1.49539400	-1.73253600
C	7.04368900	1.97008700	0.01575300
H	6.58910500	2.87798800	0.41968300
H	7.85942800	1.63022300	0.65297700
H	7.39887200	2.16481400	-0.99872500
C	6.40328800	-2.67524700	-1.85609000
H	6.94440200	-2.55636600	-2.79435800
H	7.09748400	-2.74346900	-1.01506300
H	5.77857300	-3.57158500	-1.88183200
C	0.22417700	4.94152900	-0.09401700
C	-0.92122300	5.52998700	0.45755500
C	1.28133300	5.75762400	-0.51574100
C	-1.00117400	6.91545700	0.59323200
H	-1.75652200	4.90733200	0.76279800
C	1.20311200	7.14338600	-0.37242000
H	2.16747400	5.30829700	-0.95856500
C	0.06166800	7.72430600	0.18264800
H	-1.89528300	7.36533900	1.01555800
H	2.02866100	7.76732900	-0.70219200
H	-0.00339800	8.80333000	0.28878600
C	-0.11160800	-0.43937300	-2.70948100
C	-0.78357100	0.44189600	-3.58192700
C	0.16021100	-1.74883100	-3.15182700
C	-1.13067300	0.03786200	-4.87086700
H	-0.99414000	1.45581400	-3.25208300
C	-0.17090300	-2.14148200	-4.44780100
H	0.66600000	-2.44081800	-2.48689500
C	-0.81057500	-1.24870400	-5.31289500
H	-1.63164800	0.73431400	-5.53727000
H	0.07244000	-3.14513800	-4.78576100
H	-1.06233900	-1.55627400	-6.32382000

3c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.634067 a.u.

M06 SCF energy in solution: -2612.580927 a.u.

M06 Free energy in solution: -2611.664652 a.u.

C	-0.63497400	3.08245100	-0.53838400
C	-0.44680300	2.17328500	0.68201000
C	0.68258300	1.35251300	0.84980500
C	1.95835900	1.48930000	0.04000200
H	2.04991300	2.53219900	-0.29908000
H	0.76558300	0.78586600	1.77180800
C	3.29306700	1.07725800	0.68952400
C	3.32453800	0.49227200	-1.73770000
C	1.92043400	0.61409300	-1.18374300
C	0.78148800	0.03119200	-1.54606000
H	-1.20073300	2.20201200	1.46864600
H	0.32566100	3.54119600	-0.82212000
H	3.54708100	-0.52002900	-2.08524500
H	3.48668900	1.17750100	-2.57600600
H	3.67625000	1.79794000	1.41737400
H	3.20707600	0.10710800	1.18678700
C	-2.66481900	-2.86653900	1.50073500
C	-1.49684800	-3.03320400	2.16610300
C	-1.20422300	-1.28879500	0.73719800
N	-0.61391600	-2.06312400	1.70296700
N	-2.47505400	-1.80066700	0.63576300
Rh	-0.86269100	0.40592900	-0.45514400
H	-1.20844900	-3.73924700	2.92783700
H	-3.60214400	-3.39444200	1.56583100
C	-3.53135600	-1.20468400	-0.16627600
C	-3.86193400	-1.78868300	-1.41052500
C	-4.24756400	-0.10876600	0.37834800
C	-4.88946700	-1.18524500	-2.14748700
C	-5.25794600	0.45206300	-0.41239000
C	-5.56824100	-0.07068900	-1.66469200
H	-5.16665500	-1.59897500	-3.11072900
H	-5.81873200	1.30002600	-0.03538000
H	-6.35839000	0.38016000	-2.25834400
C	0.68281500	-1.89671600	2.33913900
C	0.74722400	-1.11619700	3.51678500
C	1.79173900	-2.60878300	1.83633300
C	1.99307100	-1.00952800	4.14868400

C	3.01102300	-2.45941200	2.51065400
C	3.11503600	-1.66178200	3.64643700
H	2.08248300	-0.41734700	5.05390500
H	3.89464300	-2.96480300	2.13985800
H	4.07336400	-1.55870000	4.14665400
C	-4.03757900	0.38892800	1.80853600
H	-3.00796900	0.15849000	2.10445300
C	-4.97620100	-0.36825300	2.77541200
H	-4.81275600	-0.03175000	3.80556100
H	-6.02525300	-0.17919700	2.52143600
H	-4.81294900	-1.45016200	2.74442500
C	-4.23319700	1.90675200	1.97376900
H	-3.91872500	2.21103300	2.97846300
H	-3.66045300	2.48509800	1.24226900
H	-5.28518500	2.19538300	1.87210800
C	-0.48089700	-0.47134200	4.16115200
H	-1.28717400	-0.45022600	3.42037300
C	-0.97041800	-1.32324400	5.35320100
H	-0.20533200	-1.37391000	6.13596900
H	-1.87357300	-0.88443300	5.79230000
H	-1.20591000	-2.34918500	5.05190400
C	-0.24517000	0.98109300	4.61949400
H	0.12383200	1.61804900	3.80834400
H	-1.18385300	1.41128700	4.98573500
H	0.47652600	1.03914200	5.44098100
C	1.67908500	-3.58324500	0.66681100
H	0.80331800	-3.29769500	0.07303000
C	1.44339100	-5.01996300	1.18424800
H	1.34258200	-5.71640500	0.34390700
H	2.28639000	-5.35347300	1.79985400
H	0.53599700	-5.09443800	1.79231500
C	2.90532100	-3.56029100	-0.26301400
H	2.71815700	-4.18808000	-1.14169600
H	3.14066800	-2.54695500	-0.60095300
H	3.79788800	-3.95956200	0.22945600
C	-3.21034800	-3.07238900	-1.91831500
H	-2.22564300	-3.16522700	-1.44532100
C	-4.05276100	-4.30323100	-1.51305100
H	-5.04982800	-4.25396600	-1.96522300
H	-3.57018900	-5.22366400	-1.86041300
H	-4.18403100	-4.38260000	-0.42933700
C	-2.99429800	-3.07550300	-3.44085600
H	-3.94259700	-3.14644400	-3.98518400
H	-2.47196100	-2.17695500	-3.77854100
H	-2.39480300	-3.94569000	-3.72717400
O	-1.03563100	2.12544300	-1.50164600
C	4.24653900	0.92299800	-0.53792100
C	4.89330400	2.28700800	-0.83409400
O	4.54807100	3.04440600	-1.71436200
O	5.85325700	2.56100400	0.06445800
C	5.33128200	-0.12803200	-0.28654900
O	5.34569300	-0.91599000	0.63464300
O	6.24516000	-0.09991000	-1.27040300
C	6.51887800	3.83150500	-0.09365300
H	5.80260200	4.65051300	0.00683400
H	7.26293800	3.86888600	0.70136400
H	6.99581300	3.88772900	-1.07474000
C	7.31974200	-1.05505400	-1.16402200
H	7.95224900	-0.87725100	-2.03308100
H	7.87798600	-0.89320800	-0.23893600
H	6.92556500	-2.07423800	-1.17471500
C	-1.63994800	4.19996000	-0.31606600
C	-2.89264500	4.18195500	-0.93630100
C	-1.30248700	5.27370200	0.51949600
C	-3.79954400	5.22302200	-0.71646100
H	-3.14028300	3.35755400	-1.59670200
C	-2.21148500	6.30652000	0.74633700
H	-0.31955400	5.30912300	0.98726900
C	-3.46454300	6.28296500	0.12702100
H	-4.76723700	5.20774700	-1.21097900
H	-1.93939100	7.13407800	1.39563600
H	-4.16984600	7.09198200	0.29495000
C	0.39481400	-0.68629900	-2.76013600
C	-0.17828700	0.03631700	-3.83385300
C	0.69628700	-2.05451400	-2.93636400
C	-0.38496800	-0.58598200	-5.06268900
H	-0.42492900	1.08313200	-3.68388800
C	0.50395500	-2.66106300	-4.17422300
H	1.12889400	-2.61122400	-2.11310500
C	-0.02970200	-1.92730700	-5.23964100
H	-0.80666100	-0.02107900	-5.88886400
H	0.77482700	-3.70371400	-4.31427700
H	-0.17423600	-2.40333700	-6.20535900

TS3c [X = $C(O_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.613028 a.u.

M06 SCF energy in solution: -2612.557432 a.u.

M06 Free energy in solution: -2611.641414 a.u.

C	0.80594000	-2.27656300	-1.84770900
C	1.03470900	-1.99012300	-0.36389800
C	-0.07066500	-1.62172700	0.43486700
C	-1.50435000	-1.85382500	-0.00615300
H	-1.59128100	-2.89179800	-0.36829600
H	0.09176000	-1.54537500	1.50480700
C	-2.61332100	-1.64513300	1.04310800
C	-3.45621200	-0.88097800	-1.16032100
C	-1.93761700	-0.91133700	-1.10254700
C	-1.08645500	-0.11585600	-1.76093800
H	2.00053200	-2.20402800	0.08554500
H	-0.10383000	-2.87673800	-1.99133900
C	1.70612800	2.83346200	2.52556400
C	2.31339400	1.74152400	3.04283200
C	1.26257700	1.08580200	1.13057200
N	2.03295200	0.67711600	2.19276400
N	1.06692300	2.42279100	1.36167100
Rh	0.76547300	0.10386300	-0.60730600
H	2.92222100	1.61550300	3.92309000

H	1.66570400	3.85687200	2.86269100
C	0.34534500	3.37111900	0.53711500
C	-0.94220200	3.77249100	0.94822200
C	1.01368400	3.95403400	-0.56218300
C	-1.56170500	4.79197500	0.21197800
C	0.33795100	4.95421400	-1.26979700
C	-0.93119700	5.37761300	-0.88168700
H	-2.54752100	5.13725400	0.50828200
H	0.81679100	5.42427700	-2.12225100
H	-1.42610800	6.17397700	-1.43060600
C	2.60343900	-0.63636900	2.43447000
C	3.80817900	-0.97851000	1.78006000
C	1.98798600	-1.47585600	3.38975700
C	4.35805200	-2.23523700	2.06459000
C	2.58866400	-2.71826800	3.63362700
C	3.75257100	-3.09989200	2.97299000
H	5.28057900	-2.53598900	1.57945700
H	2.14288000	-3.39255000	4.35749500
H	4.19996700	-4.06801000	3.17935000
C	2.41355500	3.51668200	-0.98453100
H	2.89587300	3.04485500	-0.12155800
C	3.31583200	4.68839100	-1.41524000
H	4.33744200	4.32974000	-1.58075000
H	2.97859700	5.14821600	-2.35019700
H	3.34957200	5.46783000	-0.64723900
C	2.33831300	2.46420900	-2.10458800
H	3.33421900	2.10918800	-2.39003500
H	1.76254400	1.56873700	-1.78973900
H	1.82948100	2.84955200	-2.99414500
C	4.55516700	-0.00743200	0.86736100
H	3.83892400	0.73781800	0.50526400
C	5.64442400	0.74145500	1.66725600
H	6.39208400	0.04152400	2.05748100
H	6.16171700	1.46266100	1.02424100
H	5.22316900	1.28854000	2.51747400
C	5.17105800	-0.67910200	-0.37270600
H	4.43015800	-1.24386000	-0.94725900
H	5.59850500	0.08649000	-1.03020600
H	5.98598500	-1.36168800	-0.10836000
C	0.75598100	-1.05902300	4.19436800
H	0.27233500	-0.22500700	3.67251900
C	1.16573100	-0.55778300	5.59733500
H	0.28204200	-0.23430000	6.15858300
H	1.65418500	-1.35630800	6.16708500
H	1.86039900	0.28670800	5.54797500
C	-0.28951200	-2.18272200	4.33713300
H	-1.19635700	-1.78659600	4.80644300
H	-0.56990900	-2.61474400	3.37079800
H	0.07345400	-2.99806900	4.97196000
C	-1.65822600	3.16926500	2.15329200
H	-1.06905000	2.31743600	2.50892600
C	-1.75821700	4.18208600	3.31231900
H	-2.34581400	5.06061700	3.02243600
H	-2.24982900	3.72193200	4.17651700
H	-0.77106800	4.53416600	3.63213800
C	-3.05086800	2.63166600	1.77576900
H	-3.73120800	3.43922600	1.48206300
H	-2.98997800	1.92231400	0.94384500
H	-3.50562100	2.10667900	2.62082800
O	0.58293800	-0.95259500	-2.37006400
C	-3.90667200	-1.55582200	0.18158000
H	-2.66881100	-2.44248600	1.78976400
H	-2.48058900	-0.69694100	1.57345700
H	-3.84431600	0.13658300	-1.25191800
H	-3.83511300	-1.45780800	-2.01025700
C	-4.41010100	-2.98358800	-0.09284700
O	-4.19304700	-3.61266500	-1.10551300
O	-5.06646400	-3.47039700	0.97260000
C	-5.00072300	-0.74871400	0.88364100
O	-4.87283200	-0.16444600	1.93735900
O	-6.12344200	-0.74392500	0.14557500
C	-7.23945200	-0.01874800	0.69976400
H	-8.04706000	-0.13340200	-0.02251900
H	-7.52131000	-0.44156800	1.66690400
H	-6.98183300	1.03546000	0.82810700
C	-5.56409300	-4.81892500	0.84444700
H	-6.06964800	-5.03094000	1.78593600
H	-6.26093700	-4.88507400	0.00589900
H	-4.73725700	-5.51461000	0.68259000
C	-1.30723500	0.87589500	-2.81325800
C	-1.04530000	0.58666200	-4.16869800
C	-1.87098100	2.12220800	-2.47676700
C	-1.35874800	1.51548400	-5.15627400
H	-0.60065000	-0.36673300	-4.42667000
C	-2.19620700	3.04075700	-3.47420300
H	-2.06094600	2.36204400	-1.43548400
C	-1.93959000	2.74150700	-4.81342000
H	-1.15996500	1.28027400	-6.19786200
H	-2.64421800	3.99180900	-3.20282300
H	-2.19072700	3.45933300	-5.58924200
C	1.95311600	-2.97424600	-2.54926500
C	2.02483700	-4.37297400	-2.49622900
C	2.95037000	-2.26372200	-3.22670800
C	3.08765800	-5.05060400	-3.09319700
H	1.24185200	-4.93585100	-1.99165600
C	4.00873600	-2.94432900	-3.83416800
H	2.88210400	-1.18300500	-3.29376700
C	4.08339200	-4.33632700	-3.76433500
H	3.13132800	-6.13506300	-3.04591100
H	4.77299200	-2.38509000	-4.36701900
H	4.90608000	-4.86355100	-4.23888900

4c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.673414 a.u.

M06 SCF energy in solution: -2612.618161 a.u.

M06 Free energy in solution: -2611.701189 a.u.

C	0.24068500	1.95604300	-1.90178900

C	0.74933200	0.53003500	-1.77685900
C	-0.21860600	-0.45720300	-1.40519200
C	-1.72088800	-0.26656500	-1.56902100
H	-1.90147800	-0.29028100	-2.66148400
H	0.07971300	-1.49317200	-1.54221100
C	-2.57799200	-1.38892200	-0.94852300
C	-3.90973200	0.69023600	-1.01468300
C	-2.42224200	0.97571900	-1.04256400
C	-1.82808600	2.08351800	-0.57300300
H	1.69196300	0.26062600	-2.24424800
H	-0.55602100	2.04357600	-2.65279800
C	2.74324400	-2.41082300	2.47391000
C	3.31098200	-2.74432400	1.28943100
C	1.79693500	-1.11123100	0.86244200
N	2.72118200	-1.95104800	0.30558000
N	1.81216400	-1.41852100	2.19616800
Rh	0.67452600	0.41258000	0.28769100
H	4.08169300	-3.45856200	1.04883200
H	2.91353400	-2.77752200	3.47326200
C	0.95749900	-0.72827300	3.13830800
C	-0.19992900	-1.38145000	3.62305200
C	1.32391200	0.57834800	3.53672600
C	-1.03311400	-0.64863600	4.47580800
C	0.43754900	1.26626900	4.37848000
C	-0.73135300	0.66446300	4.83387200
H	-1.93367800	-1.11163700	4.86472200
H	0.68098800	2.27419400	4.70049200
H	-1.40139700	1.21208500	5.49052200
C	3.13108000	-2.00384400	-1.08372000
C	4.16390200	-1.14242000	-1.50980100
C	2.53126800	-2.95993200	-1.93322400
C	4.55522700	-1.22491200	-2.85288600
C	2.96638000	-2.99574900	-3.26405800
C	3.95940300	-2.13341000	-3.72293800
H	5.34747400	-0.57837000	-3.21689600
H	2.52938200	-3.71430800	-3.94945900
H	4.28148800	-2.18257000	-4.75933200
C	2.65101200	1.22198500	3.13742500
H	3.26570800	0.45785000	2.65050200
C	3.44123300	1.71386200	4.36643500
H	4.42790300	2.07507800	4.05623100
H	2.93477900	2.53992100	4.87725400
H	3.58772100	0.90872100	5.09389500
C	2.44721500	2.36139200	2.12491100
H	3.40320500	2.82067700	1.85026600
H	1.99871000	1.99849700	1.17906300
H	1.79088200	3.14406000	2.52125200
C	4.90449600	-0.20331200	-0.56039800
H	4.33462100	-0.14017800	0.37206900
C	6.29433000	-0.78029100	-0.21482800
H	6.92061300	-0.86249200	-1.11051200
H	6.81160300	-0.12784900	0.49775700
H	6.22027100	-1.77824800	0.23151100
C	5.03110100	1.22944400	-1.10834800
H	4.05457300	1.65712500	-1.35492700
H	5.50632200	1.87256700	-0.35886300
H	5.65423200	1.27061000	-2.00864600
C	1.50323600	-3.97562000	-1.43430900
H	1.03900900	-3.57181800	-0.52693000
C	2.19371100	-5.30416300	-1.05292000
H	1.45618900	-6.02368000	-0.67969400
H	2.68826000	-5.74783600	-1.92441800
H	2.95074300	-5.16469300	-0.27475600
C	0.37402800	-4.25365600	-2.44500000
H	-0.39682500	-4.87487000	-1.97602900
H	-0.10032000	-3.33258200	-2.80080300
H	0.73682600	-4.79989900	-3.32233300
C	-0.50540700	-2.84437400	3.31259700
H	0.04094200	-3.11767200	2.40244100
C	0.00582200	-3.74668200	4.45906100
H	-0.52539800	-3.52381200	5.39143400
H	-0.16636800	-4.80138400	4.21748400
H	1.07602700	-3.61377700	4.65063800
C	-1.99653800	-3.12356500	3.05715500
H	-2.59537600	-2.99955600	3.96654900
H	-2.42524100	-2.47775900	2.28696600
H	-2.12334300	-4.16264000	2.73351900
O	-0.40628700	2.14601300	-0.57891100
C	-4.03527300	-0.86982900	-1.06487600
H	-2.44025900	-2.35782200	-1.43698000
H	-2.33014300	-1.50717600	0.11044400
H	-4.38473500	1.11507700	-0.12539200
H	-4.42181700	1.10330400	-1.88941400
C	-4.61875300	-1.31379400	-2.41619700
O	-4.72246000	-0.60822100	-3.39591600
O	-4.93986800	-2.61805600	-2.38933800
C	-4.91945900	-1.37396500	0.07778400
O	-4.52506700	-1.94079600	1.07366200
O	-6.20314400	-1.04846300	-0.14582300
C	-7.14268800	-1.44429800	0.87374600
H	-8.11407600	-1.09812300	0.52217800
H	-7.13757500	-2.53061500	0.99032200
H	-6.88711900	-0.97700000	1.82783200
C	-5.48513200	-3.15628900	-3.61166100
H	-5.69658900	-4.20352800	-3.39773900
H	-6.39939600	-2.62375200	-3.88324300
H	-4.76010600	-3.06500600	-4.42409700
C	1.28975300	3.02005600	-2.14866500
C	2.12997000	2.88591900	-3.26378400
C	1.40035000	4.15832400	-1.34317200
C	3.07425300	3.86912000	-3.55957600
H	2.04080000	2.01811700	-3.91344500
C	2.35105700	5.13858400	-1.63908400
H	0.73546100	4.28323900	-0.49606000
C	3.19103700	4.99711400	-2.74387900
H	3.71489700	3.75533700	-4.42945800
H	2.42630500	6.01937800	-1.00741900
H	3.92492000	5.76374300	-2.97490600

C	-2.44758700	3.28657500	0.01823100
C	-1.83235100	3.93354500	1.10652500
C	-3.64617400	3.81608400	-0.48879000
C	-2.41244600	5.06188900	1.68124600
H	-0.90218000	3.54126800	1.50607400
C	-4.22319400	4.94755300	0.08874600
H	-4.11400500	3.36222100	-1.35586300
C	-3.61169700	5.57188500	1.17638100
H	-1.92848900	5.54592700	2.52507800
H	-5.14557500	5.34749600	-0.32243200
H	-4.06091300	6.45397400	1.62331000

5c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.675114 a.u.

M06 SCF energy in solution: -2612.635372 a.u.

M06 Free energy in solution: -2611.719903 a.u.

C	-0.61947300	-2.48106900	-1.58811400
C	-0.94120900	-0.98631500	-1.45862900
C	0.01621600	-0.02120700	-1.88746600
C	1.43771300	-0.49767800	-2.07675000
H	1.51397700	-1.30674500	-2.81937700
H	-0.30381100	0.92003600	-2.32395200
C	2.46688100	0.60025600	-2.39703300
C	3.16107000	-0.34944200	-0.26761500
C	1.83100200	-0.99096100	-0.66281500
C	1.26739600	-2.10249800	-0.04913100
H	-1.99652900	-0.75165200	-1.56105900
H	-0.18742200	-2.63191600	-2.58768700
H	3.03238700	0.49281900	0.42272800
H	3.84022200	-1.06696400	0.19630400
H	2.66038600	0.70548700	-3.46731500
H	2.13539500	1.57306300	-2.02043800
C	-3.11186800	2.90897100	0.94094000
C	-2.37066800	2.87119200	2.07564600
C	-1.50404800	1.33644300	0.62909900
N	-1.39370300	1.91017200	1.86452000
N	-2.57398200	1.97260000	0.06102100
Rh	-0.06135700	-0.04185600	0.20480200
H	-2.44476400	3.42551200	2.99794800
H	-3.97122400	3.50283100	0.67446900
O	0.34629800	-2.93388000	-0.62599500
C	3.73215400	0.19070200	-1.60866800
C	-0.34750300	1.54143600	2.79268300
C	-0.57449700	0.45524100	3.67039700
C	0.82718000	2.33198200	2.83246600
C	0.45250100	0.13372000	4.56711400
C	1.81344500	1.96096700	3.75516600
C	1.63131300	0.87386900	4.60817500
H	0.31971900	-0.69839500	5.25100600
H	2.72497200	2.54647300	3.82384100
H	2.40685000	0.61466200	5.32374900
C	-3.14819300	1.74516200	-1.25193100
C	-2.63885500	2.47207500	-2.35152000
C	-4.24932300	0.86878700	-1.35437200
C	-3.23839700	2.24698900	-3.59696400
C	-4.80739400	0.68807200	-2.62722000
C	-4.30379700	1.36002000	-3.73668700
H	-2.87559400	2.78072400	-4.46881800
H	-5.65395800	0.01957300	-2.74686700
H	-4.75347600	1.20568100	-4.71351600
C	-4.88274700	0.18812400	-0.14206700
H	-4.18440100	0.26666600	0.69810100
C	-1.54016700	3.52551800	-2.20201900
H	-0.92922900	3.25728500	-1.33228300
C	-1.88491200	-0.32723300	3.69794800
H	-2.58901100	0.16427600	3.01887400
C	0.99539800	3.60253900	2.00151500
H	0.20186700	3.62594200	1.24782400
C	-2.15939800	4.91506700	-1.92926100
H	-1.37083700	5.66600900	-1.80558200
H	-2.79396800	5.22626300	-2.76679000
H	-2.77384200	4.92086400	-1.02347000
C	-0.59560000	3.61371800	-3.41529600
H	-0.18666300	2.63766500	-3.69832700
H	-1.09815400	4.03110700	-4.29463500
H	0.24505900	4.27561600	-3.18154200
C	-6.18269600	0.91773200	0.26125000
H	-6.92600700	0.86423500	-0.54226900
H	-6.61859100	0.45519700	1.15399300
H	-6.00793100	1.97675100	0.48062500
C	-5.15685000	-1.31018800	-0.36294200
H	-4.25386900	-1.85300800	-0.65522500
H	-5.53360400	-1.75656700	0.56399200
H	-5.91691800	-1.47870300	-1.13361600
C	-2.52287400	-0.30857500	5.10164200
H	-3.50199300	-0.79911300	5.07297500
H	-1.90960800	-0.84222200	5.83588900
H	-2.66609000	0.71485900	5.46492900
C	-1.69521400	-1.77017800	3.19228300
H	-1.34351600	-1.78068900	2.15280000
H	-0.96612600	-2.31860700	3.79907700
H	-2.64668800	-2.31255400	3.23126400
C	0.81712200	4.84764400	2.89833900
H	1.59772600	4.89643300	3.66593300
H	0.88058700	5.76057600	2.29613200
H	-0.15168100	4.84581100	3.41011100
C	2.33659600	3.66553500	1.25051400
H	3.19187000	3.67050700	1.93543000
H	2.46015700	2.82729100	0.55857200
H	2.39055400	4.58605000	0.65960900
C	4.46775100	-0.93291100	-2.35324200
O	4.48147600	-2.09581300	-2.01351000
O	5.04729200	-0.46195300	-3.46974200
C	4.66073800	1.38242400	-1.36073400
O	4.32774100	2.54476100	-1.44796000
O	5.87509300	0.96990300	-0.96574500
C	5.76592200	-1.43038300	-4.26162500

H	6.16595000	-0.87283900	-5.10788400
H	6.57238800	-1.87419500	-3.67342400
H	5.09090700	-2.21963300	-4.60138000
C	6.83525500	2.00905500	-0.68438500
H	7.74624700	1.48915300	-0.39005400
H	7.00580400	2.61546000	-1.57689600
H	6.47567800	2.64986600	0.12430700
C	1.79934600	-2.73124000	1.19234600
C	1.76327700	-4.13293700	1.31695700
C	2.34789900	-1.97684500	2.24263500
C	2.28219000	-4.75648300	2.44914900
H	1.34099300	-4.72780300	0.51612700
C	2.85791600	-2.60582200	3.37815500
H	2.36012200	-0.89339700	2.19306900
C	2.83316300	-3.99703300	3.48401200
H	2.25915000	-5.83999900	2.52076700
H	3.27436100	-2.00434400	4.18098300
H	3.23853500	-4.48562700	4.36534700
C	-1.83730100	-3.37924000	-1.47900900
C	-2.62849700	-3.57864800	-2.61796500
C	-2.19580800	-4.00606000	-0.28004100
C	-3.76879800	-4.38042800	-2.55847800
H	-2.34650200	-3.11373500	-3.56065900
C	-3.33278800	-4.81517300	-0.22361700
H	-1.57227500	-3.88031600	0.59840600
C	-4.12340200	-5.00228400	-1.35915900
H	-4.36925300	-4.53193500	-3.45101700
H	-3.59639900	-5.30658500	0.70896400
H	-5.00323000	-5.63767900	-1.31337600

TS4c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2613.575706 a.u.

M06 SCF energy in solution: -2612.519798 a.u.

M06 Free energy in solution: -2611.605063 a.u.

C	-2.26654800	0.19270000	0.27596500
C	-1.47791200	-0.36935800	1.16940400
C	-1.75972600	1.83317300	-1.03156800
C	-0.68918300	1.59765600	-2.00087700
C	0.62598500	1.95871100	-1.82496200
C	1.10548800	2.65624400	-0.56212100
H	-0.97487300	1.07685800	-2.91311200
H	-1.54496000	2.58394600	-0.27284100
H	1.34346100	1.73757100	-2.60928500
H	0.36030500	3.42867000	-0.29781000
C	-3.15663500	1.91983900	-1.60803600
H	-3.33102500	2.94973300	-1.94022200
H	-3.25846800	1.27627100	-2.48688900
C	-3.72828300	0.14752200	-0.04231100
H	-3.89857900	-0.61779100	-0.81123400
H	-4.27543300	-0.14689200	0.85713300
C	2.84616900	-2.70687400	0.55372200
C	1.99296300	-3.35439100	-0.27090100
C	1.24285600	-1.22090300	-0.03179500
N	1.01591500	-2.43540700	-0.63930800
N	2.40313100	-1.38978300	0.67744900
Rh	-0.15232200	0.22178100	-0.19642600
H	1.98766900	-4.36752700	-0.63911700
H	3.74351200	-3.03839300	1.05043500
C	3.32208600	-0.41634900	1.27215000
C	3.13612100	0.02933400	2.59339600
C	4.47548300	-0.09044100	0.52086800
C	4.14134200	0.82696000	3.15671700
C	5.44947300	0.70010000	1.14198800
C	5.29183800	1.15309600	2.44765800
H	4.02359500	1.17844600	4.17719500
H	6.34781600	0.96152700	0.59151200
H	6.06659800	1.75647900	2.91264400
C	0.02555800	-2.70385400	-1.67375200
C	0.27414800	-2.21483000	-2.98234800
C	-1.09322300	-3.51213300	-1.37642800
C	-0.69576500	-2.46694400	-3.95992100
C	-2.02352100	-3.73583100	-2.40196500
C	-1.84268200	-3.20354600	-3.67248400
H	-0.54247100	-2.10367500	-4.97016300
H	-2.89502000	-4.35087400	-2.20153000
H	-2.57783600	-3.38886800	-4.45056800
C	4.73039500	-0.56998900	-0.90801500
H	3.84780200	-1.11478100	-1.25437500
C	5.92389400	-1.54579000	-0.97069500
H	5.77503700	-2.41576700	-0.32180800
H	6.06596100	-1.90895400	-1.99500300
H	6.85352300	-1.05677700	-0.65932900
C	4.94453100	0.60410100	-1.88356200
H	4.10719600	1.30757900	-1.85951100
H	5.85246500	1.16899900	-1.64677500
H	5.05406700	0.22440200	-2.90669900
C	1.93211700	-0.34374800	3.44179600
H	1.24558100	-0.91326300	2.81481400
C	2.34025500	-1.24773100	4.62224600
H	3.01603500	-0.72790100	5.31080000
H	1.45368200	-1.55111900	5.19010400
H	2.85180300	-2.15427500	4.27768600
C	1.16742400	0.90164500	3.92957300
H	1.77581100	1.50862600	4.61012800
H	0.86959100	1.52854700	3.08329900
H	0.26593300	0.59907700	4.47387100
C	-1.28604600	-4.22380500	-0.04169400
H	-0.59429900	-3.78510000	0.68088700
C	-0.92916500	-5.72067100	-0.17796400
H	-1.02207200	-6.22424100	0.79085000
H	-1.60130400	-6.22172400	-0.88357000
H	0.09468500	-5.86861600	-0.53888700
C	-2.70769600	-4.06941100	0.52924300
H	-2.75729700	-4.51149100	1.52971200
H	-2.99641700	-3.01756100	0.61445000
H	-3.45330200	-4.57928800	-0.09046700
C	1.59133400	-1.54854200	-3.38023300

H	1.97991000	-1.00600700	-2.51332300
C	2.63148700	-2.62533400	-3.76737300
H	2.28440100	-3.20347200	-4.63133000
H	3.58410200	-2.15497100	-4.03701000
H	2.82360200	-3.32563900	-2.94873100
C	1.45990400	-0.53343000	-4.52961400
H	1.26150300	-1.02246000	-5.48936400
H	0.65797100	0.19211500	-4.35562400
H	2.39985100	0.01754900	-4.64271100
O	1.11922900	1.65248100	0.43933700
C	-4.22128300	1.49874300	-0.58301100
C	-4.33796300	2.52190900	0.55693900
O	-4.06732800	2.30074200	1.71859200
O	-4.75033700	3.70690500	0.08841900
C	-5.58244300	1.32004000	-1.27585200
O	-5.72741200	1.19106300	-2.46991000
O	-6.57019400	1.26785200	-0.37135900
C	-7.90186100	1.07405600	-0.89970900
H	-8.55832700	1.06802800	-0.03062300
H	-8.15886700	1.89159100	-1.57671200
H	-7.95924100	0.12506700	-1.43751000
C	-4.92917500	4.75266100	1.07018100
H	-5.27599200	5.61868300	0.50807300
H	-5.67113500	4.44691200	1.81089000
H	-3.98222900	4.96754800	1.57069300
C	2.43484800	3.37953400	-0.70997000
C	3.32072500	3.46065700	0.36869800
C	2.73376700	4.06749400	-1.89406100
C	4.49490000	4.20745600	0.25740000
H	3.09195300	2.93295300	1.28777600
C	3.90981700	4.81162300	-2.00470300
H	2.04344400	4.03834500	-2.73503300
C	4.79479600	4.88266000	-0.92724300
H	5.17687900	4.26090200	1.10147100
H	4.13012200	5.33778100	-2.92940200
H	5.70844400	5.46460400	-1.00969400
C	-1.68460400	-0.99739000	2.46720300
C	-0.95583200	-2.11668400	2.90580000
C	-2.67284600	-0.45043100	3.31563500
C	-1.22600000	-2.69617400	4.14328800
H	-0.18336700	-2.53464200	2.27139900
C	-2.92368900	-1.02384300	4.56027900
H	-3.21873300	0.43299900	2.99848100
C	-2.20893600	-2.15091200	4.97453700
H	-0.66455400	-3.56901800	4.46369600
H	-3.67934200	-0.58890900	5.20793700
H	-2.41176700	-2.59937500	5.94277000

trans-**c1** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -1343.130459 a.u.

M06 SCF energy in solution: -1342.607652 a.u.

M06 Free energy in solution: -1342.238822 a.u.

C	-2.63551000	-1.51874800	-1.30839300
C	-1.34414900	-2.07332700	-0.81958400
C	-0.03740300	-1.61142900	-1.32714000
C	1.06950500	-1.56140500	-0.57978900
H	1.01329600	-1.88676700	0.45956500
H	-0.01485300	-1.30917600	-2.37388400
C	2.43444300	-1.19221500	-1.09008600
C	2.74190400	1.37063000	-0.69463900
C	1.33572700	1.70453300	-0.48448100
C	0.19833200	2.09634900	-0.33527700
H	-1.34786900	-2.48765200	0.19028100
H	-2.57479100	-0.73246200	-2.06394300
H	2.99075900	1.52077600	-1.75424700
H	3.35873400	2.07076200	-0.12057300
H	3.06709600	-2.08645600	-1.05709800
H	2.38009000	-0.89711200	-2.14332000
O	-2.17406800	-2.79794400	-1.75301300
C	3.19572700	-0.07496600	-0.31742600
C	3.10603900	-0.26797200	1.20365900
O	2.73465200	0.55820000	2.00287100
O	3.51617200	-1.51144500	1.54308000
C	4.68515600	-0.16504900	-0.71445300
O	5.12281400	-0.79465300	-1.64973300
O	5.44717200	0.59659700	0.09756500
C	6.85455200	0.61357500	-0.20512300
H	7.02314100	1.00746100	-1.21052300
H	7.30471900	1.26411000	0.54458000
H	7.26894300	-0.39562600	-0.14201800
C	3.51131900	-1.79940700	2.95285100
H	2.50254400	-1.69705400	3.36072600
H	3.86005100	-2.82841700	3.04116100
H	4.18109200	-1.11706400	3.48248800
C	-1.13411200	2.57029600	-0.13267300
C	-1.90010500	3.04770100	-1.21468900
C	-1.69526700	2.59394400	1.15921700
C	-3.18588000	3.54240600	-1.00566600
H	-1.47109300	3.03464300	-2.21215300
C	-2.98222500	3.08684800	1.35965000
H	-1.10748800	2.22747500	1.99497000
C	-3.73082600	3.56577700	0.28117700
H	-3.76247200	3.91463600	-1.84839000
H	-3.40170300	3.10041300	2.36195200
H	-4.73165200	3.95735400	0.44241200
C	-3.85520000	-1.48286500	-0.44978600
C	-4.47855200	-0.25858600	-0.17840700
C	-4.38012600	-2.65752400	0.10353500
C	-5.60276900	-0.20863000	0.64552900
H	-4.08039300	0.65756500	-0.60752700
C	-5.50680000	-2.60535500	0.92387600
H	-3.90770100	-3.60605500	-0.13322800
C	-6.12032400	-1.38126300	1.19970100
H	-6.07511400	0.74827800	0.85181000
H	-5.91064700	-3.52326600	1.34354400
H	-6.99936700	-1.34230100	1.83775600

cis-**c1** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -1343.130645 a.u.

M06 SCF energy in solution: -1342.605272 a.u.

M06 Free energy in solution: -1342.23647 a.u.

C	-2.70977400	-1.75243700	0.02965500
C	-1.93818600	-0.78482400	-0.80429800
C	-0.55822100	-1.05101600	-1.27918500
C	0.50734000	-1.12451000	-0.47651000
H	0.35561300	-0.97908900	0.59186000
H	-0.44999500	-1.17130000	-2.35727100
C	1.89483400	-1.46108100	-0.94547300
C	3.02892600	0.89183000	-0.97668800
C	1.85293800	1.70121500	-0.66680900
C	0.91526900	2.43361300	-0.43515000
H	-2.53631900	-0.12195900	-1.43367300
H	-2.18627800	-2.67200400	0.29663200
H	3.14312300	0.81411100	-2.06718600
H	3.92070900	1.40406000	-0.59919700
H	2.13225600	-2.48758500	-0.64184400
H	1.94303800	-1.45039200	-2.03915200
O	-2.12663300	-0.57009400	0.59991800
C	3.04143800	-0.56177900	-0.40577500
C	3.05848800	-0.51087100	1.13134000
O	3.14763400	0.48806700	1.80396000
O	2.97987100	-1.75885100	1.64698800
C	4.37305600	-1.19446500	-0.86567900
O	4.48404100	-2.04114800	-1.72274000
O	5.42041500	-0.64840600	-0.21472300
C	6.71692200	-1.14373900	-0.59606400
H	6.90091300	-0.95253700	-1.65627300
H	7.42920100	-0.59917300	0.02361200
H	6.78343400	-2.21854900	-0.40970700
C	3.01946900	-1.83337400	3.08327300
H	2.18062100	-1.28324200	3.51689900
H	2.94876700	-2.89476900	3.32191600
H	3.95515600	-1.41308800	3.46086700
C	-0.19987500	3.28255800	-0.15380200
C	-0.20206700	4.62281900	-0.58681600
C	-1.31237400	2.79500600	0.56009000
C	-1.28735600	5.45126900	-0.31236600
H	0.65430800	5.00232700	-1.13612100
C	-2.39257500	3.63249300	0.83005400
H	-1.32361500	1.76260400	0.89399400
C	-2.38619100	4.96054200	0.39691100
H	-1.27455900	6.48373600	-0.65184200
H	-3.24308100	3.24453800	1.38480400
H	-3.23110400	5.60956000	0.61142600
C	-4.19576000	-1.84409900	-0.00742900
C	-4.80824600	-3.08617900	-0.21648000
C	-4.99626400	-0.70394100	0.14191000
C	-6.19745000	-3.18649000	-0.29175900
H	-4.19339600	-3.97762600	-0.32128500
C	-6.38481700	-0.80586600	0.07028500
H	-4.52008100	0.25323300	0.33242600
C	-6.98973400	-2.04571800	-0.14992700
H	-6.66067800	-4.15589600	-0.45555900
H	-6.99709900	0.08393800	0.19169600
H	-8.07230700	-2.12319200	-0.20410700

c2 [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -1343.198616 a.u.

M06 SCF energy in solution: -1342.669224 a.u.

M06 Free energy in solution: -1342.291164 a.u.

C	-2.38786700	-0.99723800	-0.26159900
C	-1.91099800	-1.65822700	-1.53851200
C	-0.60576200	-1.82861400	-1.75921600
C	0.42752600	-1.39434600	-0.74664000
H	0.30267100	-2.00531800	0.16377600
H	-0.25637200	-2.26610000	-2.69382400
C	1.88598200	-1.56024900	-1.20967200
C	1.75696900	0.62699900	-0.16329400
C	0.34071500	0.09033200	-0.36347500
C	-0.77011600	0.83976700	-0.20918400
H	-2.65569700	-1.94118500	-2.27802800
H	-1.86710300	-1.44074400	0.59867700
H	2.03933700	1.33625700	-0.94954600
H	1.89170400	1.13080700	0.79696600
H	2.23995100	-2.59404500	-1.16767600
H	2.01174900	-1.20535800	-2.23821900
C	2.68260700	-0.61812600	-0.28008600
O	-2.08006700	0.41471300	-0.27467100
C	2.88364200	-1.27714400	1.08921200
O	2.32617000	-0.96464200	2.11681800
O	3.75192200	-2.30920400	0.99455500
C	4.03661900	-0.23258100	-0.87405100
O	4.38104200	-0.41471600	-2.02010900
O	4.79381000	0.40609400	0.04361400
C	6.07952900	0.85613000	-0.41670700
H	5.96436000	1.56284500	-1.24263500
H	6.54321300	1.34127700	0.44241200
H	6.68230200	0.00882400	-0.75376300
C	4.01387600	-3.01154400	2.22107200
H	4.72706900	-3.79462200	1.96255900
H	4.43861100	-2.33338400	2.96575000
H	3.09264300	-3.44531400	2.61880700
C	-0.76210900	2.29755000	0.10282900
C	-1.52404300	2.77857500	1.17994400
C	-0.05104100	3.21759200	-0.68025500
C	-1.54360200	4.13783300	1.48559500
H	-2.10126600	2.07634400	1.77311700
C	-0.07466900	4.57950300	-0.37799900
H	0.50154100	2.86815100	-1.54703200
C	-0.81580600	5.04328600	0.70962600
H	-2.13037300	4.49204800	2.32918300
H	0.47778700	5.27886500	-1.00018500
H	-0.83390300	6.10390000	0.94630100

C	-3.88182100	-1.13025600	-0.04946700
C	-4.38449200	-2.21338400	0.67948700
C	-4.77795300	-0.21529100	-0.61525000
C	-5.76036800	-2.38545100	0.83922000
H	-3.69540900	-2.92620000	1.12766400
C	-6.15302000	-0.38358000	-0.45086500
H	-4.38993100	0.63508500	-1.16645800
C	-6.64882300	-1.46964500	0.27381100
H	-6.13615900	-3.22986800	1.41109700
H	-6.83913300	0.33680800	-0.88885100
H	-7.72045500	-1.59836700	0.40110500

TS5c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in the gas: -1343.172848 a.u.

M06 SCF energy in solution: -1342.640149 a.u.

M06 Free energy in solution: -1342.261899 a.u.

O	-3.85477100	0.27267100	1.75750600
C	-3.17803400	-0.77292700	1.23932000
C	-4.28170000	0.12392700	3.12328900
O	-4.23421700	0.77830800	-1.74325800
C	-4.07680200	-0.15186900	-0.98583900
O	-5.01731100	-1.09022900	-0.74912900
C	-6.26112200	-0.91426000	-1.45068500
O	-2.91737700	-1.77532700	1.86864100
C	-2.78942900	-0.48474500	-0.21622900
C	0.04446400	-1.70614400	0.52973900
C	-0.58044500	-1.43905300	-0.80997300
C	-2.08974100	-1.70800800	-0.88867000
C	-0.43281400	0.06400400	-0.68272700
C	-1.76123500	0.68532300	-0.30839000
H	-0.02869100	-1.87311400	-1.64758100
H	-2.38948100	-2.64278400	-0.40972100
H	-2.38477700	-1.75518100	-1.94238900
H	-2.11331100	1.35472700	-1.10173000
H	-1.73820000	1.28196800	0.61011300
H	-4.95063100	-0.73484100	3.22109900
H	-4.80342600	1.04941400	3.36703200
H	-3.41951900	-0.01723100	3.77995000
H	-6.72308800	0.03676800	-1.17374300
H	-6.88851900	-1.75155800	-1.14482600
H	-6.09556900	-0.93023600	-2.53089200
H	-0.63286500	-1.71732100	1.37806200
C	1.39428900	-1.78492200	0.76273800
C	2.33866700	-1.70410500	-0.28885200
H	1.74289900	-1.74956300	1.79232100
C	0.81696700	0.66449200	-0.84073300
O	1.82052300	-0.04593200	-1.26040400
H	2.08516600	-2.19142300	-1.22170000
C	1.12657300	2.07962200	-0.45673700
C	2.44470500	2.37512400	-0.06396900
C	0.19790100	3.13355400	-0.49535100
C	2.80875500	3.66364500	0.31708300
H	3.17761200	1.57595000	-0.07229000
C	0.56821400	4.42829300	-0.12804000
H	-0.81340100	2.96329900	-0.84319600
C	1.87085900	4.69888500	0.29006400
H	3.83121100	3.86327300	0.62849700
H	-0.16664500	5.22801600	-0.17651600
H	2.15562300	5.70664600	0.58121300
C	3.78182700	-1.57782000	-0.05277700
C	4.68055000	-2.05070100	-1.02511700
C	4.30795100	-0.98734700	1.11169400
C	6.05725500	-1.96134000	-0.83334200
H	4.28801400	-2.49411400	-1.93682500
C	5.68385900	-0.89611200	1.30291600
H	3.63437900	-0.58218100	1.86081600
C	6.56407800	-1.38583100	0.33355800
H	6.73481000	-2.33789300	-1.59488400
H	6.07245700	-0.43672200	2.20790900
H	7.63764800	-1.31194500	0.48462200

cis-**c3** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -1343.206942 a.u.

M06 SCF energy in solution: -1342.68297 a.u.

M06 Free energy in solution: -1342.308247 a.u.

O	-3.88668900	-0.53148600	1.78575200
C	-3.04497000	-1.33015800	1.09540000
C	-4.30841200	-1.03132000	3.06701300
O	-4.22802900	0.74849000	-1.48920400
C	-3.97224200	-0.31534000	-0.97375200
O	-4.79383500	-1.38547700	-1.01705300
C	-6.03533300	-1.18796200	-1.71660900
O	-2.63661900	-2.38985900	1.51619100
C	-2.67137400	-0.67929900	-0.24356500
C	0.24863500	-1.05523300	0.30139600
C	-0.39073700	-1.16908200	-1.05270300
C	-1.82939100	-1.65220900	-1.13548400
C	-0.35706300	0.19635200	-0.41488900
C	-1.78265800	0.58657100	-0.01492900
H	0.25500500	-1.34724200	-1.90652700
H	-1.96329200	-2.68405700	-0.80138200
H	-2.16784800	-1.58914300	-2.17568300
H	-2.15161100	1.38269400	-0.66860800
H	-1.87831600	0.95147900	1.01146500
H	-4.83208500	-1.98347000	2.95051900
H	-4.97669900	-0.27038500	3.47033100
H	-3.44680200	-1.17572100	3.72394500
H	-6.61634200	-0.39179300	-1.24422400
H	-6.56116300	-2.14055200	-1.65039000
H	-5.84750100	-0.92277400	-2.76016300
H	-0.35756800	-1.39748900	1.13778600
C	1.70389300	-1.20994000	0.55210100
C	2.67074700	-1.38174500	-0.36560200
H	1.97447800	-1.16753000	1.60649300
C	0.58737800	1.23226400	-0.96279400
O	1.25262400	1.00379200	-1.96580700

C	0.71624500	2.55022200	-0.26233500
C	0.41591600	2.71334500	1.09771400
C	1.21144600	3.64413300	-0.98951900
C	0.59890700	3.94966000	1.71711900
H	0.06796300	1.86678300	1.68076800
C	1.37645400	4.88202200	-0.37588800
H	1.46113900	3.49782600	-2.03546800
C	1.07034400	5.03705900	0.97975000
H	0.37571600	4.06341000	2.77448800
H	1.74873100	5.72646000	-0.94960100
H	1.20428600	6.00250300	1.46059900
H	2.39510800	-1.39607600	-1.41741300
C	4.11051400	-1.53483600	-0.11035500
C	4.99263500	-1.53657900	-1.20583400
C	4.66157000	-1.69043800	1.17607000
C	6.36800900	-1.67725000	-1.02851300
H	4.58726900	-1.41749400	-2.20790100
C	6.03442100	-1.83175900	1.35465400
H	4.01013000	-1.71174700	2.04510000
C	6.89676300	-1.82483800	0.25408400
H	7.02625900	-1.67148900	-1.89348000
H	6.43520600	-1.95273600	2.35794900
H	7.96813600	-1.93699300	0.39719400

TS6c [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]
B3LYP SCF energy in gas phase: -1343.204424 a.u.
M06 SCF energy in solution: -1342.680701 a.u.
M06 Free energy in solution: -1342.305251 a.u.

O	-3.44679000	-1.23561700	1.86568000
C	-2.54171100	-1.76817000	1.01705400
C	-3.61530500	-1.93307600	3.11254000
O	-4.39833800	0.21738200	-1.22639500
C	-3.87260900	-0.80301600	-0.84504800
O	-4.45107700	-2.01987700	-0.92928000
C	-5.77218600	-2.04141200	-1.49845500
O	-1.88569200	-2.75306800	1.27494600
C	-2.45620600	-0.93041000	-0.26645600
C	0.50281000	-0.68346100	0.05226200
C	-0.20474400	-0.84578700	-1.26838800
C	-1.51839400	-1.60481300	-1.32137400
C	-0.39868400	0.43874800	-0.48865400
C	-1.84074100	0.47636300	0.02682200
H	0.41064400	-0.80396200	-2.16139400
H	-1.41738100	-2.67246600	-1.11047600
H	-1.95006300	-1.49937900	-2.32321800
H	-2.41939400	1.22178400	-0.52649200
H	-1.93504800	0.72633800	1.08719000
H	-3.94658400	-2.95896900	2.93304000
H	-4.37407700	-1.37278800	3.65904200
H	-2.67493500	-1.95387200	3.66935100
H	-6.45569500	-1.43616200	-0.89748600
H	-6.07537400	-3.08847600	-1.49019200
H	-5.75444300	-1.65283100	-2.51982900
H	0.08076000	-1.23660100	0.89133300
C	1.98920100	-0.52193100	0.11208300
C	2.84065900	-1.53683000	-0.10095100
H	2.37202700	0.46036900	0.38402400
C	0.26266400	1.69412800	-0.99743800
O	0.94970000	1.67333800	-2.01085400
C	0.09535100	2.97698000	-0.23845900
C	-0.16771900	3.01089700	1.13879400
C	0.27844700	4.18502900	-0.93001300
C	-0.25295200	4.23058100	1.81064500
H	-0.27770000	2.08408100	1.69265600
C	0.17228100	5.40180300	-0.26356400
H	0.50466500	4.14371100	-1.99065600
C	-0.09282500	5.42669200	1.10934600
H	-0.44354800	4.24665000	2.88027300
H	0.30158000	6.33236300	-0.80958100
H	-0.16968700	6.37690600	1.63123700
H	2.41902500	-2.51171800	-0.34943400
C	4.30852600	-1.50171000	-0.01888600
C	5.01934300	-2.71456900	-0.04341200
C	5.04717800	-0.30722100	0.07734400
C	6.41062500	-2.73982200	0.04153000
H	4.46732500	-3.64831000	-0.12523400
C	6.43611900	-0.33100500	0.16115500
H	4.53123800	0.64842800	0.06962600
C	7.12637200	-1.54692800	0.14649400
H	6.93491300	-3.69182400	0.02347900
H	6.98520300	0.60455400	0.23086000
H	8.21114100	-1.56144200	0.20926400

trans-**c3** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Ph, R^3 = H]
B3LYP SCF energy in gas phase: -1343.211543 a.u.
M06 SCF energy in solution: -1342.685784 a.u.
M06 Free energy in solution: -1342.310088 a.u.

O	-3.22276900	-1.50978500	1.84312100
C	-2.47988800	-1.91216600	0.79014500
C	-3.26441400	-2.41749700	2.95844600
O	-4.47728300	0.54977500	-0.74750100
C	-3.98197700	-0.54892800	-0.64512100
O	-4.65559900	-1.69782700	-0.86399700
C	-6.04153900	-1.54785300	-1.22005800
O	-1.86084000	-2.95287800	0.76976600
C	-2.51241400	-0.85309100	-0.32049100
C	0.47571700	-0.80174100	-0.44577900
C	-0.43681200	-0.66595700	-1.63835200
C	-1.78714300	-1.35951700	-1.61028300
C	-0.42563500	0.45773300	-0.62745000
C	-1.75754000	0.44094800	0.12781900
H	0.03362800	-0.48450100	-2.59994300
H	-1.71640100	-2.45005700	-1.60282100
H	-2.35742200	-1.06545400	-2.49868900
H	-2.36336900	1.30592200	-0.15738700
H	-1.65676500	0.47061000	1.21610200

H	-3.68564100	-3.37823300	2.65194600
H	-3.90111600	-1.93653100	3.70110800
H	-2.25975000	-2.57888500	3.35763800
H	-6.58649900	-1.03697300	-0.42216200
H	-6.41801400	-2.56173700	-1.35638800
H	-6.13839600	-0.97278500	-2.14442700
H	0.14663900	-1.47596700	0.34229100
C	1.94110200	-0.72991700	-0.60517700
C	2.79421900	-1.44106500	0.15281300
H	2.30860000	-0.07266900	-1.38932800
C	0.23664800	1.75312000	-1.00827200
O	0.83887600	1.85412000	-2.07259900
C	0.17398900	2.92808600	-0.08029600
C	0.07337600	2.78999800	1.31162100
C	0.29146300	4.21309000	-0.63362100
C	0.08034900	3.91677300	2.13382200
H	0.02414300	1.80174400	1.75677800
C	0.27618800	5.33770300	0.18560900
H	0.39388900	4.30538600	-1.71009200
C	0.17087700	5.19137700	1.57217900
H	0.01747900	3.79912000	3.21216800
H	0.35271100	6.32897300	-0.25290900
H	0.16543200	6.06916600	2.21297000
H	2.37503200	-2.09609800	0.91795700
C	4.26042300	-1.45970500	0.06686900
C	4.97723800	-2.33857300	0.89882600
C	4.99644900	-0.63755300	-0.80827700
C	6.36921000	-2.40220800	0.85870700
H	4.42862200	-2.98188100	1.58340600
C	6.38590900	-0.70035600	-0.84922600
H	4.47845000	0.06074600	-1.45921900
C	7.08177100	-1.58298100	-0.01724000
H	6.89626000	-3.09258200	1.51232500
H	6.93107500	-0.05477100	-1.53310200
H	8.16692100	-1.62810900	-0.05181600

VOR-**TS1** [X = $C(CO_2Me)_2$, R^1 = Me, R^2 = Me, R^3 = H]
B3LYP SCF energy in gas phase: -2230.109249 a.u.
M06 SCF energy in solution: -2229.247058 a.u.
M06 Free energy in solution: -2228.435294 a.u.

C	-0.47083300	-4.23143500	0.05452800
C	0.21428700	-2.93033300	0.25283400
C	-0.48992600	-1.69935200	0.72784800
C	-1.82964700	-1.40516100	0.18582100
H	-2.11971200	-2.17701100	-0.53130000
H	-0.34165600	-1.51402000	1.79776900
C	-2.98899900	-0.88803400	1.00508100
C	-3.47546900	0.04589700	-1.29076700
C	-1.99971500	-0.21924600	-1.31014200
C	-0.93243200	-0.19358500	-2.07110400
H	1.27549400	-2.96578200	0.48758600
H	-1.54687800	-4.26443000	0.24041800
H	-3.62544600	1.12999800	-1.33951700
H	-3.95707200	-0.39631400	-2.16733200
H	-3.33133000	-1.64771800	1.71791500
H	-2.72127400	-0.00100500	1.58564400
Rh	-0.16662600	0.07292100	-0.24613400
C	1.77904700	0.73334300	0.04293100
N	3.02784800	0.17543700	0.12840700
C	4.00423900	1.15483100	0.24867000
C	3.36674600	-1.23207700	0.21577000
N	2.01680900	2.08395300	0.12570000
C	3.36875000	2.35429200	0.25108500
C	0.98914400	3.10774300	0.14818400
C	3.56840600	-1.96616100	-0.97125200
C	3.57153600	-1.78155800	1.50018200
C	3.97880900	-3.29897600	-0.83730700
C	3.40485200	-1.34914900	-2.35725000
C	4.18533000	-3.87120400	0.41569100
C	3.98148000	-3.11978100	1.56974000
C	3.40161600	-0.98340600	2.79176300
C	2.75652200	-2.31652700	-3.36496800
C	4.76183700	-0.84048800	-2.89010600
C	2.43601600	-1.66722400	3.77932300
C	4.76604800	-0.72233200	3.46323700
C	0.69730700	3.80684400	-1.04337700
C	0.35992400	3.39804700	1.37811500
C	-0.62273300	4.39620500	1.37749500
C	0.73720800	2.71733600	2.69161400
C	-0.94596800	5.08908000	0.21441000
C	-0.28600400	4.80212600	-0.97785300
C	1.43882000	3.55311500	-2.35352800
C	-0.46672300	2.01646500	3.34923200
C	1.38765900	3.72235100	3.66509500
C	2.50684600	4.64093500	-2.59716000
C	0.48981600	3.45835700	-3.56336000
H	5.05023200	0.90503200	0.32962300
H	3.74691600	3.36060300	0.33595300
H	4.14600600	-3.89654100	-1.72699300
H	4.51423200	-4.90391100	0.49179000
H	4.15409200	-3.57421400	2.54058900
H	2.73843300	-0.48535700	-2.26226900
H	5.20666800	-0.09242700	-2.22469100
H	4.63727900	-0.38177500	-3.87774600
H	5.47556800	-1.66622100	-2.99020200
H	3.43050300	-3.13686700	-3.63576900
H	2.52072900	-1.78226800	-4.29219600
H	1.83478900	-2.75330700	-2.96635200
H	2.96780100	-0.00988900	2.54213400
H	5.24845600	-1.66088100	3.75824400
H	4.63753400	-0.11367600	4.36529200
H	5.45210900	-0.19360000	2.79262600
H	2.82377900	-2.62988600	4.12961100
H	1.45565700	-1.84889100	3.32457500
H	2.28884200	-1.03366600	4.66102900
H	-1.13050400	4.64273500	2.30489400
H	-1.70469600	5.86612700	0.23980500

H	-0.53397700	5.36507900	-1.87195600
H	1.48332900	1.94559900	2.47807100
H	2.27166300	4.19425300	3.22232100
H	1.69845600	3.21417200	4.58490400
H	0.68922100	4.51913800	3.94402000
H	-1.25088500	2.72835600	3.62792900
H	-0.15178900	1.49666900	4.26126300
H	-0.91687100	1.27972500	2.67288500
H	1.95838600	2.59198200	-2.26970100
H	2.04267500	5.62911700	-2.69248900
H	3.05798300	4.43656100	-3.52200100
H	3.23130100	4.69255800	-1.77724700
H	0.02702100	4.42361500	-3.79561200
H	-0.31446100	2.73566600	-3.38988700
H	1.04776500	3.14690000	-4.45358700
C	-0.42482500	-0.27600500	-3.45657300
H	-1.22616700	-0.02908500	-4.16599800
H	0.42177700	0.39197800	-3.63482900
H	-0.10044400	-1.30288400	-3.66497700
O	-0.11869200	-3.39306200	-1.06265400
C	0.25000100	-5.54861400	0.17021200
H	0.09561400	-5.98344400	1.16447300
H	-0.13305800	-6.25823900	-0.57180900
H	1.32367900	-5.42016200	0.00469500
C	-4.12600200	-0.52947800	0.01088100
C	-4.88991500	-1.82191200	-0.32787200
O	-4.71666400	-2.47820300	-1.33232900
O	-5.71739100	-2.16384900	0.66923700
C	-5.07510000	0.50691900	0.62740900
O	-4.87243500	1.10055400	1.66261600
O	-6.13429200	0.70411400	-0.17228300
C	-7.09897900	1.67578300	0.28589200
H	-7.87088900	1.70091100	-0.48235500
H	-7.51683200	1.36583800	1.24632600
H	-6.62725400	2.65518400	0.39491600
C	-6.47565200	-3.37819900	0.47605900
H	-7.08886500	-3.48014600	1.37049700
H	-7.09995200	-3.29261000	-0.41595900
H	-5.80258600	-4.23178000	0.36666800

VOR-**TS4** [X = $C(CO_2Me)_2$, R^1 = Me, R^2 = Me, R^3 = H]
B3LYP SCF energy in gas phase: -2230.113999 a.u.
M06 SCF energy in solution: -2229.244873 a.u.
M06 Free energy in solution: -2228.429519 a.u.

C	2.13622600	-0.20533600	0.67847400
C	1.10142400	-0.22250000	1.46712900
C	2.12223200	-1.02473200	-1.29174100
C	1.10781400	-0.65410900	-2.28548100
C	-0.06802300	-1.33896600	-2.49596000
C	-0.42341400	-2.57766200	-1.68579900
H	1.32082400	0.22918900	-2.88543900
H	2.07222000	-2.06001500	-0.95838100
H	-0.74051800	-1.00471200	-3.28242500
H	0.45007800	-3.25290200	-1.68670700
C	3.52792800	-0.54677400	-1.59195200
H	3.95614000	-1.17887400	-2.37841000
H	3.52564800	0.47945100	-1.97285500
C	3.59276200	0.12606400	0.75677300
H	3.71239300	1.20913900	0.62237800
H	3.95433400	-0.13407800	1.75620900
C	-3.66424800	1.11176000	1.25163400
C	-2.94765200	2.25009900	1.11741300
C	-1.65563100	0.52740900	0.38170900
N	-1.71752400	1.88615800	0.57937000
N	-2.87897100	0.06002800	0.77964600
Rh	0.07803200	-0.28159300	-0.24388900
H	-3.19057300	3.27616600	1.34061600
H	-4.66417400	0.93942500	1.61565500
C	-3.49780800	-1.24131400	0.55725400
C	-3.28979100	-2.28513900	1.47709900
C	-4.39119600	-1.35301700	-0.53219600
C	-3.97806300	-3.48467000	1.25721800
C	-5.05043100	-2.57747700	-0.70020900
C	-4.84340100	-3.63633200	0.17851200
H	-3.84255200	-4.30887400	1.95028400
H	-5.74487000	-2.69823300	-1.52626100
H	-5.36986400	-4.57519100	0.03164800
C	-0.71911000	2.84252700	0.13252000
C	-0.65556400	3.14604500	-1.25170200
C	0.08960200	3.49883900	1.08677300
C	0.32041300	4.06134200	-1.66517200
C	1.03700500	4.41511200	0.60986800
C	1.16739900	4.68019900	-0.74908300
H	0.40320700	4.31523800	-2.71636800
H	1.67448600	4.93698300	1.31605500
H	1.91131400	5.39255900	-1.09447600
C	-4.71556700	-0.20448200	-1.48976100
H	-4.06678100	0.64324100	-1.25188400
C	-6.17245100	0.27059800	-1.30365100
H	-6.37270300	0.56916900	-0.26885800
H	-6.37982300	1.13043400	-1.95071300
H	-6.88452700	-0.52101700	-1.56152100
C	-4.45553900	-0.56382300	-2.96515900
H	-3.40778500	-0.83392900	-3.13389300
H	-5.07553500	-1.40290800	-3.29859300
H	-4.69170700	0.29256000	-3.60738300
C	-2.41528500	-2.13629600	2.71496400
H	-1.83460500	-1.21632600	2.60513900
C	-3.28772100	-1.98635300	3.97946300
H	-3.89466700	-2.88281800	4.14973800
H	-2.65825500	-1.83599000	4.86437400
H	-3.97119900	-1.13311000	3.90046100
C	-1.41411300	-3.29639800	2.86813100
H	-1.92103600	-4.25394700	3.03004700
H	-0.78384400	-3.38698600	1.97818900
H	-0.77279100	-3.12866000	3.74187800
C	-0.08077200	3.31742800	2.59240700

H	-0.65891200	2.40330300	2.76214400
C	-0.88304100	4.49425500	3.19151600
H	-1.03716100	4.34283400	4.26572200
H	-0.34516800	5.43949000	3.05760100
H	-1.86624700	4.60601600	2.72266800
C	1.25992200	3.17200500	3.33774300
H	1.07902800	2.89751200	4.38265700
H	1.89571500	2.40407600	2.88638800
H	1.82309300	4.11128400	3.34587600
C	-1.67882500	2.62197700	-2.25961300
H	-2.04832200	1.65489000	-1.90658200
C	-2.88423900	3.58713100	-2.33132700
H	-2.56863300	4.57691300	-2.68024100
H	-3.63623400	3.20625800	-3.03184000
H	-3.36549300	3.71269800	-1.35609100
C	-1.10803700	2.39588300	-3.67029700
H	-0.85833000	3.33690800	-4.17198600
H	-0.20522600	1.77636800	-3.65203500
H	-1.85475300	1.89173300	-4.29331000
C	0.82087400	-0.28890200	2.92481200
H	0.55787200	-1.32041300	3.18314600
H	-0.01433300	0.35067900	3.21789000
H	1.70553000	-0.01202800	3.50958600
O	-0.67345300	-2.12214000	-0.36243600
C	-1.61432200	-3.35924900	-2.22450200
H	-1.82834600	-4.20511400	-1.56515800
H	-2.50967900	-2.73642500	-2.27728100
H	-1.38624900	-3.74989400	-3.22428100
C	4.40227000	-0.60185400	-0.32909500
C	4.65471600	-2.05946100	0.08909300
O	4.16249800	-2.59307800	1.05918800
O	5.45856400	-2.67133000	-0.79248900
C	5.73590900	0.12005300	-0.57122800
O	5.97401600	0.81583300	-1.53177900
O	6.57400200	-0.08501800	0.45578900
C	7.86371900	0.55901900	0.35530300
H	8.39543300	0.28337400	1.26511600
H	8.39398900	0.19968900	-0.52935800
H	7.74049600	1.64238400	0.28923200
C	5.78287000	-4.04962000	-0.50467500
H	6.44126900	-4.36552500	-1.31282100
H	6.28942400	-4.12135700	0.46026300
H	4.87440200	-4.65607000	-0.48333700

VOR-**TS1** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Me, R^3 = H]
B3LYP SCF energy in gas phase: -2421.84828 a.u.
M06 SCF energy in solution: -2420.889884 a.u.
M06 Free energy in solution: -2420.027295 a.u.

C	0.67224000	-3.93776700	-1.23322800
C	-0.10711500	-2.68103400	-1.11978300
C	0.48126300	-1.32765300	-1.37201200
C	1.84310200	-1.06276800	-0.87781300
H	2.21199000	-1.92595400	-0.31969600
H	0.23994900	-0.94587700	-2.36967600
C	2.92230900	-0.38093500	-1.69189600
C	3.44065500	0.49990600	0.57604800
C	2.06270100	-0.07026700	0.73030000
C	1.15064400	-0.38003100	1.63155700
H	-1.17659300	-2.75597700	-1.29913900
H	1.73217500	-3.84879300	-1.48383700
H	3.34681000	1.58979600	0.49277500
H	4.06179200	0.27937800	1.44710500
H	3.26269400	-1.03795800	-2.50054100
H	2.56987700	0.54570700	-2.15303400
Rh	0.11531300	0.18260100	-0.02431600
C	-1.89502300	0.72122100	-0.15967700
N	-3.10504200	0.11319300	-0.37795900
C	-4.14858300	1.02334100	-0.27655000
C	-3.35203100	-1.24814900	-0.81370000
N	-2.22921400	2.03691100	0.06665700
C	-3.59802200	2.23315200	-0.00384700
C	-1.27770600	3.11688700	0.25595700
C	-3.52188200	-2.26174100	0.15077300
C	-3.51150000	-1.47588400	-2.19903100
C	-3.84490600	-3.54326300	-0.31625200
C	-3.41794300	-2.00167700	1.65022300
C	-3.99778500	-3.80165200	-1.67585100
C	-3.83141900	-2.77785100	-2.60483500
C	-3.40048800	-0.37075600	-3.24775400
C	-2.64702900	-3.11144900	2.38878900
C	-4.82115600	-1.80724100	2.26408700
C	-2.42763000	-0.73023100	-4.38742900
C	-4.78981800	-0.01463600	-3.81784200
C	-1.01842600	3.58244500	1.56417000
C	-0.69263900	3.69991100	-0.88965400
C	0.21924500	4.74388200	-0.68759600
C	-1.04613600	3.28379800	-2.31507800
C	0.51670800	5.20357800	0.59155900
C	-0.10379100	4.63469400	1.70065000
C	-1.73373700	3.03360600	2.79617500
C	0.19198500	2.82111300	-3.10595800
C	-1.78004700	4.42109900	-3.05518700
C	-2.91388400	3.94795700	3.19221200
C	-0.79352400	2.83942400	4.00040400
H	-5.17547600	0.72539100	-0.41672800
H	-4.04625200	3.20388700	0.13568500
H	-3.98645000	-4.34856400	0.39668600
H	-4.25768700	-4.80169700	-2.01173700
H	-3.96674100	-2.98866500	-3.66124900
H	-2.86170800	-1.06910200	1.79124500
H	-5.35781800	-0.97267500	1.79876800
H	-4.74335000	-1.60161600	3.33792500
H	-5.43177400	-2.70868000	2.13828500
H	-3.20789300	-4.05279400	2.40748200
H	-2.47881800	-2.81759800	3.42987800
H	-1.67362400	-3.30141100	1.92559100
H	-3.00577700	0.52707400	-2.76205500

H	-5.23627800	-0.87139400	-4.33491300
H	-4.70855800	0.80712600	-4.53832600
H	-5.48390800	0.29469300	-3.02887600
H	-2.78068100	-1.58508900	-4.97419000
H	-1.43078600	-0.97739900	-4.00552800
H	-2.32669800	0.11702500	-5.07480200
H	0.69063300	5.21182000	-1.54653300
H	1.22137000	6.01966100	0.72468500
H	0.12120800	5.02053000	2.68940800
H	-1.73426800	2.43468100	-2.26557600
H	-2.68249800	4.73153300	-2.51728100
H	-2.07766200	4.09239400	-4.05734200
H	-1.14035700	5.30307700	-3.17042400
H	0.91893400	3.63019000	-3.23627800
H	-0.10041900	2.47512200	-4.10395600
H	0.70297400	1.99757100	-2.59293200
H	-2.14717900	2.05119300	2.53945800
H	-2.55661400	4.94888600	3.45966800
H	-3.44200900	3.53531300	4.05911900
H	-3.63805200	4.06050900	2.37856400
H	-0.44125800	3.79608100	4.40071800
H	0.08272500	2.23703500	3.74165000
H	-1.32740700	2.33122800	4.81086600
O	0.34755800	-3.37311100	0.05115000
C	4.08767100	-0.06109000	-0.72290300
C	4.84235800	-1.35989300	-0.39375600
O	4.72820900	-1.97953500	0.64339900
O	5.59712800	-1.75116000	-1.42932500
C	5.04052600	0.97364000	-1.33306500
O	4.81162900	1.61410100	-2.33397800
O	6.13539300	1.11065000	-0.56930000
C	7.10613700	2.07728900	-1.02616200
H	7.90842900	2.05117500	-0.28975000
H	7.47699300	1.79817200	-2.01496500
H	6.65584800	3.07140700	-1.07519900
C	6.35218500	-2.96831000	-1.24199500
H	6.89859600	-3.11449800	-2.17286300
H	7.03999100	-2.85716500	-0.40092100
H	5.67834200	-3.80675400	-1.05072700
C	0.96091000	-0.90437500	2.95149800
C	-0.21996000	-0.68202800	3.68821600
C	2.00344400	-1.66719300	3.53045100
C	-0.34834600	-1.19031600	4.97612300
H	-1.02189300	-0.10765900	3.23638200
C	1.86724100	-2.16714800	4.82075900
H	2.90138900	-1.86228900	2.95111400
C	0.69455200	-1.92955000	5.54569200
H	-1.25773100	-1.01062000	5.54236600
H	2.67123600	-2.74933200	5.26112500
H	0.59104300	-2.32369200	6.55256200
C	0.03259200	-5.25722100	-1.57767500
H	0.14633300	-5.47090900	-2.64676700
H	0.50992700	-6.06961100	-1.01799100
H	-1.03331200	-5.24822500	-1.33218100

VOR-**TS4** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Me, R^3 = H]

B3LYP SCF energy in gas phase: -2421.848661 a.u.

M06 SCF energy in solution: -2420.885547 a.u.

M06 Free energy in solution: -2420.018868 a.u.

C	2.07226100	-0.21124000	0.12553300
C	1.14380200	-0.64103300	0.94754700
C	1.94127700	-0.31424500	-1.99399900
C	0.86917600	0.39972600	-2.69745500
C	-0.32872800	-0.15848800	-3.07881300
C	-0.65870900	-1.61534700	-2.79453400
H	1.06022900	1.44810400	-2.91929200
H	1.89101800	-1.39985600	-2.06474600
H	-1.04485000	0.45330400	-3.62224700
H	0.19442000	-2.23295500	-3.12717100
C	3.32968000	0.25567900	-2.20701600
H	3.72021800	-0.12193100	-3.15877800
H	3.29682600	1.34670800	-2.28359600
C	3.49303100	0.24742800	0.22074300
H	3.50402200	1.33889100	0.34152900
H	3.94843300	-0.19636400	1.10999100
C	-3.64232400	0.62432700	1.51191700
C	-2.92984000	1.74836900	1.75373400
C	-1.70671000	0.43811000	0.35440700
N	-1.74595700	1.63497500	1.03181100
N	-2.90492900	-0.16625600	0.62949500
Rh	-0.00706000	-0.06549800	-0.59093300
H	-3.14831000	2.61531100	2.35605500
H	-4.61492200	0.31232100	1.85665200
C	-3.56980100	-1.27970400	-0.04750400
C	-3.31467100	-2.60705800	0.34397400
C	-4.54926100	-0.95011000	-1.01340100
C	-4.04583200	-3.62036600	-0.28860300
C	-5.24973900	-2.00732800	-1.60842800
C	-4.99950500	-3.33025600	-1.25814900
H	-3.86889600	-4.65321000	-0.00554600
H	-6.01173300	-1.78748100	-2.35008600
H	-5.55867500	-4.13315500	-1.73034800
C	-0.79056700	2.71984200	0.85693400
C	-0.83289400	3.45273000	-0.35880300
C	0.08260900	3.06879600	1.91103700
C	0.11666200	4.46613900	-0.53509800
C	1.00169000	4.10173600	1.67540000
C	1.03916400	4.77671000	0.46110500
H	0.11821500	5.04191500	-1.45417200
H	1.68750000	4.39010300	2.46536900
H	1.76295800	5.57104500	0.30171400
C	-4.92158000	0.48085900	-1.40611800
H	-4.23542500	1.17167400	-0.90912100
C	-6.34632400	0.83109800	-0.92635700
H	-6.45546500	0.69370100	0.15492700
H	-6.58355900	1.87510800	-1.16083200
H	-7.09654900	0.19996800	-1.41530700

C	-4.79138800	0.73519200	-2.92065900
H	-3.77189000	0.54738200	-3.27427900
H	-5.46850500	0.10055400	-3.50228100
H	-5.04371400	1.77700000	-3.15003500
C	-2.33890300	-2.97160400	1.45152200
H	-1.75605000	-2.08067500	1.68640100
C	-3.09771600	-3.38175000	2.73058600
H	-3.69378300	-4.28670700	2.56557400
H	-2.38956700	-3.58919500	3.54080800
H	-3.78033900	-2.59279900	3.06827900
C	-1.33785100	-4.06175300	1.02784700
H	-1.83156500	-5.02465100	0.85250000
H	-0.81270500	-3.76771200	0.11462600
H	-0.59840300	-4.21423400	1.82214800
C	0.00628000	2.45710700	3.30626000
H	-0.60327800	1.55251100	3.25015000
C	-0.69944000	3.43261900	4.27496600
H	-0.79567800	2.97926100	5.26783600
H	-0.12750700	4.36111200	4.38268900
H	-1.70277200	3.70413000	3.92811700
C	1.38072600	2.05454900	3.87157500
H	1.25097700	1.52477800	4.82099300
H	1.92089300	1.39101100	3.18995600
H	2.01061100	2.92839500	4.06994400
C	-1.94734100	3.27747600	-1.39071400
H	-2.29066800	2.23993500	-1.35854500
C	-3.14495700	4.18141500	-1.01762800
H	-2.85247700	5.23741700	-1.03575100
H	-3.96331900	4.04536700	-1.73395600
H	-3.53107400	3.95718100	-0.01817400
C	-1.51639300	3.56400800	-2.83955900
H	-1.31414700	4.62705700	-3.00879400
H	-0.61816400	3.00420300	-3.11982800
H	-2.32227200	3.28078600	-3.52525400
O	-0.80258000	-1.71864200	-1.38521000
C	4.27468900	-0.11290100	-1.05203500
C	4.61860600	-1.60999200	-1.06156300
O	4.31260100	-2.39869300	-0.19233300
O	5.28190500	-1.93587800	-2.17904600
C	5.56102700	0.72576500	-1.13260800
O	5.67262300	1.74235100	-1.77898300
O	6.51392800	0.20909100	-0.34385800
C	7.76703200	0.92894700	-0.31271300
H	8.40446400	0.36818100	0.36960300
H	8.20353100	0.96445500	-1.31323500
H	7.60800200	1.94672100	0.05053600
C	5.69604900	-3.31559100	-2.29323900
H	6.21966100	-3.38111300	-3.24606800
H	6.35986800	-3.57622800	-1.46605800
H	4.82493900	-3.97471500	-2.28182300
C	1.11674800	-1.30254900	2.24352200
C	0.07125000	-1.13714300	3.16882800
C	2.19280700	-2.15525100	2.57652200
C	0.11289100	-1.77449800	4.40663900
H	-0.77139900	-0.50555800	2.91475700
C	2.22163800	-2.79921700	3.81128200
H	2.98406400	-2.32451300	1.85251600
C	1.18844500	-2.60620800	4.73218300
H	-0.69676400	-1.62805700	5.11575500
H	3.05140400	-3.45709700	4.05284800
H	1.21578100	-3.10765900	5.69527700
C	-1.90409900	-2.12231500	-3.51086300
H	-1.75659200	-2.07800500	-4.59746300
H	-2.09358200	-3.16256400	-3.23204100
H	-2.78517600	-1.53470800	-3.24366400

VOR-**TS1** [X = $C(CO_2Me)_2$, R^1 = Me, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2421.841758 a.u.

M06 SCF energy in solution: -2420.884734 a.u.

M06 Free energy in solution: -2420.025378 a.u.

C	-2.55198600	2.76583700	-0.13769600
C	-1.99826500	1.39708300	0.09730600
C	-0.61416200	1.17994900	0.62049400
C	0.46924200	2.03043500	0.09077900
H	0.06911300	2.71315700	-0.66295100
H	-0.60143800	0.98054800	1.69787500
C	1.56271100	2.65151100	0.92803200
C	2.67434500	2.38141000	-1.32114800
C	1.55195600	1.38617600	-1.34820200
C	0.93745000	0.50557800	-2.10052600
H	-2.71691100	0.61571500	0.33199500
H	-1.87980300	3.60151600	0.06856600
H	3.61805700	1.82536000	-1.30670500
H	2.66421500	2.99808900	-2.22404700
H	1.15239500	3.40901800	1.60641900
H	2.08133000	1.91371300	1.54621600
Rh	0.61549300	-0.20204900	-0.26116200
C	-0.06496700	-2.13170700	0.08603600
N	-1.27040500	-2.77453400	0.18887600
C	-1.09412900	-4.13800000	0.37795600
C	-2.59253600	-2.18008200	0.21224300
N	0.85744900	-3.14010000	0.22696400
C	0.24346500	-4.36762000	0.40644600
C	2.29578000	-2.95168100	0.25487900
C	-3.27212700	-1.97566200	-1.00613700
C	-3.17928700	-1.92041400	1.46959900
C	-4.57875100	-1.47662900	-0.93377600
C	-2.65874800	-2.32635800	-2.35880100
C	-5.18079600	-1.19734700	0.29066100
C	-4.48744700	-1.41845400	1.47705800
C	-2.47503900	-2.20236400	2.79570500
C	-2.95992800	-1.27185800	-3.43999200
C	-3.12272600	-3.72430200	-2.82162400
C	-2.47729900	-0.98200000	3.73610000
C	-3.09950200	-3.42682400	3.49741700
C	3.03586700	-3.17693800	-0.92662900
C	2.90172400	-2.60390100	1.48170200

C	4.29322200	-2.44289300	1.48828400
C	2.12206000	-2.45197200	2.78552800
C	5.04724400	-2.63944400	0.33510600
C	4.42446000	-3.00920200	-0.85447500
C	2.38867800	-3.64048700	-2.22971100
C	2.33294100	-1.07109200	3.43511900
C	2.47946200	-3.58374600	3.77158100
C	2.54056300	-5.16733100	-2.40289800
C	2.94543500	-2.91079800	-3.46671300
H	-1.93256900	-4.80806900	0.48253800
H	0.80729500	-5.27650800	0.54389100
H	-5.13605200	-1.31047000	-1.84973300
H	-6.19392000	-0.80757000	0.32027900
H	-4.97246100	-1.20759500	2.42519300
H	-1.57130800	-2.36131500	-2.23467700
H	-2.85228600	-4.50268200	-2.09959300
H	-2.66247000	-3.98094600	-3.78266300
H	-4.21065300	-3.75224600	-2.95140200
H	-4.01644400	-1.27349100	-3.73043300
H	-2.38199000	-1.49175900	-4.34472400
H	-2.70486900	-0.26264400	-3.09987700
H	-1.42811600	-2.44378400	2.58546500
H	-4.15052300	-3.24458300	3.74806100
H	-2.56574700	-3.64862200	4.42843900
H	-3.05989800	-4.31969300	2.86380000
H	-3.48992900	-0.71165200	4.05380200
H	-2.03366800	-0.10206700	3.25696200
H	-1.89958100	-1.20336500	4.64039300
H	4.79322800	-2.17358000	2.41358400
H	6.12631600	-2.51779600	0.36606200
H	5.02839200	-3.17743300	-1.74017200
H	1.05444900	-2.54323500	2.56177300
H	2.28815600	-4.57050200	3.33559800
H	1.88282500	-3.49461300	4.68638300
H	3.53652200	-3.54519400	4.05716400
H	3.37594200	-0.91166100	3.72868500
H	1.71828500	-0.98080800	4.33795800
H	2.05655700	-0.26026200	2.75045400
H	1.31694800	-3.41789400	-2.17366500
H	3.59809900	-5.44904600	-2.45974600
H	2.05274900	-5.49816000	-3.32669900
H	2.09405700	-5.72019500	-1.56975100
H	3.98318300	-3.19293700	-3.67496500
H	2.91278200	-1.82306400	-3.34493700
H	2.35768000	-3.17657100	-4.35255400
C	0.60256800	0.11072700	-3.48467000
H	1.31214400	0.56710900	-4.18796800
H	0.61319600	-0.97301000	-3.62667700
H	-0.39915000	0.47995600	-3.73711400
O	-2.11235900	1.93316600	-1.22417900
C	2.57221300	3.29840200	-0.05744300
C	2.02353000	4.67621700	-0.46879000
O	1.43440500	4.89868400	-1.50466500
O	2.21843000	5.57881100	0.50260900
C	3.95078700	3.44643400	0.59970900
O	4.26479000	2.96313000	1.66408700
O	4.77656500	4.13972800	-0.19876400
C	6.11813800	4.33531600	0.29790800
H	6.63037900	4.91050000	-0.47244200
H	6.09279000	4.88546900	1.24120100
H	6.60830200	3.37138400	0.45362800
C	1.72156100	6.90966300	0.23982600
H	1.97831000	7.49261800	1.12341400
H	2.20242900	7.32036200	-0.65056700
H	0.63972600	6.88715200	0.08916400
C	-4.00133600	3.09026900	-0.02999700
C	-4.95886600	2.42591300	-0.80635900
C	-4.41354700	4.08202400	0.87030900
C	-6.31053000	2.74532200	-0.67484700
H	-4.63461500	1.67709600	-1.52153000
C	-5.76606200	4.39340200	1.00673500
H	-3.67368000	4.61442600	1.46448300
C	-6.71831900	3.72491700	0.23388000
H	-7.04707200	2.23637700	-1.29086300
H	-6.07499700	5.16338900	1.70794000
H	-7.77113500	3.97369600	0.33197600

VOR-**TS4** [X = $C(CO_2Me)_2$, R^1 = Me, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2421.841412 a.u.

M06 SCF energy in solution: -2420.87943 a.u.

M06 Free energy in solution: -2420.015234 a.u.

C	2.34763800	-0.12057000	0.74783400
C	1.41564900	0.26873200	1.57335100
C	2.03132700	-1.49072100	-0.92376800
C	1.04520900	-1.13810800	-1.94217000
C	-0.26194200	-1.56715800	-1.95754500
C	-0.82434700	-2.46638000	-0.86691200
H	1.38910500	-0.47281100	-2.73223300
H	1.79260600	-2.36696400	-0.32366300
H	-0.91176500	-1.25238500	-2.76908900
H	-0.06547300	-3.23613700	-0.63801200
C	3.48040400	-1.41137500	-1.34813000
H	3.73381400	-2.32688100	-1.89589500
H	3.64686300	-0.57370800	-2.03251300
C	3.83770200	-0.05678600	0.65340400
H	4.11805800	0.87420000	0.14293000
H	4.24817500	-0.02672100	1.66733900
C	-2.87594300	2.56367200	1.10712300
C	-1.97004400	3.38782600	0.53671600
C	-1.17115000	1.26286500	0.37651300
N	-0.92805500	2.58498400	0.08611700
N	-2.39518300	1.25926800	0.99026900
Rh	0.26827500	-0.09386000	-0.00302700
H	-1.96534500	4.45653300	0.39747300
H	-3.82831100	2.76416600	1.57027400
C	-3.31415900	0.16939400	1.30997200
C	-3.23818000	-0.47200300	2.55986200

C	-4.36802700	-0.06679100	0.39897900
C	-4.25324400	-1.38290400	2.88171300
C	-5.35631900	-0.98243300	0.77908000
C	-5.30624700	-1.63278800	2.00782700
H	-4.22733200	-1.88710500	3.84279800
H	-6.18079800	-1.18226200	0.10189500
H	-6.09118400	-2.33001000	2.28748100
C	0.16732200	3.09825000	-0.72023500
C	0.08317300	2.96340400	-2.12844400
C	1.22178000	3.79499700	-0.09060400
C	1.14329800	3.47263000	-2.88810700
C	2.24693500	4.29224200	-0.90739700
C	2.22033200	4.11957000	-2.28692600
H	1.11635900	3.38397200	-3.96880900
H	3.07218900	4.83327700	-0.45577500
H	3.02675600	4.51305200	-2.89933000
C	-4.50431000	0.64583900	-0.94606600
H	-3.60950800	1.25419600	-1.10788800
C	-5.71633700	1.60097800	-0.95329000
H	-5.65408800	2.34713000	-0.15363000
H	-5.77576400	2.13470900	-1.90877400
H	-6.65471000	1.05117400	-0.82051000
C	-4.59388600	-0.34454900	-2.12348000
H	-3.74286700	-1.03134400	-2.13840200
H	-5.50412800	-0.95183200	-2.07539700
H	-4.61830400	0.20503700	-3.07212200
C	-2.14926100	-0.18008900	3.58257800
H	-1.40410400	0.45873400	3.10194200
C	-2.71456100	0.59635300	4.78978000
H	-3.46311900	0.00537900	5.32943700
H	-1.91350200	0.84322500	5.49653400
H	-3.19227400	1.53217500	4.47811300
C	-1.43389700	-1.46778400	4.03490300
H	-2.11910300	-2.15440900	4.54365900
H	-0.99700100	-1.99576500	3.18079900
H	-0.63607100	-1.23131400	4.74917600
C	1.24931600	4.09176500	1.40620300
H	0.53358700	3.42475700	1.89733700
C	0.79897500	5.54402800	1.68039500
H	0.78604500	5.74266600	2.75793400
H	1.48555600	6.25923500	1.21356500
H	-0.20343600	5.74587600	1.28906400
C	2.63041600	3.84752100	2.04320900
H	2.56224800	3.94397400	3.13231500
H	3.01431800	2.84941300	1.81013700
H	3.37041700	4.57931300	1.70224200
C	-1.15182300	2.39909700	-2.83000000
H	-1.63431800	1.68635500	-2.15483400
C	-2.16304700	3.53280400	-3.11499300
H	-1.72821900	4.28036100	-3.78822800
H	-3.06244000	3.12931800	-3.59401600
H	-2.47193200	4.04479400	-2.19826900
C	-0.83921600	1.64410900	-4.13398600
H	-0.50692500	2.31729000	-4.93149300
H	-0.06281400	0.88412900	-3.99421000
H	-1.74417800	1.14414000	-4.49601000
C	1.32312400	0.71726000	2.98673900
H	0.94032300	-0.11094500	3.59225800
H	0.64443700	1.56360500	3.11439200
H	2.31060800	0.98926100	3.37638800
O	-0.99909900	-1.62610000	0.26359600
C	4.41010200	-1.24524900	-0.13538600
C	4.39473900	-2.51165700	0.73598600
O	3.87620800	-2.58872700	1.82854300
O	4.99246100	-3.52955500	0.10117100
C	5.84089900	-0.93564900	-0.60006000
O	6.14507200	-0.64684200	-1.73463600
O	6.69026200	-0.97900700	0.43693000
C	8.07370300	-0.69268800	0.13158100
H	8.60260500	-0.78218000	1.07956000
H	8.45340700	-1.41351000	-0.59578100
H	8.16957000	0.31705000	-0.27397300
C	5.04980500	-4.78128600	0.82140400
H	5.57676500	-5.46919000	0.16156300
H	5.59286600	-4.64884300	1.75959300
H	4.04071500	-5.14218400	1.03364000
C	-2.08986100	-3.21345400	-1.25452500
C	-3.06596800	-3.49559700	-0.29380800
C	-2.23782100	-3.72269800	-2.55168800
C	-4.17954300	-4.26653700	-0.63160700
H	-2.95357100	-3.10503600	0.71143700
C	-3.35334300	-4.49165800	-2.88841200
H	-1.47582800	-3.53436600	-3.30557600
C	-4.32827400	-4.76525000	-1.92729100
H	-4.93275400	-4.47835400	0.12223400
H	-3.45671800	-4.87857600	-3.89833000
H	-5.19502900	-5.36689000	-2.18602800

VOR-**TS1** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Me, R^3 = Me]

B3LYP SCF energy in gas phase: -2461.163289 a.u.

M06 SCF energy in solution: -2460.186299 a.u.

M06 Free energy in solution: -2459.299557 a.u.

C	0.54960600	-4.06003300	-0.92100200
C	-0.07455900	-2.71395600	-0.76385200
C	0.51319400	-1.39835300	-1.18167300
C	1.85967400	-1.03573900	-0.70917500
H	2.23582300	-1.82396600	-0.05465700
H	0.26399100	-1.13148000	-2.21438200
C	2.93382800	-0.42136300	-1.58369200
C	3.39877200	0.71215300	0.57738900
C	2.02975000	0.12992000	0.77112100
C	1.11204600	-0.09339300	1.69322300
H	-1.16233400	-2.70592900	-0.74623300
H	3.28537700	1.78408400	0.37356800
H	4.00886400	0.60001900	1.47634600
H	3.29894900	-1.14991900	-2.31603100
H	2.56868400	0.44465500	-2.14214100

Rh	0.08657400	0.25534800	-0.02591300
C	-1.93575900	0.73653400	-0.22773900
N	-3.14216700	0.09913100	-0.37049600
C	-4.19144600	1.00917000	-0.38033300
C	-3.39588000	-1.30615500	-0.62863900
N	-2.27909000	2.06811500	-0.16354000
C	-3.64878000	2.24621500	-0.25779100
C	-1.33566300	3.16979100	-0.10224700
C	-3.56978200	-2.18626600	0.45915400
C	-3.57391900	-1.70726700	-1.97133200
C	-3.93911900	-3.50556900	0.16463000
C	-3.41008100	-1.74481800	1.91014200
C	-4.12370800	-3.92993800	-1.14873100
C	-3.93568000	-3.04070500	-2.20274500
C	-3.42986400	-0.75480500	-3.15715600
C	-2.65774400	-2.78476200	2.76137600
C	-4.78165000	-1.41342900	2.53595900
C	-2.45716900	-1.29271100	-4.22440600
C	-4.80424500	-0.44320400	-3.78566800
C	-1.08381700	3.79082600	1.14168000
C	-0.75514900	3.61939100	-1.30888800
C	0.15321100	4.68289500	-1.23035100
C	-1.10956400	3.03930900	-2.67577000
C	0.44662700	5.29175200	-0.01405100
C	-0.17497800	4.85656700	1.15351800
C	-1.80227800	3.39053800	2.42791400
C	0.11498600	2.42205500	-3.37663300
C	-1.78025300	4.10217700	-3.57048400
C	-2.98929800	4.33976100	2.70475100
C	-0.86756800	3.34993600	3.65119700
H	-5.21615200	0.68957500	-0.48399200
H	-4.10267300	3.22400300	-0.23820900
H	-4.09124700	-4.20845400	0.97677200
H	-4.41879100	-4.95585600	-1.35049200
H	-4.08628400	-3.38236300	-3.22223500
H	-2.81119700	-0.82815600	1.91402500
H	-5.30233600	-0.62360200	1.98292300
H	-4.65750400	-1.07455100	3.57101000
H	-5.43096300	-2.29647200	2.54849300
H	-3.25255100	-3.69197900	2.91621500
H	-2.44097200	-2.36954400	3.75071500
H	-1.70772800	-3.07292100	2.29946500
H	-3.01462100	0.18952600	-2.79155600
H	-5.27239800	-1.35080900	-4.18288200
H	-4.69446800	0.26726900	-4.61269800
H	-5.49326100	-0.00701100	-3.05428100
H	-2.83496500	-2.20475900	-4.69908300
H	-1.47503800	-1.52233800	-3.79619100
H	-2.31717000	-0.54751600	-5.01553300
H	0.62297800	5.04936600	-2.13813800
H	1.14761300	6.12092600	0.02242500
H	0.04380100	5.35907200	2.08979200
H	-1.83774400	2.23561400	-2.53075600
H	-2.67167700	4.52293200	-3.09251300
H	-2.08372200	3.65779100	-4.52509100
H	-1.09812200	4.93036400	-3.79157200
H	0.88887200	3.17020100	-3.58022900
H	-0.17755800	1.97702300	-4.33461100
H	0.56743600	1.63727600	-2.75811200
H	-2.20973400	2.38222600	2.28917600
H	-2.63834800	5.36743300	2.85235300
H	-3.52155700	4.03158800	3.61173400
H	-3.70902800	4.35084700	1.87955800
H	-0.52110000	4.35053200	3.93152000
H	0.01225800	2.72408500	3.47289900
H	-1.40348000	2.94306800	4.51574200
O	0.52370800	-3.37631000	0.35794800
C	4.07736600	0.02392000	-0.64045800
C	4.85645000	-1.21039400	-0.15363400
O	4.79678500	-1.66802000	0.96811800
O	5.57293600	-1.74657700	-1.15208600
C	5.02099800	1.00441100	-1.34772200
O	4.78224300	1.54945600	-2.40150900
O	6.11907300	1.21797600	-0.60656100
C	7.07794000	2.14927500	-1.15326300
H	7.88336500	2.19745400	-0.42142100
H	7.44772500	1.78639200	-2.11491100
H	6.61689300	3.13030000	-1.28904800
C	6.36078600	-2.90934600	-0.81394300
H	6.87230500	-3.18833200	-1.73429900
H	7.07931800	-2.65960800	-0.03026500
H	5.71318200	-3.71821200	-0.46787500
C	0.92609800	-0.46314700	3.06546900
C	-0.26197700	-0.18017200	3.76910000
C	1.98153300	-1.13050100	3.73258600
C	-0.38548600	-0.53554200	5.10783400
H	-1.07315400	0.32103300	3.25169100
C	1.85000000	-1.47772900	5.07255900
H	2.88654500	-1.37297700	3.18288200
C	0.66960600	-1.18121900	5.76236200
H	-1.30046200	-0.30839700	5.64740500
H	2.66398300	-1.98707700	5.57977600
H	0.56973900	-1.45658500	6.80831400
C	-0.36695300	-5.26623900	-0.98518000
H	-0.54987600	-5.56078300	-2.02504000
H	0.09597200	-6.11707400	-0.47133700
H	-1.32692900	-5.05546100	-0.50780100
C	1.91513400	-4.28773200	-1.53598000
H	2.55254000	-3.40233600	-1.51793400
H	2.43351500	-5.08762200	-0.99420700
H	1.80899700	-4.60878900	-2.57855300

VOR-**TS4** [X = $C(CO_2Me)_2$, R^1 = Ph, R^2 = Me, R^3 = Me]

B3LYP SCF energy in gas phase: -2461.160969 a.u.

M06 SCF energy in solution: -2460.179017 a.u.

M06 Free energy in solution: -2459.284443 a.u.

C	2.08890600	-0.08508300	0.18349300

C	1.16046300	-0.42754800	1.04689400
C	1.99385300	-0.47897400	-1.89261200
C	0.94860200	0.18060000	-2.68562300
C	-0.27248300	-0.33742000	-3.05508100
C	-0.78203400	-1.72860300	-2.69894200
H	1.17797100	1.19829400	-2.99947600
H	1.91399600	-1.55983600	-1.81879900
H	-0.91091100	0.28996800	-3.67250000
C	3.39628700	0.03182600	-2.16393400
H	3.79754500	-0.49910700	-3.03433900
H	3.38355600	1.09663600	-2.41532400
C	3.50342300	0.40118200	0.23615700
H	3.50517400	1.49760100	0.17463200
H	3.94135800	0.11323000	1.19544100
C	-3.53333800	0.71995400	1.61437600
C	-2.86685500	1.89603400	1.64569900
C	-1.69516800	0.46826500	0.31632500
N	-1.74713500	1.74222300	0.83513100
N	-2.83842100	-0.14459400	0.76751600
Rh	0.02890200	-0.08332800	-0.57877300
H	-3.08214000	2.82370700	2.15081000
H	-4.45240400	0.41428700	2.08657200
C	-3.51510900	-1.34921800	0.28000400
C	-3.10166300	-2.62690500	0.70433500
C	-4.65365900	-1.15857300	-0.54331500
C	-3.83006900	-3.73099700	0.24270700
C	-5.34462700	-2.30255200	-0.96194400
C	-4.93591700	-3.57744600	-0.58547200
H	-3.53193900	-4.72635300	0.55553200
H	-6.22315400	-2.19027000	-1.58957900
H	-5.48991700	-4.44874500	-0.92347900
C	-0.87148600	2.83971900	0.44695500
C	-1.03453000	3.39495400	-0.84987200
C	0.04249700	3.37643200	1.38137600
C	-0.16702900	4.42810800	-1.22310400
C	0.87430200	4.41934900	0.94841400
C	0.79122700	4.92531700	-0.34287200
H	-0.25809300	4.87119700	-2.20867300
H	1.58838000	4.84965200	1.64318500
H	1.44929700	5.73114400	-0.65559300
C	-5.20970700	0.20806900	-0.95906500
H	-4.49051400	0.98273100	-0.67892600
C	-6.53003400	0.50876300	-0.21538000
H	-6.41347500	0.46141900	0.87241100
H	-6.89423500	1.50966500	-0.47332500
H	-7.30739500	-0.21204700	-0.49171700
C	-5.43635900	0.34026600	-2.47869300
H	-4.51565900	0.18182400	-3.04818300
H	-6.18201300	-0.37228700	-2.84649300
H	-5.80808400	1.34524300	-2.70946900
C	-1.97804100	-2.84814200	1.70472100
H	-1.39568800	-1.92907500	1.76309100
C	-2.56965500	-3.12124400	3.10408500
H	-3.16336000	-4.04273700	3.10749500
H	-1.76780300	-3.23254800	3.84191800
H	-3.22414400	-2.30522200	3.43355300
C	-1.00379500	-3.96580900	1.29238600
H	-1.47854400	-4.95370400	1.30642200
H	-0.60555800	-3.78132600	0.29094000
H	-0.16600100	-4.00056000	1.99814100
C	0.10246600	2.95165800	2.84493400
H	-0.45559100	2.01996600	2.95451000
C	-0.58178200	4.01191800	3.73667000
H	-0.58502700	3.68424200	4.78227300
H	-0.05188900	4.96974500	3.68611100
H	-1.61948500	4.19610900	3.43652800
C	1.53537800	2.68876800	3.34386400
H	1.50514600	2.28219100	4.36013300
H	2.05722300	1.96589100	2.71001500
H	2.13108800	3.60746400	3.37691600
C	-2.18597800	3.00822200	-1.77834100
H	-2.43985300	1.95950600	-1.59990100
C	-3.43290700	3.85848400	-1.44232700
H	-3.22872200	4.92339400	-1.60156600
H	-4.27264600	3.57569800	-2.08741300
H	-3.74791100	3.72887400	-0.40191400
C	-1.85653700	3.14507100	-3.27535700
H	-1.77707400	4.19236200	-3.58605600
H	-0.91672500	2.64761200	-3.53804300
H	-2.65925800	2.69742900	-3.87147500
O	-0.62742100	-1.83164000	-1.28277900
C	4.31422900	-0.15502900	-0.94537600
C	4.65735300	-1.63396800	-0.71299200
O	4.36752900	-2.26797800	0.27954000
O	5.30501800	-2.14106500	-1.77070400
C	5.60360600	0.66476600	-1.12539100
O	5.71345400	1.60066600	-1.88431200
O	6.55935800	0.24045100	-0.28722600
C	7.81273400	0.95846000	-0.34255000
H	8.45464800	0.47399200	0.39198700
H	8.24234400	0.88567700	-1.34402600
H	7.65610600	2.00949400	-0.08975900
C	5.72446500	-3.51919200	-1.65781800
H	6.23430200	-3.74267400	-2.59403800
H	6.40181900	-3.63512800	-0.80895500
H	4.85712700	-4.16937300	-1.52217100
C	1.14268200	-0.87412000	2.43315500
C	0.08461800	-0.59717600	3.31753700
C	2.24784900	-1.61676000	2.90579000
C	0.14611200	-1.00948200	4.64665700
H	-0.78580800	-0.05874800	2.96154700
C	2.29528900	-2.03814100	4.23271100
H	3.04845200	-1.87712100	2.22041200
C	1.25221600	-1.72842800	5.10925600
H	-0.67383400	-0.77849700	5.32050700
H	3.14833900	-2.61283200	4.58165600
H	1.29456600	-2.05448100	6.14447300
C	-2.26353600	-1.84557900	-3.07609200

H	-2.39631400	-1.77410000	-4.16278700
H	-2.66060400	-2.80630400	-2.73842200
H	-2.84333500	-1.05512100	-2.59834000
C	-0.00083000	-2.86031100	-3.39582500
H	-0.15318200	-2.82553300	-4.48041800
H	1.07299900	-2.81296500	-3.19989500
H	-0.37092700	-3.82359600	-3.02919600

VOR-**TS1** [X = O, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2193.727543 a.u.

M06 SCF energy in solution: -2192.783766 a.u.

M06 Free energy in solution: -2191.970791 a.u.

C	3.59332100	0.80688100	-1.64347500
C	2.40837300	0.17762300	-0.98491800
C	1.13751200	-0.09354500	-1.72824000
C	0.65332000	0.94569800	-2.64618500
H	1.30376400	1.82272100	-2.61994300
H	1.05836600	-1.13175800	-2.06642100
C	0.10175600	0.70876500	-4.03642900
C	-1.25768800	2.51568200	-3.46257100
C	-0.75484600	2.10969300	-2.10113200
C	-0.70883600	2.43409000	-0.82732400
H	2.61246300	-0.48221100	-0.14623200
H	3.47439600	1.07993700	-2.69456200
H	-2.29935400	2.17227200	-3.56239400
H	-1.23714200	3.60077400	-3.60157500
H	0.90608600	0.45687500	-4.73595500
H	-0.64240300	-0.10236100	-4.04769600
Rh	-0.67494400	0.40007000	-0.87507600
C	-1.05565100	-0.98285000	0.64303600
N	-0.34269500	-1.65896000	1.59925200
C	-1.17936600	-2.42578700	2.39663100
C	1.09902300	-1.73934600	1.74420200
N	-2.35576300	-1.37106000	0.86868300
C	-2.44343500	-2.25075500	1.93341600
C	-3.49416000	-1.00230400	0.04579700
C	1.76409800	-0.79406800	2.55099600
C	1.76110800	-2.83398600	1.14421900
C	3.14266900	-0.96553500	2.73434100
C	1.04106500	0.35216300	3.25057100
C	3.82634800	-2.02476500	2.14405000
C	3.14073200	-2.94720500	1.35886900
C	1.03897400	-3.90579300	0.32920800
C	1.79553200	1.68835300	3.12062300
C	0.78271800	0.00895400	4.73320400
C	1.70744700	-4.16860400	-1.03415600
C	0.92576700	-5.21972100	1.13131300
C	-4.34252900	0.04124300	0.47728500
C	-3.74434700	-1.75466400	-1.12356500
C	-4.85805400	-1.39570800	-1.89345700
C	-2.91044100	-2.96680300	-1.53159200
C	-5.69342900	-0.35076300	-1.51024000
C	-5.44140000	0.35098400	-0.33457600
C	-4.14482700	0.77488200	1.80195500
C	-2.41997100	-2.88500000	-2.98894600
C	-3.69864000	-4.27171100	-1.29125000
C	-5.03865500	0.16057000	2.90213200
C	-4.41002000	2.28825300	1.69861700
H	-0.79632600	-3.02569600	3.20678000
H	-3.38282700	-2.67233000	2.25318900
H	3.68835800	-0.26079200	3.35300700
H	4.89622200	-2.13162300	2.29602700
H	3.68367400	-3.77462200	0.91285600
H	0.06777700	0.48090900	2.76588100
H	0.18603900	-0.90390500	4.84106800
H	0.24271000	0.82548900	5.22624700
H	1.72505500	-0.14324900	5.27168700
H	2.73971300	1.67906000	3.67662400
H	1.18908000	2.50165700	3.53230600
H	2.01658600	1.92541600	2.07466300
H	0.02178600	-3.55643100	0.12500800
H	1.91669100	-5.62947400	1.35702300
H	0.37369600	-5.97235800	0.55723100
H	0.40382400	-5.07028000	2.08258200
H	2.70890200	-4.59794500	-0.92459600
H	1.80405600	-3.25026000	-1.62403700
H	1.10977000	-4.88197600	-1.61248900
H	-5.08342000	-1.95317200	-2.79741800
H	-6.55467300	-0.09345600	-2.12029000
H	-6.11656900	1.14676100	-0.03821700
H	-2.01997100	-3.00321900	-0.89661700
H	-4.00809200	-4.36680100	-0.24465600
H	-3.08280100	-5.14238700	-1.54352600
H	-4.60200700	-4.30899900	-1.91023000
H	-3.24920000	-2.90799800	-3.70415600
H	-1.76901500	-3.73686400	-3.21584800
H	-1.85304800	-1.96351400	-3.16558100
H	-3.10082300	0.64232100	2.11009500
H	-6.09832100	0.26120900	2.64158400
H	-4.87584300	0.67310100	3.85693600
H	-4.83388500	-0.90431000	3.05327600
H	-5.47075500	2.50463900	1.53325700
H	-3.83948700	2.75025700	0.88707100
H	-4.12625700	2.78038200	2.63519500
O	2.73845100	1.55057600	-0.75700800
C	4.99716000	0.54593500	-1.22117800
C	5.41542300	0.76839300	0.09700800
C	5.91697700	0.06681300	-2.16360900
C	6.73487000	0.50555400	0.46581700
H	4.70888900	1.16594800	0.81837700
C	7.23338700	-0.20366400	-1.79036600
H	5.60376700	-0.09102700	-3.19354800
C	7.64513400	0.01506100	-0.47377800
H	7.05727300	0.69438000	1.48630900
H	7.93867900	-0.57449900	-2.52858100
H	8.67280300	-0.18535300	-0.18444800
C	-0.64401000	3.51306900	0.11624700

C	-1.01086400	3.34517700	1.46648900
C	-0.20196300	4.78357900	-0.32133300
C	-0.95427200	4.41879800	2.34882000
H	-1.33677700	2.36748800	1.80479300
C	-0.15490900	5.85352100	0.56489500
H	0.10513300	4.91394600	-1.35457600
C	-0.53063900	5.67431600	1.90051400
H	-1.24326700	4.28275300	3.38692000
H	0.18191000	6.82622000	0.21925500
H	-0.48972800	6.51121600	2.59149200
O	-0.44374800	1.94083600	-4.47697600

VOR-**TS4** [X = O, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2193.724345 a.u.

M06 SCF energy in solution: -2192.778474 a.u.

M06 Free energy in solution: -2191.959815 a.u.

C	2.22515800	0.32378400	2.24174500
C	1.99263900	1.10927600	1.21996300
C	0.82658600	-0.86388500	3.31515300
C	0.00220700	-1.82766400	2.59195600
C	-1.26227100	-1.55970500	2.10902400
C	-1.93130000	-0.21140900	2.33948400
H	0.44799000	-2.80160700	2.39532200
H	0.29750400	-0.04244100	3.79421000
H	-1.80568300	-2.33567000	1.57929200
H	-1.73956800	0.08770900	3.38542000
C	1.93906200	-1.43844900	4.17562600
H	1.53262400	-1.71935900	5.15236800
H	2.36927500	-2.33665100	3.70194800
C	3.37512400	-0.00160700	3.15855000
H	4.01201500	-0.75917900	2.66964500
H	3.97502100	0.89619400	3.32903000
C	-0.27125300	0.27184700	-3.14150600
C	0.72538900	-0.64096100	-3.10503500
C	0.13686200	-0.16679700	-0.96091900
N	0.96419000	-0.91775200	-1.76269400
N	-0.65258000	0.54194800	-1.82611600
Rh	0.47356100	-0.21998400	1.02234100
H	1.27926100	-1.12551100	-3.89285700
H	-0.77296600	0.74336300	-3.97087000
C	-1.91178800	1.26033400	-1.61449600
C	-1.90697800	2.62364900	-1.26757900
C	-3.10161500	0.56790000	-1.93950000
C	-3.13920700	3.29097000	-1.24217300
C	-4.29959200	1.29108900	-1.90678200
C	-4.32375300	2.63977300	-1.56722700
H	-3.16142200	4.34482600	-0.98195800
H	-5.22805800	0.78703200	-2.15637200
H	-5.26462200	3.18304800	-1.56002000
C	1.83864700	-1.98965000	-1.30518100
C	1.24505800	-3.22614400	-0.93551200
C	3.23969400	-1.81261600	-1.33751200
C	2.09774000	-4.24252100	-0.48964600
C	4.03945100	-2.87372300	-0.88809300
C	3.47940200	-4.06686900	-0.44899600
H	1.67897300	-5.19853000	-0.19535000
H	5.11912600	-2.76511800	-0.90091300
H	4.11930200	-4.87514000	-0.10627600
C	-3.15109900	-0.90308300	-2.35178100
H	-2.14630700	-1.32499700	-2.25941100
C	-3.57847200	-1.06002700	-3.82608200
H	-2.91334900	-0.51524900	-4.50511700
H	-3.56534100	-2.11675900	-4.11664300
H	-4.59465400	-0.68375800	-3.98714300
C	-4.07337700	-1.72920100	-1.43367900
H	-3.78293100	-1.63921400	-0.38275500
H	-5.11729300	-1.40780100	-1.51240900
H	-4.03546000	-2.78749800	-1.71898500
C	-0.64028700	3.40695300	-0.96560900
H	0.19773500	2.70926800	-0.98995400
C	-0.38158200	4.48259100	-2.03981300
H	-1.17734600	5.23574000	-2.05165000
H	0.56298800	4.99972200	-1.83802400
H	-0.32432500	4.04561700	-3.04374100
C	-0.67321800	4.02455500	0.44551400
H	-1.47588200	4.76458400	0.54250200
H	-0.82695600	3.25004300	1.20349200
H	0.27336000	4.53553700	0.65408000
C	3.91943900	-0.57905000	-1.92198700
H	3.16209500	0.19750100	-2.05210800
C	4.49676700	-0.89767000	-3.31916100
H	4.94356800	0.00074300	-3.75934100
H	5.27625500	-1.66534200	-3.25840100
H	3.72704100	-1.26471400	-4.00715500
C	5.02038700	-0.00683100	-1.01013500
H	5.40108000	0.93118000	-1.42743200
H	4.64380000	0.20319500	-0.00430700
H	5.87017700	-0.69189300	-0.91945400
C	-0.24338200	-3.52004200	-1.12629800
H	-0.80029500	-2.59014200	-0.97838500
C	-0.50486600	-4.00391600	-2.57148700
H	0.03734800	-4.93540100	-2.77020500
H	-1.57337100	-4.19751000	-2.71986700
H	-0.19152700	-3.26627900	-3.31637400
C	-0.81248100	-4.55171400	-0.13551100
H	-0.44802500	-5.56400400	-0.34080600
H	-0.56278900	-4.31473600	0.90445200
H	-1.90366800	-4.58324200	-0.22471100
O	-1.26109400	0.68827500	1.46761400
C	-3.44113000	-0.22072500	2.16660500
C	-4.10671300	0.89721600	1.65545900
C	-4.19021900	-1.30956400	2.63423100
C	-5.50168000	0.91882500	1.60277900
H	-3.53180600	1.74291600	1.29498800
C	-5.58465500	-1.28772700	2.57729200
H	-3.69055300	-2.17692500	3.06161600
C	-6.24446100	-0.17089900	2.06068700

H	-6.00841800	1.79256300	1.20278800
H	-6.15278800	-2.13896100	2.94186800
H	-7.32984100	-0.14907200	2.02102800
C	2.58804800	2.33411000	0.70011300
C	2.68389000	2.61665400	-0.67290400
C	3.10501900	3.27052400	1.62113700
C	3.30865500	3.78103300	-1.11509000
H	2.27191300	1.91821700	-1.39142900
C	3.71432200	4.44061200	1.17612400
H	3.00618300	3.08405500	2.68645500
C	3.82575700	4.69571100	-0.19359100
H	3.38615700	3.97891200	-2.18018500
H	4.10106600	5.15387200	1.89790700
H	4.30613800	5.60568800	-0.54072100
O	2.92811800	-0.46310600	4.40867500

VOR-**TS1** [X = NTs, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2992.795599 a.u.

M06 SCF energy in solution: -2991.695077 a.u.

M06 Free energy in solution: -2990.765194 a.u.

C	0.36981800	3.77411100	-0.36925200
C	0.96019600	2.40185400	-0.39219500
C	0.24194900	1.23802800	-1.00013200
C	-1.19199700	1.09546700	-0.70783600
H	-1.53584100	1.88959100	-0.04196900
H	0.56061800	1.03792200	-2.02774700
C	-2.23444100	0.71211600	-1.72791200
C	-3.17037000	-0.33957800	0.28018500
C	-1.73864000	-0.11731000	0.66305100
C	-0.88163300	-0.19877000	1.66006500
H	2.04489100	2.34170400	-0.40114200
H	-0.62902100	3.87960300	-0.79877300
H	-3.31860100	-1.41321600	0.09541200
H	-3.85265500	-0.03418000	1.08155500
H	-2.43280700	1.54302200	-2.41061300
H	-1.91022200	-0.15268300	-2.32413100
Rh	0.19748200	-0.57256700	-0.01903600
C	2.08766800	-1.43938900	-0.19489700
N	3.39545600	-1.02905900	-0.22285000
C	4.25616400	-2.11366100	-0.31369100
C	3.89981500	0.32945500	-0.29740600
N	2.17161700	-2.80899100	-0.28675400
C	3.48703700	-3.23151600	-0.36071600
C	1.03227800	-3.70228000	-0.40538500
C	4.17947000	1.02525200	0.89625600
C	4.18199400	0.86028300	-1.57600900
C	4.74583100	2.30107100	0.77672800
C	3.93632500	0.42500300	2.27732800
C	5.02061600	2.85829100	-0.46910400
C	4.74178800	2.14345400	-1.63018100
C	3.95419300	0.08569300	-2.87300500
C	3.32299400	1.43686100	3.26255800
C	5.24105600	-0.17129400	2.84735300
C	3.19583900	0.90657400	-3.93373800
C	5.29357000	-0.42204600	-3.44868000
C	0.55948500	-4.37069700	0.74584000
C	0.47631700	-3.90498700	-1.68779600
C	-0.62983000	-4.75919800	-1.78172800
C	1.06640400	-3.30226300	-2.96044700
C	-1.14225100	-5.40099000	-0.65858000
C	-0.54397600	-5.21838700	0.58556400
C	1.24359700	-4.25733600	2.10608300
C	0.03334400	-2.49272300	-3.76520900
C	1.70360100	-4.40314800	-3.83491600
C	2.22078000	-5.43436500	2.32069500
C	0.24782000	-4.18308100	3.27819500
H	5.32643800	-1.98596400	-0.34655300
H	3.75119200	-4.27328300	-0.44882200
H	4.97912400	2.86554300	1.67319700
H	5.45272800	3.85234500	-0.53498900
H	4.97051400	2.58502700	-2.59498800
H	3.21778200	-0.39341700	2.16466400
H	5.65481700	-0.94496300	2.19099600
H	5.05890200	-0.62357100	3.82905500
H	6.00508600	0.60463800	2.97145500
H	4.02706900	2.23688100	3.51682400
H	3.05780800	0.93343900	4.19788000
H	2.41536000	1.89471700	2.85556600
H	3.33941300	-0.79155300	-2.64684700
H	5.95338300	0.41457800	-3.70467400
H	5.12146100	-1.00594900	-4.35992100
H	5.82687400	-1.05922100	-2.73503500
H	3.78297700	1.76016500	-4.28878600
H	2.24705600	1.29505800	-3.54716800
H	2.97581900	0.27948800	-4.80479700
H	-1.08753900	-4.93335500	-2.75055900
H	-1.99988000	-6.06045600	-0.75570900
H	-0.93783600	-5.74897400	1.44588000
H	1.86711100	-2.61214900	-2.67734800
H	2.47514600	-4.95506000	-3.28663500
H	2.16844900	-3.96250100	-4.72411800
H	0.95367900	-5.12678400	-4.17295900
H	-0.78650100	-3.12009600	-4.13093000
H	0.50995500	-2.03211300	-4.63798200
H	-0.40712400	-1.69513600	-3.15581600
H	1.83344500	-3.33295800	2.11247800
H	1.68374000	-6.38958400	2.31860300
H	2.73168800	-5.33615000	3.28520800
H	2.98523500	-5.48192400	1.53819000
H	-0.28367400	-5.13015100	3.42008900
H	-0.49753300	-3.39486500	3.13302800
H	0.78417700	-3.97497900	4.21041200
O	0.40503500	2.94756600	0.80790500
C	1.19293000	5.01486600	-0.38747800
C	2.17718200	5.25036700	0.58090700
C	0.97997700	5.96325000	-1.39699300
C	2.94259500	6.41556800	0.53175900

H	2.32145700	4.52785700	1.37777900
C	1.75226800	7.12353300	-1.44898500
H	0.20566200	5.79528000	-2.14268200
C	2.73634200	7.35196800	-0.48442100
H	3.69493300	6.59888400	1.29423800
H	1.57919100	7.85236600	-2.23564800
H	3.33165800	8.25995200	-0.51863000
C	-0.70535200	-0.06360500	3.07788500
C	0.37271200	-0.66741900	3.75532400
C	-1.64296300	0.69262600	3.81928500
C	0.50035400	-0.53407100	5.13392600
H	1.09790800	-1.23774100	3.18486200
C	-1.51205900	0.81647000	5.19774700
H	-2.46262700	1.18040200	3.30047600
C	-0.44178300	0.20372000	5.85818000
H	1.33101500	-1.00737900	5.64943000
H	-2.23844400	1.39648800	5.75910500
H	-0.34033200	0.30437000	6.93482300
N	-3.45195800	0.45820700	-0.93420500
S	-4.79711700	-0.07834200	-1.86069400
O	-4.68871100	0.66327100	-3.11875900
O	-4.84112300	-1.54714200	-1.84841100
C	-6.17462300	0.53305400	-0.90732700
C	-6.46951000	1.90062100	-0.93296700
C	-6.96159600	-0.36340200	-0.18363600
C	-7.56062900	2.36704100	-0.20851800
H	-5.86123600	2.57985700	-1.52095700
C	-8.05237300	0.12577100	0.53618100
H	-6.73085000	-1.42311400	-0.19979700
C	-8.36960300	1.49036800	0.53575900
H	-7.79740900	3.42780200	-0.22557300
H	-8.67156700	-0.56729500	1.09937500
C	-9.56790900	2.01137900	1.29107100
H	-9.32719700	2.92907700	1.83901100
H	-10.38727700	2.25286500	0.60199100
H	-9.94446700	1.27457900	2.00655400

VOR-**TS4** [X = NTs, R^1 = Ph, R^2 = Ph, R^3 = H]

B3LYP SCF energy in gas phase: -2992.789637 a.u.

M06 SCF energy in solution: -2991.686194 a.u.

M06 Free energy in solution: -2990.751165 a.u.

C	-1.69641600	-0.87429600	0.50327900
C	-0.66560400	-1.21768500	1.24098400
C	-1.95168600	0.94918300	-0.60223300
C	-0.96783700	1.27649300	-1.63245200
C	0.13359500	2.07969100	-1.43903500
C	0.42632900	2.72899600	-0.09481800
H	-1.12033400	0.81641300	-2.60720800
H	-2.00623000	1.62328300	0.25003600
H	0.80959400	2.26016300	-2.26934800
H	-0.52817500	3.10598300	0.31458900
C	-3.30984300	0.51196600	-1.10782600
H	-3.91015900	1.40848200	-1.30331300
H	-3.21600400	-0.04836700	-2.05081800
C	-3.07091200	-1.40499900	0.24935100
H	-3.02148900	-2.13194400	-0.58010000
H	-3.43636700	-1.92678900	1.13584600
C	4.12911100	-1.67293500	0.05536400
C	3.48610600	-2.48285400	-0.81561000
C	2.04712900	-0.83066800	-0.21103300
N	2.21091700	-1.95495900	-0.98709500
N	3.25567400	-0.64204600	0.40505500
Rh	0.21242800	-0.01546600	-0.10693900
H	3.80754800	-3.37149900	-1.33438500
H	5.13210100	-1.70599700	0.44888600
C	3.81803700	0.52151400	1.09555500
C	3.63382900	0.68815900	2.48036600
C	4.68052600	1.35266900	0.34339900
C	4.33677800	1.72511600	3.10861500
C	5.36317400	2.36452400	1.02896900
C	5.20128500	2.55001000	2.39797500
H	4.21675000	1.87042000	4.17787600
H	6.03489700	3.01586600	0.47840900
H	5.75112900	3.33459000	2.91041200
C	1.27385300	-2.43353900	-1.99642000
C	1.19835700	-1.72760400	-3.22596700
C	0.54472000	-3.62153200	-1.76900800
C	0.27604100	-2.18332200	-4.17508000
C	-0.35678500	-4.02951600	-2.76313700
C	-0.50961100	-3.30996200	-3.94178300
H	0.18664800	-1.66484600	-5.12340700
H	-0.93581400	-4.93486900	-2.61368800
H	-1.21676200	-3.64429200	-4.69557200
C	4.92837300	1.19566400	-1.15632200
H	4.27370300	0.40673900	-1.53685700
C	6.38077800	0.76287400	-1.44540400
H	6.63612400	-0.17431900	-0.93875900
H	6.52805000	0.61565400	-2.52146400
H	7.09562200	1.52363200	-1.11315200
C	4.58445600	2.48128000	-1.93441700
H	3.55535400	2.80273100	-1.74832100
H	5.24128700	3.31178600	-1.65486400
H	4.71086300	2.31272000	-3.01068600
C	2.74885100	-0.21561100	3.32203600
H	2.27220900	-0.93204500	2.65220100
C	3.57731100	-1.01854800	4.34462200
H	4.05521500	-0.36076400	5.07934400
H	2.93063200	-1.71342400	4.89174700
H	4.36817500	-1.60026800	3.85663200
C	1.62215500	0.57578100	4.01356900
H	2.02187500	1.30267000	4.73017900
H	1.02118500	1.11646700	3.27562900
H	0.96783500	-0.10734200	4.56670300
C	0.76178900	-4.52372200	-0.55879800
H	1.32768300	-3.96241900	0.18829000
C	1.61110900	-5.75171600	-0.95714600
H	1.80673900	-6.37937400	-0.08065000

H	1.08890300	-6.36457000	-1.70031400
H	2.57599000	-5.46300700	-1.38870100
C	-0.55124100	-4.98236500	0.10141700
H	-0.33267400	-5.53166600	1.02309200
H	-1.19296000	-4.13495200	0.36078600
H	-1.12208000	-5.65323900	-0.54944400
C	2.15783900	-0.59425500	-3.58886900
H	2.42935800	-0.06508800	-2.67104400
C	3.45408900	-1.17659300	-4.19834200
H	3.23382700	-1.72597200	-5.12070000
H	4.15455400	-0.37043200	-4.44479600
H	3.95933200	-1.86179000	-3.51094200
C	1.56474100	0.44749400	-4.55421700
H	1.43518000	0.04547600	-5.56480500
H	0.59084900	0.81952500	-4.21827200
H	2.24552900	1.30163100	-4.63677800
O	0.90915300	1.67862300	0.72787500
C	1.36568200	3.92192900	-0.16445400
C	2.27133500	4.17536200	0.86986300
C	1.25269100	4.84122000	-1.21659900
C	3.06052500	5.32666300	0.84420800
H	2.36115600	3.46793100	1.68651300
C	2.04409300	5.99071600	-1.24166900
H	0.53505900	4.67367400	-2.01770500
C	2.95134700	6.23633100	-0.20910100
H	3.76231400	5.51202300	1.65256200
H	1.94742700	6.69421700	-2.06392600
H	3.56474200	7.13280200	-0.22428000
C	-0.48447900	-2.02755400	2.43864000
C	0.64365500	-2.83618900	2.65891900
C	-1.50266600	-2.00513500	3.41645000
C	0.73977100	-3.62098600	3.80617800
H	1.44063200	-2.85325500	1.92533300
C	-1.39548400	-2.77883000	4.56890300
H	-2.36693400	-1.36327900	3.27424300
C	-0.27746200	-3.59433500	4.76419800
H	1.61209000	-4.25040300	3.95586600
H	-2.18478000	-2.74641900	5.31397300
H	-0.19682800	-4.20221400	5.66048300
N	-3.95642000	-0.27900100	-0.06280100
S	-5.57463800	-0.77539000	-0.42996600
O	-5.66888100	-1.07145300	-1.86523300
O	-5.87267400	-1.79572200	0.57649000
C	-6.49592200	0.71092400	-0.08916100
C	-7.00499900	1.46178100	-1.15015700
C	-6.73255000	1.07706200	1.24025400
C	-7.74984900	2.60702800	-0.86781600
H	-6.83472600	1.14201600	-2.17272500
C	-7.47770300	2.22219700	1.49869300
H	-6.34988500	0.46700000	2.05160000
C	-7.99886200	3.00410800	0.45304500
H	-8.15228300	3.19501200	-1.68825600
H	-7.66769400	2.51271200	2.52866800
C	-8.83455300	4.22422900	0.75350100
H	-9.86202400	3.93629600	1.01102100
H	-8.43322800	4.78429000	1.60473600
H	-8.88773000	4.89803800	-0.10668200

VCP-**TS1** [X = O, R^1 = H]

B3LYP SCF energy in gas phase: -1695.711476 a.u.

M06 SCF energy in solution: -1694.993812 a.u.

M06 Free energy in solution: -1694.30725 a.u.

C	-3.34583200	3.45232700	0.88915700
C	-2.49088700	2.19246800	0.71769400
C	-1.02866700	2.24358800	0.99107500
C	-0.19135000	3.31353900	0.43299400
H	-0.74210000	3.91700100	-0.28966700
H	-0.78426700	1.94443200	2.02126800
C	-3.15581200	2.84654000	-0.47011900
C	0.77930600	4.18696800	1.19551600
C	1.91048300	4.19532900	-0.85741000
C	1.04383200	2.98378300	-1.06139100
C	0.66360000	2.02380400	-1.85176900
H	-2.95809800	1.27731400	1.06479100
H	-3.98456700	2.30486900	-0.91512700
H	-2.54602500	3.38249300	-1.19333600
H	-4.30285500	3.34249400	1.39062700
H	-2.83237200	4.38508900	1.10840400
H	2.93481100	3.83637600	-0.66908300
H	1.92681600	4.83708700	-1.74360500
H	0.24717000	4.88587800	1.84980300
H	1.47591900	3.59331200	1.80747200
O	1.45003900	4.98300400	0.23085100
Rh	0.37722400	1.18384600	-0.06832100
C	0.08852100	-0.87406700	-0.03648800
N	-0.97733300	-1.72564200	-0.15134600
C	-0.56017200	-3.04812800	-0.15351300
C	-2.38286300	-1.37704000	-0.20904800
N	1.17348600	-1.71195900	0.04068700
C	0.79257900	-3.03989600	-0.03095200
C	2.55150100	-1.28277500	0.18753500
C	-2.95683100	-1.07529400	-1.45985100
C	-3.13413900	-1.44788000	0.98391400
C	-4.33178300	-0.80591700	-1.48543500
C	-2.16396300	-1.09905200	-2.76340600
C	-5.09829700	-0.84991900	-0.32387100
C	-4.50507900	-1.17296300	0.89457400
C	-2.53015400	-1.85082700	2.32868000
C	-2.32360600	0.20228200	-3.57139700
C	-2.55262100	-2.32647500	-3.61424000
C	-2.83339000	-0.83270700	3.44500900
C	-3.00338400	-3.26082000	2.74106600
C	3.35870200	-1.19457000	-0.96777600
C	3.04047600	-1.02424900	1.48548600
C	4.38018300	-0.63169800	1.59989300
C	2.19046500	-1.17731200	2.74412300
C	5.19713000	-0.51963000	0.47821000

C	4.69169900	-0.80411700	-0.78796300
C	2.85056100	-1.55354200	-2.36209900
C	2.05394900	0.15717100	3.50265500
C	2.74572600	-2.28147300	3.66653200
C	3.36351700	-2.94566700	-2.78897500
C	3.22285500	-0.49761300	-3.42016200
H	-1.26118800	-3.86352600	-0.23644400
H	1.50862400	-3.84519200	0.01402400
H	-4.81131900	-0.57706300	-2.43231700
H	-6.16486400	-0.64854600	-0.37021400
H	-5.11832900	-1.22487000	1.78908200
H	-1.10249800	-1.19497500	-2.51447500
H	-2.40023100	-3.26196900	-3.06458100
H	-1.94634800	-2.36649700	-4.52628400
H	-3.60583200	-2.28470700	-3.91397700
H	-3.35364200	0.34697200	-3.91526100
H	-1.68730100	0.17072800	-4.46364900
H	-2.04104800	1.07607100	-2.97473600
H	-1.44120900	-1.88936500	2.21921500
H	-4.08898700	-3.28696600	2.88722200
H	-2.53078800	-3.56211500	3.68253300
H	-2.75342500	-4.00994200	1.98183500
H	-3.90601200	-0.76255200	3.65540300
H	-2.47738600	0.17093800	3.18651600
H	-2.33865000	-1.13746700	4.37385900
H	4.79188900	-0.42274100	2.58266500
H	6.23540400	-0.22119500	0.59188700
H	5.34615900	-0.72927400	-1.65064100
H	1.18276000	-1.48359900	2.44482200
H	2.80872800	-3.24310200	3.14585500
H	2.09534700	-2.40943100	4.53900200
H	3.74822100	-2.03437400	4.03280500
H	3.02175900	0.51481800	3.87091100
H	1.39192500	0.03911300	4.36797700
H	1.63830000	0.94037100	2.85546700
H	1.75669500	-1.60212700	-2.32429300
H	4.45766200	-2.95912700	-2.84804000
H	2.96946600	-3.21209800	-3.77602500
H	3.06009500	-3.72565500	-2.08215500
H	4.30262900	-0.46089400	-3.59987800
H	2.90072400	0.50501100	-3.11858900
H	2.74472000	-0.74125700	-4.37554000
H	0.66751200	1.67132200	-2.87278400

VCP-**TS3** [X = O, R^1 = H]

B3LYP SCF energy in gas phase: -1695.731611 a.u.

M06 SCF energy in solution: -1695.020879 a.u.

M06 Free energy in solution: -1694.33037 a.u.

C	-1.62199200	2.54190400	0.36859600
C	-0.98621000	1.82811900	1.17993000
C	-1.08678300	2.63096600	-2.43588600
C	-1.12608900	1.26571800	-2.72647300
C	0.09339000	0.50612700	-2.94099100
C	1.31867600	1.04733100	-3.60940100
C	1.56455100	1.12521400	-2.14011900
H	2.18789000	0.35647000	-1.71024400
H	1.69405200	2.11753300	-1.71671900
H	-2.07769000	0.74606000	-2.81091000
H	-0.17817600	3.20308700	-2.61150900
H	0.00313300	-0.57312400	-2.92985100
H	1.20127800	1.99137900	-4.13610300
C	-2.34155700	3.45942900	-2.33997700
H	-2.37974900	4.15659600	-3.18355200
H	-3.23644700	2.81781900	-2.38470300
C	-2.65189700	3.54512700	-0.01145100
H	-3.62493500	3.03197600	-0.09575700
H	-2.72163200	4.27883400	0.79760600
H	1.89776500	0.31666800	-4.16902700
C	1.31015300	-1.95249100	1.77500600
C	0.00983100	-2.31658400	1.71706700
C	0.24934000	-0.45196200	0.42477000
N	-0.63289100	-1.39715700	0.89526500
N	1.45244500	-0.82026700	0.97713700
Rh	-0.34433300	1.18931900	-0.72727600
O	-2.38196700	4.27991900	-1.18175900
H	-0.52058100	-3.13593200	2.17429400
H	2.14912800	-2.38491800	2.29567700
C	2.76772300	-0.25356500	0.73035800
C	3.62340900	-0.93686100	-0.16811900
C	3.18014300	0.88960200	1.44391100
C	4.89318800	-0.39018900	-0.39035400
C	4.45851300	1.39586300	1.16853300
C	5.30296800	0.77370900	0.25540400
H	5.57507600	-0.88741500	-1.07306800
H	4.80320900	2.27914700	1.69712600
H	6.29137300	1.18140200	0.06394800
C	-2.04529400	-1.51812200	0.57324600
C	-3.00317600	-1.12167800	1.53155600
C	-2.40836400	-2.12041500	-0.65393700
C	-4.35507100	-1.24467200	1.18063400
C	-3.77382800	-2.21171900	-0.94896600
C	-4.73911800	-1.76143000	-0.05147300
H	-5.11802600	-0.94419200	1.89143300
H	-4.09069300	-2.66274000	-1.88315700
H	-5.79301300	-1.84514700	-0.30113800
C	2.34897600	1.53488700	2.54757100
H	1.36992500	1.04851300	2.55988700
C	3.24827700	-2.25603700	-0.84770900
H	2.17536400	-2.42557000	-0.70806800
C	-2.64477900	-0.67144100	2.94740100
H	-1.57454400	-0.44000100	2.97603000
C	-1.38579400	-2.77602700	-1.58177900
H	-0.42807800	-2.25942500	-1.45536300
C	3.99440400	-3.43505700	-0.18543900
H	3.68856500	-4.38455200	-0.63868000
H	5.07782000	-3.33408800	-0.31404200
H	3.79441700	-3.49344700	0.88942400

C	3.51546500	-2.25790700	-2.36579100
H	3.00168600	-1.43615100	-2.87679000
H	4.58273900	-2.17247000	-2.59490800
H	3.16423400	-3.19851400	-2.80406300
C	-1.17000500	-4.25198100	-1.17524300
H	-2.10415700	-4.81731800	-1.26689400
H	-0.42440700	-4.72358600	-1.82583600
H	-0.82158300	-4.34466100	-0.14181900
C	-1.76288700	-2.70568200	-3.07320300
H	-2.61368700	-3.35328400	-3.30950800
H	-2.02507100	-1.69022800	-3.39038500
H	-0.92372300	-3.05169000	-3.68722600
C	-2.88849600	-1.82109400	3.95090600
H	-2.58732900	-1.51729100	4.95971700
H	-3.94971300	-2.09172400	3.98339200
H	-2.32677900	-2.72364300	3.68755300
C	-3.40985300	0.58647100	3.40163000
H	-3.03415400	0.92071700	4.37529000
H	-3.29925700	1.40991500	2.68967800
H	-4.47997100	0.38815400	3.52260100
C	2.99643100	1.28315400	3.92636800
H	3.98306900	1.75425400	3.99541500
H	2.37031000	1.70202400	4.72230600
H	3.12381000	0.21260400	4.12156200
C	2.12351900	3.04017600	2.31339100
H	3.06659900	3.59711100	2.33404400
H	1.63762300	3.22724300	1.35015700
H	1.48501100	3.45379100	3.10242200
H	-0.76345800	1.46980000	2.16460200

VCP-**TS4** [X = O, R^1 = H]

B3LYP SCF energy in gas phase: -1695.743336 a.u.

M06 SCF energy in solution: -1695.014462 a.u.

M06 Free energy in solution: -1694.324132 a.u.

C	-2.14094800	-2.35954100	-1.10054800
C	-2.18897100	-1.07250700	-1.02482800
C	-0.34800400	-3.44050500	-1.25749300
C	0.87198500	-3.14565400	-0.50228900
C	1.87789800	-2.31258100	-0.95249800
C	1.84422600	-1.67175900	-2.33187300
C	0.59693700	-0.78192900	-2.35480100
H	0.81822700	0.28163500	-2.42500000
H	-0.15743200	-1.05338200	-3.09867200
H	0.97606400	-3.62182900	0.47204900
H	-0.26195800	-3.32884000	-2.33783700
H	2.77148900	-2.20734800	-0.34656500
H	1.82791300	-2.43752600	-3.12005900
C	-1.07262800	-4.72559800	-0.88961100
H	-0.52557300	-5.58488300	-1.28933700
H	-1.14762400	-4.83489500	0.20572000
C	-3.02964600	-3.57558900	-1.09722100
H	-3.43623700	-3.70263200	-0.07942900
H	-3.86443800	-3.42264700	-1.78743100
H	2.75397100	-1.08586400	-2.47554100
C	1.16432500	2.43273100	1.28150700
C	-0.16376300	2.68582000	1.28626300
C	0.13710300	0.67335200	0.24890600
N	-0.77884800	1.61587000	0.65235100
N	1.34291300	1.21225100	0.64320400
Rh	-0.24063600	-1.18768500	-0.51003400
O	-2.34202500	-4.73390400	-1.50034700
H	-0.73315100	3.51484000	1.67515400
H	1.99827400	2.99374100	1.67044200
C	2.67497400	0.65668700	0.50397000
C	3.48362700	1.10366900	-0.56432100
C	3.15028500	-0.21128500	1.51128800
C	4.78319600	0.58418500	-0.64460300
C	4.46011000	-0.69054300	1.38061100
C	5.26380700	-0.31060700	0.30762800
H	5.43495200	0.90038700	-1.45264600
H	4.86275200	-1.35860300	2.13525600
H	6.27702600	-0.69405700	0.22758600
C	-2.21814700	1.59728900	0.49629100
C	-2.99799500	0.99691700	1.50512400
C	-2.77846900	2.24234700	-0.62522100
C	-4.38911000	1.01885100	1.33907700
C	-4.17531100	2.23255500	-0.73751300
C	-4.97340600	1.62234000	0.22827100
H	-5.02322400	0.56589600	2.09520600
H	-4.64479900	2.71666000	-1.58855300
H	-6.05436300	1.63002200	0.12129800
C	2.32582900	-0.56987900	2.74652600
H	1.27376500	-0.35702700	2.52866000
C	2.74203300	0.31419900	3.94282700
H	2.62183600	1.37989800	3.72128300
H	2.13047200	0.08107100	4.82180000
H	3.79174800	0.14404500	4.20740000
C	2.41635400	-2.05816200	3.13125900
H	2.16089600	-2.71245300	2.29065600
H	3.41800100	-2.33425500	3.47761200
H	1.72226400	-2.27305400	3.95112300
C	3.03687700	2.18582200	-1.54876100
H	1.94639800	2.27537800	-1.48823000
C	3.63893400	3.55118800	-1.14585300
H	4.73324000	3.52341400	-1.19485000
H	3.29049700	4.33633800	-1.82602200
H	3.36042100	3.84004800	-0.12726900
C	3.39193500	1.87968700	-3.01593100
H	4.47451800	1.85983500	-3.18031400
H	2.98346200	0.92120400	-3.35076600
H	2.98324200	2.66195800	-3.66466800
C	-1.93871500	2.94846100	-1.68740400
H	-0.88212600	2.77217800	-1.46126100
C	-2.16933300	4.47331000	-1.64757400
H	-1.52904700	4.97445400	-2.38202400
H	-3.20897900	4.72604600	-1.88375800
H	-1.94228400	4.88947900	-0.65977200

C	-2.19731400	2.39104100	-3.10093500
H	-1.54691900	2.89207100	-3.82668800
H	-1.99632900	1.31511300	-3.15212300
H	-3.23199400	2.55636900	-3.42078800
C	-2.39466600	0.37143900	2.75998600
H	-1.30452700	0.37873100	2.65550800
C	-2.74100100	1.20607700	4.01054600
H	-3.82215500	1.22783200	4.18757900
H	-2.26536500	0.77690000	4.89954100
H	-2.39956900	2.24216100	3.90977000
C	-2.82409100	-1.09686400	2.94608400
H	-3.90382100	-1.18730300	3.10827200
H	-2.56626300	-1.70236200	2.06941000
H	-2.32428700	-1.52783500	3.82102200
H	-2.93609500	-0.30046300	-1.12864100

VCP-**TS1** [X = O, R^1 = Ph]

B3LYP SCF energy in gas phase: -1926.773251 a.u.

M06 SCF energy in solution: -1925.938943 a.u.

M06 Free energy in solution: -1925.176972 a.u.

C	2.09465400	-2.87254800	3.23410900
C	1.79047500	-1.88255800	2.10924100
C	0.89202300	-0.71520300	2.35474000
C	-0.37566000	-0.88950500	3.07749600
H	-0.57657300	-1.93711700	3.30933000
H	1.45303000	0.19080900	2.61420500
C	-0.85047200	-0.00679600	4.21464700
C	-2.93610200	-0.45076200	3.27895000
C	-2.03620300	-0.86106300	2.14177400
C	-1.99444200	-1.42280900	0.95264800
H	2.63898700	-1.63947700	1.47975500
H	1.56113900	-2.75470300	4.17431800
H	-3.37549800	0.52846200	3.03094700
H	-3.75065800	-1.16343100	3.43947100
H	-0.27970900	-0.20963100	5.12695000
H	-0.75267000	1.06122300	3.96656800
Rh	-0.48469600	-0.06256600	0.95679300
C	0.56257700	0.74085000	-0.67194200
N	1.69900900	0.46360500	-1.38929500
C	1.85982800	1.35793400	-2.43733200
C	2.72365500	-0.51993800	-1.09173900
N	0.03840500	1.84330700	-1.30735900
C	0.82013200	2.22875700	-2.38216400
C	-1.12749500	2.59087400	-0.86976400
C	2.60022200	-1.82219100	-1.61685000
C	3.85842500	-0.09166400	-0.36818800
C	3.64903600	-2.71688600	-1.36668000
C	1.42549600	-2.24829300	-2.49219700
C	4.77299000	-2.33005400	-0.64165600
C	4.87623000	-1.03034300	-0.15355900
C	4.03716900	1.33764200	0.14035000
C	0.90625700	-3.65700100	-2.15412900
C	1.80605600	-2.15586900	-3.98602200
C	4.40959500	1.39420500	1.63456100
C	5.08594300	2.09217300	-0.70412200
C	-2.36744300	2.36292900	-1.50702500
C	-0.95365200	3.57412700	0.12910800
C	-2.08593500	4.29739300	0.52517200
C	0.40442400	3.92178900	0.73385500
C	-3.32751400	4.07112100	-0.06102200
C	-3.46088300	3.12246500	-1.07142500
C	-2.53338000	1.39292700	-2.67442100
C	0.40390200	3.82293200	2.27065200
C	0.86480200	5.32137400	0.27467900
C	-2.46467100	2.14654900	-4.02137600
C	-3.83655400	0.57595700	-2.59830000
H	2.69878400	1.29586000	-3.11204600
H	0.57377700	3.08123300	-2.99463400
H	3.59260400	-3.72706300	-1.75869400
H	5.57697100	-3.03984800	-0.46831800
H	5.76556600	-0.73564800	0.39494100
H	0.60290900	-1.54782000	-2.31474600
H	2.11611000	-1.14284900	-4.26526900
H	0.95340500	-2.43337500	-4.61640400
H	2.63359000	-2.83456400	-4.22190400
H	1.64059900	-4.43360500	-2.39408100
H	0.00672900	-3.87433500	-2.73925400
H	0.64708700	-3.74590900	-1.09422400
H	3.08424500	1.86455800	0.02755300
H	6.07242600	1.62281200	-0.61892500
H	5.17733500	3.12957900	-0.36320100
H	4.81663000	2.10738400	-1.76578700
H	5.39698100	0.96103500	1.82789600
H	3.68397700	0.85609100	2.25440400
H	4.44043100	2.43576000	1.97333400
H	-1.98928100	5.06071800	1.29123800
H	-4.19098900	4.64854900	0.25690700
H	-4.43013000	2.97598300	-1.53604400
H	1.14163700	3.20216300	0.36499600
H	0.91390600	5.38946600	-0.81763000
H	1.86050500	5.54449700	0.67413200
H	0.18080800	6.10166900	0.62631000
H	-0.27514800	4.55130800	2.72699200
H	1.40810600	4.01869300	2.66341200
H	0.09315300	2.82526800	2.60260200
H	-1.69712100	0.68427300	-2.64819800
H	-3.28076900	2.87347900	-4.10132600
H	-2.55581300	1.44386700	-4.85735300
H	-1.52251100	2.69138500	-4.14159100
H	-4.72010300	1.20422400	-2.75399800
H	-3.94613300	0.06964900	-1.63430200
H	-3.84387800	-0.18661300	-3.38456300
C	-2.59275800	-2.41306100	0.09980300
C	-2.41251800	-2.39999900	-1.29749200
C	-3.38616900	-3.43211400	0.67740800
C	-3.01760600	-3.36675100	-2.09427500
H	-1.79656500	-1.62444000	-1.74023800

C	-3.99370400	-4.39041000	-0.12612400
H	-3.51726700	-3.45988300	1.75525800
C	-3.81091400	-4.36101400	-1.51282800
H	-2.87695600	-3.34614800	-3.17108900
H	-4.60535500	-5.16507000	0.32664800
H	-4.28373000	-5.11282400	-2.13784500
O	-2.19249800	-0.37264700	4.48757700
H	3.12227500	-3.20578700	3.34611400
H	1.80110500	-3.95145600	1.30081400
H	0.25155200	-3.52043600	2.14984300
C	1.31183000	-3.31178400	2.02927500

VCP-**TS3** [X = O, R^1 = Ph]

B3LYP SCF energy in gas phase: -1926.775351 a.u.

M06 SCF energy in solution: -1925.952152 a.u.

M06 Free energy in solution: -1925.1861 a.u.

C	2.29435500	0.48954100	1.52425300
C	1.74642800	1.33087700	0.75807900
C	0.97486800	-0.96410700	3.62791900
C	0.29016200	-1.85021300	2.81363800
C	-1.11355200	-1.69981600	2.47165300
C	-2.13778000	-1.13230000	3.40913400
C	-1.80557400	-0.00787600	2.49186500
H	-2.51084500	0.18623600	1.69811100
H	-1.32866800	0.86594000	2.92888200
H	0.82278800	-2.69944100	2.39195100
H	0.44629600	-0.20300000	4.19804900
H	-1.49911800	-2.33997800	1.68797400
H	-1.82117500	-1.02884200	4.44505200
C	2.41186400	-1.20524300	4.01444200
H	2.49152300	-1.28154400	5.10340500
H	2.76683900	-2.15224900	3.57691600
C	3.47380600	-0.04523400	2.25618100
H	3.77473100	-1.01600600	1.83142800
H	4.29986200	0.66087700	2.11879700
H	-3.13239100	-1.56272500	3.31413400
C	-1.44208800	0.23624900	-2.53217300
C	-0.35298800	-0.52752000	-2.77332900
C	-0.44259200	-0.16223300	-0.52374100
N	0.25025800	-0.78280700	-1.54437100
N	-1.51218700	0.43932800	-1.15382000
Rh	0.27097900	-0.16746200	1.38343800
O	3.29059900	-0.14775300	3.65277800
H	0.04745100	-0.92163800	-3.69341000
H	-2.18900400	0.63999500	-3.19678800
C	-2.75192200	0.93973700	-0.56319300
C	-3.86256300	0.05732000	-0.54295200
C	-2.85042200	2.26884100	-0.10077400
C	-5.06368600	0.53484600	-0.00338300
C	-4.07794200	2.68399300	0.43446900
C	-5.17336900	1.83059400	0.49137500
H	-5.93027200	-0.11845900	0.02109900
H	-4.17594100	3.70184500	0.79802100
H	-6.11553000	2.17798300	0.90557000
C	1.32082500	-1.76639200	-1.39963800
C	2.64385500	-1.43156100	-1.76131900
C	0.97021500	-3.07865000	-0.99114400
C	3.63474600	-2.40849200	-1.58272800
C	2.00482700	-4.00718500	-0.82698500
C	3.32935600	-3.67346300	-1.09734400
H	4.66062800	-2.17343600	-1.84696600
H	1.76933300	-5.01707100	-0.50935500
H	4.11482100	-4.41224800	-0.96540800
C	-1.71834300	3.27584000	-0.21232700
H	-0.81404300	2.73196300	-0.47926100
C	-3.83690900	-1.36434600	-1.10430100
H	-2.80700700	-1.61865700	-1.36562400
C	3.02998600	-0.11709800	-2.42994200
H	2.20761200	0.58632200	-2.29778800
C	-0.47760000	-3.55080900	-0.86396900
H	-1.09485400	-2.69233800	-0.58412100
C	-4.67433200	-1.45996600	-2.39754900
H	-4.61640800	-2.47079000	-2.81661900
H	-5.72929300	-1.23717700	-2.20336400
H	-4.32307200	-0.75722000	-3.16049200
C	-4.31731000	-2.41245600	-0.08107900
H	-3.74027500	-2.36736700	0.84984300
H	-5.37280500	-2.27922600	0.17844800
H	-4.21014700	-3.42062100	-0.49694000
C	-0.98414600	-4.06342500	-2.23212100
H	-0.39147900	-4.92342000	-2.56362600
H	-2.03024800	-4.38346700	-2.15908400
H	-0.92076900	-3.29347400	-3.00722000
C	-0.69434800	-4.64347200	0.19954000
H	-0.25615200	-5.60057200	-0.10216100
H	-0.26303700	-4.37545200	1.17014600
H	-1.76691700	-4.81777700	0.33957300
C	3.22043400	-0.33030600	-3.94872000
H	3.44886900	0.62222600	-4.43990400
H	4.04910200	-1.01902300	-4.14851600
H	2.32508000	-0.74891300	-4.42199800
C	4.28925400	0.53419500	-1.82983300
H	4.44757000	1.51845100	-2.28282200
H	4.19493100	0.67279300	-0.74898700
H	5.18908300	-0.06044300	-2.02132000
C	-2.00712900	4.28411700	-1.34407800
H	-2.89854800	4.88302800	-1.12494000
H	-1.16067600	4.96850200	-1.46488200
H	-2.17449500	3.77758700	-2.30168400
C	-1.42755000	4.00869700	1.11024100
H	-2.25821800	4.65384100	1.41719200
H	-1.22828800	3.30347800	1.92495100
H	-0.54355000	4.64424700	0.99384000
C	1.91465700	2.57612100	0.02328700
C	1.44466200	2.81447100	-1.27831900
C	2.64898600	3.59270500	0.67101900
C	1.72529800	4.01904600	-1.92420500

H	0.86309900	2.05877400	-1.79266400
C	2.91411100	4.79847900	0.02599000
H	3.00555300	3.42761300	1.68333800
C	2.45864700	5.01540700	-1.27699600
H	1.36545800	4.17854700	-2.93666500
H	3.48108600	5.56778100	0.54221300
H	2.67098200	5.95323700	-1.78158600

VCP-**TS4** [X = O, R^1 = Ph]

B3LYP SCF energy in gas phase: -1926.795258 a.u.

M06 SCF energy in solution: -1925.95722 a.u.

M06 Free energy in solution: -1925.188987 a.u.

C	2.47688900	0.57530700	1.81758000
C	1.86259400	1.23148600	0.86538900
C	1.64866400	-0.66271200	3.13683200
C	0.66045700	-1.70397700	2.79477800
C	-0.70927500	-1.50659500	2.77371700
C	-1.35815700	-0.19904300	3.20730800
H	1.05890200	-2.68189600	2.52858300
H	1.27384400	0.10774600	3.80985200
H	-1.34236700	-2.36134900	2.55291600
H	-1.20834300	-0.01875200	4.28190400
C	3.00078400	-1.19442200	3.60532200
H	2.92458100	-1.54598700	4.63821900
H	3.32769200	-2.03329000	2.96741900
C	3.90098100	0.41339300	2.29532700
H	4.44184700	-0.23574300	1.58466700
H	4.40303600	1.38338100	2.32719600
C	-1.99592600	-0.03776900	-2.38441500
C	-1.00886200	-0.89530400	-2.72638100
C	-0.64948300	-0.25884500	-0.56512900
N	-0.19415500	-1.03635600	-1.60683400
N	-1.78593800	0.33619900	-1.05542500
Rh	0.48532200	-0.25837400	1.11457000
H	-0.80703500	-1.41913800	-3.64690700
H	-2.83812900	0.33704000	-2.94326400
C	-2.83913400	1.03984500	-0.33202400
C	-2.81507100	2.44790800	-0.24982400
C	-3.91739000	0.27244000	0.16934400
C	-3.87889900	3.07584000	0.41198900
C	-4.94919900	0.95773300	0.82364300
C	-4.92929500	2.34286900	0.95424400
H	-3.88726500	4.15768700	0.49438200
H	-5.79110900	0.39843500	1.21927800
H	-5.74304600	2.85268300	1.46203200
C	0.88561500	-2.00858800	-1.51133300
C	0.61326400	-3.25880000	-0.89371600
C	2.13196100	-1.73047200	-2.11660500
C	1.66839700	-4.17296900	-0.79335500
C	3.14412100	-2.69326700	-1.99206100
C	2.92649800	-3.89016900	-1.32075700
H	1.49709500	-5.13395800	-0.32122300
H	4.11230400	-2.50500600	-2.44439000
H	3.72667200	-4.62015700	-1.23676100
C	-4.05343600	-1.23369500	-0.05068000
H	-3.09028500	-1.62070400	-0.39447400
C	-5.08850000	-1.52283900	-1.16043200
H	-4.82280100	-1.03162400	-2.10221400
H	-5.15591700	-2.60032300	-1.34910500
H	-6.08409300	-1.16894800	-0.87031700
C	-4.42505900	-2.00685400	1.22856000
H	-3.71531500	-1.81818100	2.04058400
H	-5.42362800	-1.74322400	1.59251400
H	-4.43144900	-3.08370300	1.02507600
C	-1.72234800	3.29544300	-0.88816100
H	-0.87707400	2.64032900	-1.10972900
C	-2.21226800	3.89127800	-2.22526600
H	-3.07013700	4.55550700	-2.07029200
H	-1.41418700	4.47678100	-2.69575400
H	-2.51963600	3.11013600	-2.92986900
C	-1.20456900	4.40654400	0.04312400
H	-1.96527900	5.17193200	0.23196800
H	-0.88219400	4.00457700	1.00951300
H	-0.34579600	4.90519600	-0.41675400
C	2.39295400	-0.49545400	-2.97161000
H	1.57943300	0.21459800	-2.80074700
C	2.36953500	-0.86924200	-4.47042200
H	2.51444000	0.02483600	-5.08702500
H	3.17002400	-1.57747000	-4.71168400
H	1.42054100	-1.33207400	-4.76323600
C	3.71456100	0.21198500	-2.61939400
H	3.80121700	1.14560600	-3.18472200
H	3.76937300	0.45793600	-1.55463800
H	4.58416700	-0.40384200	-2.87293300
C	-0.79337000	-3.67990900	-0.46922500
H	-1.33696100	-2.78439800	-0.15510900
C	-1.54494000	-4.29338500	-1.67356400
H	-1.03100100	-5.19307800	-2.03018100
H	-2.56230500	-4.57943200	-1.38258300
H	-1.62014300	-3.59400800	-2.51148200
C	-0.82601100	-4.67157800	0.70746800
H	-0.45536400	-5.66158200	0.42074300
H	-0.23070400	-4.32814200	1.55999300
H	-1.85881300	-4.80640800	1.04682700
C	2.13842500	2.46665500	0.13722200
C	1.74501200	2.65702300	-1.19751500
C	2.83276000	3.50957000	0.78662700
C	2.06913800	3.83025800	-1.87700100
H	1.19015200	1.87356100	-1.69942500
C	3.14544100	4.68578300	0.11020300
H	3.11197600	3.39698100	1.83022700
C	2.77253000	4.84776100	-1.22721500
H	1.76864900	3.95306800	-2.91387300
H	3.67883100	5.47795300	0.62756100
H	3.02105700	5.76344700	-1.75563600
H	-2.43680800	-0.25685300	3.04177200
C	-0.73777800	0.88865900	2.32593000

H	-0.08291800	1.59251200	2.84729200
H	-1.45793200	1.43233900	1.72291400
O	3.93546000	-0.14230200	3.58749000

VCP-**TS1** [X = NTs, R^1 = H]

B3LYP SCF energy in gas phase: -2494.779378 a.u.

M06 SCF energy in solution: -2493.905399 a.u.

M06 Free energy in solution: -2493.103978 a.u.

C	-0.13443400	-4.34124700	1.10648100
C	0.66660300	-3.06137800	0.85275500
C	0.05471300	-1.72896200	1.11660600
C	-1.30382400	-1.41229700	0.64470200
H	-1.72082600	-2.22126900	0.04374700
H	0.29896700	-1.34552100	2.11700800
C	-2.36557600	-0.74987300	1.48294500
C	-3.02472500	-0.02329800	-0.79225200
C	-1.57441500	-0.33968600	-0.96950300
C	-0.57127600	-0.38666400	-1.79995600
H	1.71127200	-3.11524900	1.14056800
H	-1.17972500	-4.23715800	1.38653000
H	-3.14008800	1.06446800	-0.89521100
H	-3.63416900	-0.50545400	-1.56597300
H	-2.73054600	-1.42965500	2.25862100
H	-1.97493300	0.15080500	1.97816800
Rh	0.36965000	-0.08730900	-0.07569400
C	2.35277700	0.50546000	-0.15411000
N	3.57319600	-0.10472300	-0.26490100
C	4.59142800	0.83266900	-0.35221300
C	3.84870600	-1.52726300	-0.25334900
N	2.65027900	1.84525800	-0.16791100
C	4.01105700	2.05963900	-0.28926500
C	1.66939700	2.90869600	-0.05499500
C	3.78099700	-2.24105400	-1.46623600
C	4.26050100	-2.11565800	0.96180300
C	4.11471600	-3.60144600	-1.42851900
C	3.43029000	-1.58185100	-2.79727300
C	4.50862000	-4.21612700	-0.24286200
C	4.58474200	-3.47849300	0.93637100
C	4.40702400	-1.32626800	2.26204900
C	2.32364300	-2.33889200	-3.55466900
C	4.68975000	-1.42620600	-3.67539300
C	3.66393400	-1.98143700	3.44229900
C	5.89616800	-1.11916400	2.61078500
C	1.16781000	3.49445900	-1.23776300
C	1.28338900	3.33149200	1.23433600
C	0.33250400	4.35685000	1.31504400
C	1.87718400	2.75011400	2.51487100
C	-0.19530300	4.94172300	0.16752600
C	0.22493200	4.51975000	-1.09164900
C	1.65389200	3.09269300	-2.62850700
C	0.79395700	2.14654100	3.42961700
C	2.70818600	3.80759600	3.27004900
C	2.68387200	4.11301000	-3.15948900
C	0.50386000	2.91761100	-3.63811800
H	5.62498300	0.53928300	-0.44567300
H	4.43536900	3.05087700	-0.31523800
H	4.08250100	-4.18279300	-2.34478600
H	4.77268300	-5.26995700	-0.24034000
H	4.91215900	-3.96542000	1.84988600
H	3.04882900	-0.57739900	-2.58901300
H	5.46384900	-0.83885900	-3.16912800
H	4.44071700	-0.92005600	-4.61497600
H	5.12213500	-2.40187100	-3.92436200
H	2.65190600	-3.33461800	-3.87242200
H	2.04460800	-1.78765000	-4.46034100
H	1.43029100	-2.46071400	-2.93306500
H	3.96317000	-0.33614700	2.11421000
H	6.39714800	-2.07781800	2.78597700
H	5.99557300	-0.51689700	3.52071200
H	6.43372900	-0.60669000	1.80537900
H	4.08443500	-2.95981200	3.69872700
H	2.59954100	-2.12215900	3.22362100
H	3.74523500	-1.34888300	4.33311500
H	0.00689100	4.70633400	2.29009600
H	-0.92982700	5.73709400	0.25440900
H	-0.18336800	4.99910600	-1.97554100
H	2.55995100	1.93886600	2.24092100
H	3.50484800	4.21631700	2.63882900
H	3.17218900	3.36414300	4.15820400
H	2.08438600	4.64452400	3.60267300
H	0.08686400	2.90653800	3.77880000
H	1.25267700	1.68917700	4.31352200
H	0.21406800	1.37525600	2.90740200
H	2.16092500	2.12485100	-2.54541800
H	2.23257200	5.10619900	-3.26402100
H	3.05578400	3.80590700	-4.14347300
H	3.54422800	4.20874400	-2.48818000
H	0.01389400	3.86921300	-3.86998300
H	-0.26158500	2.23023900	-3.26180800
H	0.89319900	2.51757700	-4.58106200
N	-3.47195200	-0.48099700	0.54340900
S	-4.77161500	0.41943700	1.22219900
O	-4.80778400	-0.00401400	2.62318400
O	-4.61509500	1.83456300	0.85921500
C	-6.18519600	-0.22887000	0.35083100
C	-6.68039400	-1.49161500	0.69449700
C	-6.80080600	0.54666800	-0.63246300
C	-7.79845500	-1.97951500	0.02748900
H	-6.20556000	-2.07060600	1.47961500
C	-7.92162400	0.03788800	-1.28930600
H	-6.41774600	1.53483100	-0.86314100
C	-8.43759100	-1.22566200	-0.97251400
H	-8.19068400	-2.95839800	0.29096300
H	-8.40752200	0.63823000	-2.05374800
C	-9.66872300	-1.75938700	-1.66304600
H	-9.88865700	-1.20515000	-2.58016500
H	-9.55517000	-2.81789900	-1.92122700

H	-10.54667000	-1.67902300	-1.00928100
C	0.26462500	-3.96237000	-0.29007400
H	0.37763100	-5.16251700	1.59921300
H	1.06261800	-4.52121400	-0.76928300
H	-0.50927900	-3.62994900	-0.97797100
H	-0.29310500	-0.36407800	-2.84361000

VCP-**TS3** [X = NTs, R^1 = H]

B3LYP SCF energy in gas phase: -2494.796089 a.u.

M06 SCF energy in solution: -2493.929919 a.u.

M06 Free energy in solution: -2493.123274 a.u.

C	-1.50862400	-0.45390700	0.40221400
C	-0.62692700	0.00399100	1.16925700
C	-1.27712400	-0.46076200	-2.44076000
C	-0.02627000	-1.06012900	-2.59335300
C	1.15742200	-0.27892200	-2.90706800
C	1.16531500	0.92673600	-3.79491700
C	1.15824100	1.42259100	-2.38828400
H	2.10079900	1.75804000	-1.98321000
H	0.28863400	1.99358100	-2.07514000
H	0.08310100	-2.13703600	-2.49007400
H	-1.45231200	0.55458800	-2.78973400
H	2.11222300	-0.77530200	-2.78621500
H	0.26427300	1.09913400	-4.37864000
C	-2.52070000	-1.28761200	-2.26926400
H	-3.10849400	-1.23612500	-3.19090600
H	-2.26197000	-2.34370400	-2.09068500
C	-2.82763700	-1.07354200	0.13980200
H	-2.75078900	-2.16321800	0.28666400
H	-3.52002200	-0.68755300	0.89576200
H	2.07895700	1.07054500	-4.36664400
C	3.74228800	0.62359500	1.82337600
C	3.54815000	-0.70577300	1.97174900
C	1.98997600	0.04379900	0.48363300
N	2.47875700	-1.05378500	1.15370700
N	2.79566500	1.07335300	0.90662900
Rh	0.28638700	-0.03913500	-0.72498500
H	4.06268000	-1.43719200	2.57348500
H	4.45679400	1.29501200	2.27122800
C	2.82313800	2.44688800	0.43466500
C	3.80963700	2.79969700	-0.51829900
C	1.94289400	3.39372100	0.99510000
C	3.83825100	4.13014300	-0.95377000
C	2.01386100	4.70797200	0.51169700
C	2.94052800	5.07296900	-0.45891900
H	4.58027300	4.43573500	-1.68452700
H	1.34588200	5.46006600	0.92003800
H	2.98058400	6.09878700	-0.81380200
C	2.03456600	-2.43277600	1.02771700
C	1.24530800	-2.99410000	2.05419000
C	2.49346800	-3.19197300	-0.07430200
C	0.83660600	-4.32633000	1.89856700
C	2.04863000	-4.51532800	-0.17583400
C	1.21390400	-5.07410100	0.78924900
H	0.22446200	-4.78772500	2.66677000
H	2.37425000	-5.12712300	-1.01010100
H	0.88277200	-6.10383100	0.68960800
C	0.99721900	3.07508500	2.14806000
H	1.02572800	1.99511200	2.31631400
C	4.86592100	1.81938400	-1.03422200
H	4.55698800	0.80394100	-0.76335500
C	0.90145800	-2.26162800	3.35008900
H	1.11446300	-1.19637400	3.21062100
C	3.52879000	-2.65862500	-1.06391300
H	3.40617900	-1.57178000	-1.12986100
C	6.22850200	2.08762900	-0.35773000
H	6.97285800	1.35730400	-0.69422500
H	6.59874300	3.08732500	-0.61080400
H	6.16399800	2.02539100	0.73327600
C	5.03480300	1.85168400	-2.56610800
H	4.08852400	1.68271500	-3.09146300
H	5.43831500	2.80837700	-2.91387200
H	5.73818900	1.07202300	-2.87829800
C	4.95807100	-2.93234500	-0.54202700
H	5.13070700	-4.00929400	-0.43689400
H	5.70367300	-2.53794900	-1.24219400
H	5.13385200	-2.46782900	0.43320300
C	3.38423100	-3.23223700	-2.48559000
H	3.67160000	-4.28799500	-2.53052200
H	2.35939400	-3.15463200	-2.86541000
H	4.04735000	-2.69590600	-3.17375000
C	1.80084700	-2.76067700	4.50314200
H	1.58417500	-2.20705600	5.42368700
H	1.62696000	-3.82422000	4.70087300
H	2.86558600	-2.63759200	4.27766000
C	-0.58080900	-2.39412300	3.74917300
H	-0.79079100	-1.76259200	4.61988200
H	-1.24807600	-2.09310200	2.93614000
H	-0.83513800	-3.42161200	4.02969900
C	1.48608200	3.74945200	3.44784900
H	1.47650100	4.84140200	3.35846800
H	0.83464200	3.47714400	4.28602700
H	2.50815100	3.44516900	3.69922700
C	-0.46092500	3.46279600	1.84129200
H	-0.57215500	4.54430100	1.70683100
H	-0.82334500	2.96699800	0.93490000
H	-1.11246300	3.17075300	2.67302600
N	-3.36414200	-0.75304700	-1.18810400
S	-5.03693000	-1.19205500	-1.34851100
O	-5.33319300	-1.01551500	-2.77169400
O	-5.26684600	-2.47847400	-0.67835600
C	-5.84009600	0.09050800	-0.40263400
C	-6.44034800	-0.23382900	0.81530700
C	-5.90511900	1.38782600	-0.92074800
C	-7.10031000	0.76619700	1.52948000
H	-6.40178100	-1.25373400	1.18301300
C	-6.56766700	2.37018400	-0.19194500

H	-5.45624800	1.61646500	-1.88163200
C	-7.17641600	2.07762500	1.04068700
H	-7.57154300	0.51945200	2.47719700
H	-6.62418300	3.38052900	-0.58868200
C	-7.92552600	3.14490400	1.80072200
H	-7.46564400	4.12976000	1.66925100
H	-8.96109500	3.21972900	1.44413000
H	-7.96452500	2.92372500	2.87175400
H	-0.25151600	0.24765500	2.14316700

VCP-**TS4** [X = NTs, R^1 = H]

B3LYP SCF energy in gas phase: -2494.810258 a.u.

M06 SCF energy in solution: -2493.925397 a.u.

M06 Free energy in solution: -2493.118631 a.u.

C	1.36110400	-0.03519600	1.28511900
C	0.14478000	-0.13430800	1.72145600
C	1.88408100	-0.44947100	-0.64863500
C	1.06489700	-0.12940200	-1.83766800
C	0.14012200	-0.98792900	-2.40106700
C	-0.09319400	-2.39310500	-1.86555100
H	1.22133900	0.85007300	-2.28770800
H	2.04525100	-1.51498000	-0.49014700
H	-0.36133300	-0.67696700	-3.31332600
H	0.80883000	-3.01121800	-1.97955800
C	3.18261400	0.32876800	-0.54093700
H	3.88467600	-0.03805700	-1.29773600
H	3.02279600	1.40442400	-0.71412500
C	2.70543200	0.40306800	1.78493400
H	2.66778600	1.49083700	1.96279200
H	2.93048300	-0.08627600	2.73552300
C	-4.61631900	0.46454000	0.46264800
C	-4.11477700	1.70405700	0.25909400
C	-2.39655700	0.22322700	0.04512600
N	-2.75745600	1.54550400	0.00447700
N	-3.56039500	-0.43785400	0.32603500
Rh	-0.43238800	-0.16321100	-0.19083300
H	-4.58371500	2.67468700	0.27083100
H	-5.61523800	0.12748600	0.68770400
C	-3.78549200	-1.86667900	0.42756100
C	-3.59084400	-2.50173500	1.67156600
C	-4.27177900	-2.54657200	-0.71120000
C	-3.85178500	-3.87668600	1.73759500
C	-4.51561200	-3.91967500	-0.58239400
C	-4.30069200	-4.58098300	0.62397600
H	-3.71261500	-4.40132400	2.67762000
H	-4.89076900	-4.47722200	-1.43484900
H	-4.49884400	-5.64627100	0.70045100
C	-1.83818700	2.63115700	-0.27646600
C	-1.59986500	2.98137200	-1.62757500
C	-1.26606100	3.33597400	0.80742900
C	-0.71375200	4.03821700	-1.86897500
C	-0.38859500	4.38452900	0.49949700
C	-0.10741400	4.72637400	-0.81993800
H	-0.50637100	4.33953200	-2.89024600
H	0.07079100	4.94913700	1.30395500
H	0.57315800	5.54592700	-1.03274200
C	-4.59606700	-1.83883800	-2.02592300
H	-4.14705100	-0.84021500	-1.99878200
C	-6.12215300	-1.65834100	-2.17867600
H	-6.55081000	-1.09622000	-1.34217300
H	-6.35320400	-1.11757700	-3.10332700
H	-6.62931100	-2.62878900	-2.22024800
C	-4.02069200	-2.55999000	-3.25885700
H	-2.93736400	-2.69873200	-3.17786600
H	-4.47299700	-3.54623400	-3.40772400
H	-4.22100700	-1.97243000	-4.16171600
C	-3.17361300	-1.74795800	2.93142200
H	-2.82908300	-0.75234700	2.63336500
C	-4.38355600	-1.55415500	3.87028900
H	-4.78061300	-2.51899900	4.20531100
H	-4.09130500	-0.98389600	4.75940900
H	-5.19668400	-1.01374000	3.37323600
C	-2.01213900	-2.43366300	3.67514800
H	-2.30677800	-3.40513900	4.08594900
H	-1.15123400	-2.59543300	3.01740400
H	-1.68875800	-1.81408500	4.51994800
C	-1.63387200	3.05327400	2.26247500
H	-2.05721100	2.04432600	2.31578200
C	-2.72060600	4.04116500	2.74214900
H	-3.00856100	3.81852600	3.77565400
H	-2.35060000	5.07208900	2.70938200
H	-3.62231600	3.99143700	2.12302700
C	-0.42571000	3.09969400	3.21639800
H	-0.72904800	2.76935200	4.21608900
H	0.38719600	2.45165100	2.87370500
H	-0.02614800	4.11376700	3.32292000
C	-2.33615200	2.31112700	-2.78656300
H	-2.61600900	1.30045500	-2.46973900
C	-3.63675700	3.07941000	-3.11259000
H	-3.41315300	4.10592700	-3.42429700
H	-4.17531200	2.58760700	-3.93053700
H	-4.30914900	3.13009100	-2.25032500
C	-1.48253500	2.16975200	-4.05964000
H	-1.28737500	3.13750300	-4.53419600
H	-0.51508200	1.69777100	-3.85597300
H	-2.01381800	1.55590400	-4.79519900
N	3.72150400	0.04560700	0.78740300
S	5.26529800	0.74283800	1.11848700
O	5.33229000	2.07313500	0.49946900
O	5.43586200	0.56969000	2.56173500
C	6.35622100	-0.35359800	0.23278800
C	6.97089300	0.08977200	-0.93972000
C	6.61404600	-1.62661900	0.75195700
C	7.84574700	-0.76737000	-1.60697500
H	6.77773500	1.09168400	-1.30808600
C	7.48977800	-2.46515200	0.07030600
H	6.14545500	-1.94443500	1.67741600

C	8.12010700	-2.05129000	-1.11581200
H	8.33021100	-0.42855400	-2.51884300
H	7.69730700	-3.45521800	0.46778400
C	9.09710200	-2.95860600	-1.82289800
H	9.19676000	-2.69655400	-2.88056800
H	10.09428200	-2.88152400	-1.37037300
H	8.79162000	-4.00791900	-1.75573400
H	-0.88243500	-2.87910400	-2.44460200
C	-0.51494200	-2.22062700	-0.40281200
H	-1.52098400	-2.57086800	-0.19531100
H	0.18408900	-2.63162700	0.33131500
H	-0.33878300	-0.11969800	2.68778700

VCP-**TS1** [X = NTs, R^1 = Me]

B3LYP SCF energy in gas phase: -2534.102602 a.u.

M06 SCF energy in solution: -2533.207902 a.u.

M06 Free energy in solution: -2532.378809 a.u.

C	0.17685900	-4.29620600	-1.13599300
C	-0.62707400	-3.02868000	-0.84395400
C	-0.03538000	-1.68402100	-1.10747200
C	1.33269400	-1.36633100	-0.66564900
H	1.77813200	-2.18654700	-0.10122900
H	-0.30083900	-1.29940100	-2.10083900
C	2.36643800	-0.68536300	-1.52681000
C	3.05423200	0.07310900	0.71444500
C	1.62198500	-0.31156100	0.92683800
C	0.66911000	-0.40985700	1.81837600
H	-1.67853400	-3.08909000	-1.10352800
H	1.21378200	-4.17971800	-1.44135500
H	3.12299000	1.16843300	0.76775400
H	3.70287900	-0.34800300	1.49201500
H	2.71482300	-1.35375000	-2.31929800
H	1.95789300	0.22056600	-1.99753600
Rh	-0.34545700	-0.06824600	0.12472900
C	-2.34812200	0.48529200	0.14563800
N	-3.56985500	-0.13380000	0.20606500
C	-4.59795200	0.79700800	0.25137100
C	-3.84765800	-1.55493800	0.12454500
N	-2.65847800	1.82395700	0.14753500
C	-4.02542100	2.02761800	0.21178500
C	-1.69176200	2.89975000	0.02208600
C	-3.85908900	-2.31977800	1.30911900
C	-4.19114700	-2.08974200	-1.13557000
C	-4.19953300	-3.67368400	1.19432700
C	-3.59320800	-1.70610200	2.68119800
C	-4.52653400	-4.23538000	-0.03769100
C	-4.52642800	-3.44966100	-1.18665500
C	-4.25631000	-1.25059900	-2.41096200
C	-2.79301700	-2.63380600	3.61284900
C	-4.91974800	-1.28974800	3.35396500
C	-3.45273200	-1.86944400	-3.57116100
C	-5.72143700	-1.01527000	-2.83557900
C	-1.22090500	3.53367200	1.19297000
C	-1.29737200	3.29564300	-1.27389100
C	-0.36514600	4.33676000	-1.37162400
C	-1.87007900	2.67777200	-2.54722500
C	0.13508400	4.96514600	-0.23532100
C	-0.29604700	4.57262100	1.02967400
C	-1.72401300	3.16540600	2.58675500
C	-0.77041200	2.09491100	-3.45520900
C	-2.73156800	3.70104300	-3.31601700
C	-2.84889000	4.12499200	3.03202300
C	-0.60304200	3.13778500	3.64241900
H	-5.63256000	0.49642300	0.29755900
H	-4.45868100	3.01518900	0.21452300
H	-4.22451000	-4.29509600	2.08331200
H	-4.79634900	-5.28592300	-0.09927500
H	-4.80126900	-3.89499600	-2.13778200
H	-2.99629900	-0.80010500	2.53293400
H	-5.47317600	-0.56429300	2.74822100
H	-4.72706200	-0.83416900	4.33204500
H	-5.56754400	-2.16006000	3.50851500
H	-3.37858900	-3.50365500	3.92971600
H	-2.50986000	-2.09309300	4.52273900
H	-1.88036700	-3.00037000	3.13047600
H	-3.81349200	-0.27127200	-2.20192300
H	-6.22063000	-1.96149800	-3.07279300
H	-5.76357500	-0.38069700	-3.72788200
H	-6.29924900	-0.52504000	-2.04437700
H	-3.86705700	-2.83214600	-3.88917800
H	-2.40448200	-2.03194100	-3.29731600
H	-3.47630500	-1.20253700	-4.44009400
H	-0.03351800	4.66508500	-2.35197000
H	0.85529200	5.77198700	-0.33546400
H	0.09029500	5.08660500	1.90367800
H	-2.52917200	1.85070600	-2.26365600
H	-3.54268800	4.09160800	-2.69169100
H	-3.17861900	3.23408500	-4.20084400
H	-2.13272100	4.55329300	-3.65549700
H	-0.08654800	2.87051300	-3.81593100
H	-1.21705800	1.61375000	-4.33266400
H	-0.16881800	1.34707400	-2.92457100
H	-2.15029800	2.15655600	2.53725900
H	-2.48019900	5.15523200	3.09123500
H	-3.22441700	3.84287900	4.02217000
H	-3.69413100	4.11361200	2.33585400
H	-0.22126200	4.14078900	3.86065600
H	0.24296200	2.52186200	3.31911100
H	-0.98743100	2.73076700	4.58444200
N	3.49185400	-0.42400600	-0.60941900
S	4.79980500	0.44099900	-1.31448400
O	4.82805000	-0.01662100	-2.70501100
O	4.66700400	1.86688300	-0.98592600
C	6.20449900	-0.20932100	-0.42880100
C	6.67834900	-1.48796900	-0.74214100
C	6.83251800	0.57799500	0.53703300
C	7.78696400	-1.97968500	-0.06212700

H	6.19410900	-2.07677300	-1.51410000
C	7.94359900	0.06532800	1.20745200
H	6.46608900	1.57765600	0.74408800
C	8.43775700	-1.21414200	0.92124600
H	8.16230100	-2.97120200	-0.30201600
H	8.43899800	0.67481000	1.95850400
C	9.65827800	-1.75311500	1.62656000
H	9.88283600	-1.18530100	2.53425400
H	9.52823300	-2.80491600	1.90371900
H	10.53997000	-1.69762300	0.97524400
C	-0.18732900	-3.93873300	0.27711000
H	-0.33939400	-5.11868600	-1.62237800
H	-0.96469600	-4.51470000	0.77036500
H	0.60387100	-3.60921900	0.94655800
C	0.36281100	-0.53552600	3.26119500
H	0.08030200	-1.56775100	3.50162000
H	1.24791000	-0.28367300	3.86057600
H	-0.46158900	0.11458600	3.56647300

VCP-**TS3** [X = NTs, R^1 = Me]

B3LYP SCF energy in gas phase: -2534.109146 a.u.

M06 SCF energy in solution: -2533.224118 a.u.

M06 Free energy in solution: -2532.392664 a.u.

C	-1.56943200	-0.08578600	0.25470100
C	-0.86657500	0.61877200	1.02239400
C	-1.22714700	-0.02354300	-2.60029700
C	-0.01910000	-0.69602800	-2.69239700
C	1.26123700	-0.03270500	-2.86314400
C	1.44950300	1.22062400	-3.66485800
C	1.41169300	1.67175400	-2.24637200
H	2.36256000	1.88639200	-1.78225500
H	0.58519200	2.31544900	-1.95635400
H	-0.01278900	-1.78002500	-2.61425900
H	-1.30723200	1.03236000	-2.84869500
H	2.14737900	-0.64363400	-2.73331500
H	0.60842600	1.50896200	-4.29197400
C	-2.52172100	-0.78557700	-2.53605400
H	-3.09566000	-0.59330500	-3.44743600
H	-2.31874200	-1.86755600	-2.48620600
C	-2.81670100	-0.79776000	-0.10738900
H	-2.65824100	-1.88678500	-0.09219300
H	-3.55547600	-0.56201100	0.66667400
H	2.40452700	1.29725200	-4.18004700
C	3.71581800	0.02492900	1.94900600
C	3.09949200	-1.15591800	2.17060200
C	1.90602900	-0.06219900	0.55670700
N	2.00191900	-1.21182500	1.31657200
N	2.99824400	0.68424400	0.95147100
Rh	0.33094300	0.22236700	-0.72497600
H	3.33534700	-1.96481800	2.84269900
H	4.59969000	0.46084700	2.38606300
C	3.58229300	1.85820900	0.31748900
C	4.61398600	1.64597600	-0.63158500
C	3.19677300	3.15189000	0.72372400
C	5.19777100	2.77536900	-1.21905200
C	3.81461300	4.24261200	0.09583800
C	4.79522800	4.06219000	-0.87290700
H	5.98959400	2.64507000	-1.95004100
H	3.53525800	5.24985900	0.38770700
H	5.26260600	4.92322700	-1.34191500
C	1.22415500	-2.43608400	1.16827800
C	0.27749800	-2.78173200	2.15634800
C	1.52871600	-3.29984100	0.08677700
C	-0.44683800	-3.96890300	1.97453200
C	0.76663000	-4.46659000	-0.04441100
C	-0.22638100	-4.79148000	0.87656600
H	-1.18633500	-4.25758800	2.71430700
H	0.96729100	-5.14459300	-0.86656300
H	-0.80422600	-5.70305600	0.75403300
C	2.21575100	3.40828100	1.85914600
H	1.73555000	2.45913400	2.10279700
C	5.15490200	0.26337300	-0.99576600
H	4.47339600	-0.49192800	-0.59457900
C	0.07774300	-1.98752800	3.44453500
H	0.54442000	-1.00689600	3.31637400
C	2.71891500	-3.07005300	-0.84459900
H	2.87789600	-1.99078300	-0.93128000
C	6.53588500	0.03157400	-0.34452100
H	6.90312500	-0.97410900	-0.57768000
H	7.27151900	0.75338800	-0.71649100
H	6.49397000	0.13124900	0.74485300
C	5.24877500	0.03344500	-2.51666500
H	4.29189200	0.21154800	-3.01956600
H	5.99305500	0.68565700	-2.98543700
H	5.55170700	-0.99962500	-2.72060700
C	3.99771800	-3.68742400	-0.23257100
H	3.88206500	-4.77060300	-0.11336300
H	4.85965300	-3.51152200	-0.88700700
H	4.22921400	-3.26396300	0.74936400
C	2.52191900	-3.62299300	-2.26825400
H	2.52885900	-4.71797700	-2.28695200
H	1.58099200	-3.29216200	-2.72043900
H	3.34456700	-3.29138200	-2.91169800
C	0.78786200	-2.68987500	4.62375500
H	0.68533100	-2.09658200	5.53942000
H	0.34974900	-3.67653500	4.81105700
H	1.85667200	-2.83629600	4.43457100
C	-1.40515900	-1.76035800	3.79462200
H	-1.48730500	-1.09141500	4.65859500
H	-1.95448600	-1.31564700	2.95948400
H	-1.90651500	-2.69556300	4.06571800
C	2.96668000	3.88481900	3.12127800
H	3.46943100	4.84255900	2.94596500
H	2.26676000	4.02100000	3.95362900
H	3.72810400	3.16176800	3.43417800
C	1.10935000	4.40810100	1.47423900
H	1.51418100	5.40095800	1.25103700

H	0.54802500	4.06989200	0.59571300
H	0.40580900	4.53149200	2.30549600
N	-3.35578700	-0.35163100	-1.40163100
S	-5.02802900	-0.76787000	-1.60584000
O	-5.31882900	-0.46709700	-3.00953500
O	-5.27004100	-2.10667000	-1.05226100
C	-5.83273300	0.43117000	-0.55645700
C	-6.48332600	-0.00203000	0.59956900
C	-5.85670100	1.77561100	-0.94185600
C	-7.15405200	0.93410400	1.38748400
H	-6.47453600	-1.05429000	0.86328500
C	-6.52967100	2.69252300	-0.14148400
H	-5.36690500	2.09079000	-1.85717700
C	-7.19040700	2.28898600	1.03209200
H	-7.66559100	0.60255500	2.28718400
H	-6.55443800	3.73879000	-0.43520900
C	-7.94908400	3.29098800	1.86780500
H	-7.42252400	4.24982300	1.92103900
H	-8.93777500	3.48861700	1.43375900
H	-8.10566000	2.92801200	2.88800700
C	-0.69117100	1.35112000	2.29549700
H	-0.66302400	2.42882900	2.11338900
H	-1.52950300	1.13978800	2.96875100
H	0.23509200	1.07734500	2.80634900

VCP-**TS4** [X = NTs, R^1 = Me]

B3LYP SCF energy in gas phase: -2534.127632 a.u.

M06 SCF energy in solution: -2533.225246 a.u.

M06 Free energy in solution: -2532.389964 a.u.

C	1.44323600	0.05472800	1.27476100
C	0.26571000	-0.02079700	1.82714700
C	1.89504700	-0.58965400	-0.57218200
C	1.04186900	-0.40726300	-1.76819000
C	0.07146300	-1.29838100	-2.18308700
C	-0.18102500	-2.62175900	-1.47486200
H	1.21008900	0.50015600	-2.34592900
H	2.05077800	-1.63062500	-0.29201700
H	-0.45258200	-1.08695300	-3.11130300
H	0.68524000	-3.29229300	-1.57272700
C	3.20656300	0.17455900	-0.62291400
H	3.87755600	-0.30985900	-1.34060000
H	3.04679400	1.21458100	-0.94779000
C	2.79032100	0.58576000	1.67163800
H	2.74600600	1.68755700	1.68057700
H	3.04440200	0.25055500	2.68031800
C	-4.59800300	0.54785700	0.33310200
C	-4.05033000	1.76498900	0.11915400
C	-2.35974700	0.23403100	0.07803800
N	-2.68367900	1.56460600	-0.03988900
N	-3.56192900	-0.38749900	0.29843300
Rh	-0.39280500	-0.20839900	-0.06889200
H	-4.49252000	2.74642800	0.06208500
H	-5.61972800	0.24595700	0.49665300
C	-3.85909200	-1.80992600	0.31781900
C	-3.87759000	-2.49465100	1.55134000
C	-4.21738200	-2.42822400	-0.90190500
C	-4.20256000	-3.85714600	1.52590300
C	-4.53112400	-3.79306500	-0.86297400
C	-4.51339900	-4.50415100	0.33315600
H	-4.22261300	-4.41835500	2.45389200
H	-4.81030500	-4.30202800	-1.78012600
H	-4.76259100	-5.56142700	0.33932900
C	-1.74771000	2.61157100	-0.41076800
C	-1.47503800	2.81156300	-1.78773800
C	-1.21050600	3.44551500	0.59555900
C	-0.57380200	3.82889900	-2.12363400
C	-0.31905800	4.44987200	0.19411800
C	0.00817200	4.63211100	-1.14554000
H	-0.33920500	4.01090800	-3.16689200
H	0.11422800	5.10717400	0.94047600
H	0.70106400	5.41821900	-1.43182900
C	-4.36432200	-1.65896500	-2.21440900
H	-3.86435900	-0.69157100	-2.10417000
C	-5.85578400	-1.38013600	-2.50501000
H	-6.33217400	-0.82388500	-1.69115500
H	-5.96284900	-0.79244000	-3.42379000
H	-6.40982300	-2.31629800	-2.63697600
C	-3.71937300	-2.36770200	-3.41960000
H	-2.66097300	-2.58668000	-3.24595700
H	-4.22057000	-3.31129000	-3.65988200
H	-3.79256900	-1.73031800	-4.30793800
C	-3.62810900	-1.79225700	2.88287200
H	-3.05658300	-0.88089300	2.67921700
C	-4.96617900	-1.36954600	3.52866100
H	-5.59217500	-2.24495800	3.73519400
H	-4.78618000	-0.85134000	4.47747100
H	-5.53693200	-0.69607100	2.88064800
C	-2.81086000	-2.64349000	3.87190600
H	-3.37804600	-3.50767000	4.23392200
H	-1.88462000	-3.01805500	3.42177400
H	-2.54943400	-2.04529800	4.75174900
C	-1.63138300	3.34916600	2.05893500
H	-2.06991600	2.35822600	2.21876300
C	-2.72213100	4.39701200	2.37463500
H	-3.04648000	4.30736700	3.41746200
H	-2.33997600	5.41322300	2.22617400
H	-3.60382200	4.27748500	1.73631200
C	-0.45367900	3.50878800	3.03804900
H	-0.78499900	3.29354100	4.05977300
H	0.37159800	2.83223400	2.79476400
H	-0.06107400	4.53100500	3.03856600
C	-2.20279200	2.04361900	-2.89042300
H	-2.50831400	1.07345700	-2.48577000
C	-3.48199700	2.80136300	-3.31270000
H	-3.23138900	3.78693600	-3.72111900
H	-4.01868700	2.24183200	-4.08742900
H	-4.16605300	2.95061500	-2.47159200

C	-1.33487800	1.76592900	-4.13115900
H	-1.11291400	2.68016300	-4.69188800
H	-0.38092900	1.29569400	-3.87049600
H	-1.86975800	1.09635700	-4.81361300
N	3.78832300	0.08951900	0.71553400
S	5.32472200	0.85621800	0.89082100
O	5.35131200	2.07023400	0.06390400
O	5.53260400	0.92252900	2.33829100
C	6.42157300	-0.34882300	0.16821300
C	7.00009700	-0.09058200	-1.07585900
C	6.72398400	-1.51254000	0.88225400
C	7.88392800	-1.02494300	-1.61493600
H	6.77250800	0.83271300	-1.59782400
C	7.60818300	-2.43127800	0.32599400
H	6.28313000	-1.68507100	1.85845000
C	8.20316700	-2.20388200	-0.92662200
H	8.34001300	-0.82891100	-2.58176100
H	7.84980400	-3.33746500	0.87530400
C	9.19080100	-3.19092300	-1.49936900
H	10.20407300	-2.98235500	-1.13191500
H	8.94604900	-4.21803000	-1.21019900
H	9.22316100	-3.13966000	-2.59203000
H	-1.02768600	-3.13019400	-1.94223400
C	-0.50145300	-2.27258600	-0.01762500
H	-1.49009500	-2.58965000	0.30014600
H	0.24757600	-2.60082400	0.70916800
C	-0.26968400	-0.00145700	3.21675000
H	-0.57816900	-1.01147500	3.50722800
H	0.48881200	0.33547500	3.93374900
H	-1.14618600	0.64482000	3.30770800

VCP-**TS1** [X = NTs, R^1 = Ph]

B3LYP SCF energy in gas phase: -2725.841048 a.u.

M06 SCF energy in solution: -2724.850335 a.u.

M06 Free energy in solution: -2723.973423 a.u.

C	0.00621600	-2.48330300	-3.72892500
C	-0.75717800	-1.67465200	-2.68030000
C	-0.14856600	-0.45101600	-2.07733100
C	1.24644400	-0.46142500	-1.61167100
H	1.71602400	-1.44022300	-1.72420600
H	-0.44895100	0.46385700	-2.60126200
C	2.22970400	0.64537100	-1.90733000
C	3.00350600	-0.04410600	0.31125400
C	1.61803000	-0.61285200	0.25739800
C	0.75593700	-1.36260700	0.91267300
H	-1.81719700	-1.56520900	-2.87969600
H	1.03390400	-2.19877200	-3.94172600
H	2.99284400	0.82744500	0.98161600
H	3.72338000	-0.76922700	0.70754900
H	2.54104400	0.61654800	-2.95511200
H	1.78707800	1.63186300	-1.70693100
Rh	-0.36651700	0.00714100	-0.07655700
C	-2.36307300	0.54160300	0.25423400
N	-3.61193400	0.15348800	-0.16092200
C	-4.60054000	0.89670800	0.46783200
C	-3.94745600	-0.79425900	-1.20729600
N	-2.61789800	1.55605300	1.14782100
C	-3.97578800	1.78140500	1.28647400
C	-1.60338000	2.37681800	1.78654800
C	-4.14573900	-2.14797600	-0.86930500
C	-4.16276100	-0.29249600	-2.51010200
C	-4.53664800	-3.01601900	-1.89741300
C	-4.02933300	-2.66500200	0.56146700
C	-4.73777900	-2.55562700	-3.19568400
C	-4.55817800	-1.20771900	-3.49452900
C	-4.03293300	1.18703800	-2.86840200
C	-3.30624400	-4.02057200	0.65037000
C	-5.42562800	-2.75347700	1.21496900
C	-3.17885100	1.42365900	-4.12906100
C	-5.42522300	1.83178800	-3.03743900
C	-1.18716600	2.05876400	3.09805200
C	-1.11754200	3.50094900	1.08279000
C	-0.14041400	4.28175400	1.71325800
C	-1.65652100	3.93050600	-0.27977600
C	0.31604000	3.97167000	2.99064300
C	-0.21110000	2.88037300	3.67633100
C	-1.80678900	0.92235100	3.90777900
C	-0.54173000	4.12397800	-1.32416400
C	-2.50754400	5.21116800	-0.14440600
C	-2.92803800	1.45845000	4.82518600
C	-0.77342400	0.14179500	4.74045000
H	-5.64721600	0.73226600	0.26710800
H	-4.36710200	2.54670600	1.93756200
H	-4.70246600	-4.06496600	-1.67501000
H	-5.04941000	-3.24672500	-3.97383500
H	-4.73588100	-0.85759900	-4.50650200
H	-3.43951400	-1.94191300	1.13489600
H	-5.93359300	-1.78289500	1.22120600
H	-5.34261100	-3.09777400	2.25229600
H	-6.06557800	-3.46103700	0.67547800
H	-3.88455100	-4.82475100	0.18245300
H	-3.16029000	-4.29871600	1.69923900
H	-2.32230800	-3.98348600	0.17202000
H	-3.53124500	1.69732200	-2.03990500
H	-5.97582500	1.36598500	-3.86248100
H	-5.32772200	2.90048300	-3.25933200
H	-6.03296000	1.72817600	-2.13218500
H	-3.66008200	1.02838900	-5.03010300
H	-2.19199300	0.95530500	-4.04739700
H	-3.03320800	2.49832100	-4.28507500
H	0.25943400	5.15082800	1.20030200
H	1.07377200	4.59208300	3.46050300
H	0.13625500	2.66799500	4.68179000
H	-2.31681600	3.14213400	-0.65474100
H	-3.33353800	5.07173600	0.56183400
H	-2.93357200	5.49111400	-1.11451800
H	-1.90374900	6.05316200	0.21186000

H	0.13757400	4.93914200	-1.05368200
H	-0.97692300	4.36954900	-2.29945100
H	0.06085900	3.21561000	-1.43740700
H	-2.26486800	0.21685300	3.20466700
H	-2.52749000	2.17550300	5.55068100
H	-3.39078200	0.63668300	5.38341800
H	-3.71557900	1.96516900	4.25765000
H	-0.36415300	0.74955300	5.55451600
H	0.06196100	-0.21104800	4.12741900
H	-1.24806100	-0.73164200	5.20057400
C	0.62040200	-2.48445800	1.80166500
C	-0.53752700	-2.68554700	2.57883000
C	1.68294800	-3.41229700	1.90761100
C	-0.62373800	-3.77009500	3.44610800
H	-1.35770000	-1.98071900	2.49288100
C	1.59223200	-4.49014500	2.78132000
H	2.57274400	-3.27497000	1.29995000
C	0.43940800	-4.67237800	3.55251700
H	-1.51813100	-3.91343100	4.04555200
H	2.41632600	-5.19316800	2.85849900
H	0.36916500	-5.51650600	4.23219000
N	3.39861500	0.33860700	-1.06194600
S	4.66522700	1.49831900	-1.15566800
O	4.66563800	1.92361800	-2.55669100
O	4.51097100	2.47263400	-0.06672800
C	6.10620600	0.50309400	-0.81786600
C	6.59997900	-0.34563200	-1.81456000
C	6.74041200	0.61025900	0.42042100
C	7.73564500	-1.10340200	-1.55078400
H	6.10914800	-0.39731800	-2.78076100
C	7.87884700	-0.15880800	0.66420000
H	6.35713800	1.29564400	1.16871700
C	8.39375600	-1.02315100	-0.31100200
H	8.12646800	-1.76292500	-2.32143300
H	8.37946600	-0.07727000	1.62531200
C	9.64377000	-1.82913600	-0.05473300
H	9.54389400	-2.85333100	-0.43037500
H	10.50629300	-1.38126600	-0.56470300
H	9.88012800	-1.87720000	1.01228500
C	-0.29640800	-3.08080200	-2.38350700
H	-0.54651000	-2.83002100	-4.59723100
H	-1.06573400	-3.84468200	-2.31852300
H	0.52622600	-3.23140200	-1.68875900

VCP-**TS3** [X = NTs, R^1 = Ph]

B3LYP SCF energy in gas phase: -2725.839654 a.u.

M06 SCF energy in solution: -2724.862394 a.u.

M06 Free energy in solution: -2723.979403 a.u.

C	-1.48623000	-0.29451300	0.09753500
C	-0.86495800	0.67507100	0.62799500
C	-1.05300100	-1.35142700	-2.51714100
C	0.20828800	-1.88938500	-2.32001900
C	1.43085100	-1.22268900	-2.73222700
C	1.54613000	-0.37453700	-3.96310000
C	1.41514400	0.58820600	-2.83515100
H	2.32639600	1.05365300	-2.49065800
H	0.52616100	1.21254300	-2.81882700
H	0.30404000	-2.84848000	-1.81763200
H	-1.20275900	-0.48732800	-3.16080600
H	2.36059600	-1.63894900	-2.36435400
H	0.71021400	-0.43234000	-4.65705900
C	-2.29107800	-2.12830300	-2.16931500
H	-2.83664300	-2.36536600	-3.08765900
H	-2.01839600	-3.07874300	-1.68292300
C	-2.68100600	-1.17094200	0.04664700
H	-2.46064800	-2.14472800	0.51087000
H	-3.45835800	-0.68829300	0.64935700
H	2.51272600	-0.41868200	-4.46002300
C	3.72150400	0.80482500	1.65820600
C	3.22545400	-0.29038900	2.27685700
C	1.99003100	0.04165700	0.38945700
N	2.17698800	-0.76523000	1.49351300
N	2.98287900	0.99427800	0.48995400
Rh	0.40273300	-0.24653500	-0.85748200
H	3.51905600	-0.78355500	3.18945000
H	4.53850700	1.45900400	1.91737700
C	3.49335600	1.88808400	-0.54769700
C	4.62814200	1.45047500	-1.27877100
C	2.92198000	3.16068600	-0.75735300
C	5.14448100	2.30940200	-2.25699200
C	3.48062500	3.97068600	-1.75634800
C	4.57441200	3.55419600	-2.50518000
H	6.01468600	2.00004400	-2.82750200
H	3.05475000	4.95293700	-1.93492400
H	4.99290400	4.20301800	-3.26923000
C	1.55140300	-2.06362300	1.73595400
C	0.59172300	-2.20635000	2.76100700
C	2.00705200	-3.17579000	0.98172900
C	0.00136700	-3.46796200	2.92956600
C	1.37432100	-4.40643600	1.19200200
C	0.36372000	-4.55089900	2.13943600
H	-0.74521700	-3.60193200	3.70551400
H	1.69328100	-5.27428600	0.62529100
H	-0.11247400	-5.51639200	2.28447400
C	1.77829200	3.71431000	0.07580300
H	1.39744500	2.90823100	0.69952600
C	5.33973400	0.11909100	-1.03818200
H	4.73789900	-0.47932700	-0.34998200
C	0.24777300	-1.10275400	3.75495600
H	0.62347800	-0.15840500	3.36006200
C	3.23279600	-3.11343400	0.07105400
H	3.29956100	-2.10304800	-0.34346600
C	6.71357200	0.34207600	-0.37065000
H	7.19952200	-0.61870400	-0.16671000
H	7.37836000	0.92380200	-1.01870700
H	6.62063700	0.88166300	0.57759900
C	5.50597900	-0.70465900	-2.33061800

H	4.54697500	-0.87208000	-2.83442700
H	6.17309600	-0.21417100	-3.04726600
H	5.94191600	-1.68307500	-2.09958300
C	4.51505800	-3.36451800	0.89848900
H	4.49309900	-4.36454600	1.34594400
H	5.40330100	-3.30147300	0.25880900
H	4.63076300	-2.63731000	1.70777600
C	3.19609000	-4.09802700	-1.11267900
H	3.31487500	-5.13596000	-0.78469700
H	2.26301200	-4.03754600	-1.68308900
H	4.02614500	-3.88595200	-1.79560900
C	0.96123800	-1.36162700	5.10124500
H	0.75746400	-0.54483400	5.80277900
H	0.61022700	-2.29350200	5.55856300
H	2.04771300	-1.44349700	4.98325600
C	-1.26440400	-0.93126700	3.98695500
H	-1.44348100	-0.05875800	4.62400300
H	-1.80130900	-0.77771100	3.04656800
H	-1.70246200	-1.79887700	4.49206400
C	2.28405200	4.82748800	1.01687000
H	2.65771700	5.68972400	0.45270600
H	1.46951600	5.17346400	1.66228000
H	3.09876200	4.47239500	1.65842000
C	0.60054200	4.21420100	-0.78098700
H	0.87952000	5.06817200	-1.40837700
H	0.21863000	3.42276800	-1.43572800
H	-0.22008500	4.53612500	-0.13140500
C	-0.99266000	1.77131500	1.57958900
C	-0.00027500	2.17249400	2.48866000
C	-2.23272000	2.44550500	1.59830400
C	-0.24815900	3.19424800	3.40623000
H	0.96656800	1.68347600	2.48757300
C	-2.46939100	3.47406300	2.50711700
H	-3.00469100	2.15790500	0.89062500
C	-1.48047400	3.85021700	3.41970100
H	0.52815300	3.47956000	4.11054500
H	-3.43044900	3.98040700	2.50374500
H	-1.66763300	4.64843400	4.13181100
N	-3.19556500	-1.33517000	-1.32076300
S	-4.83831500	-1.88480000	-1.36384400
O	-5.07509000	-2.24547000	-2.76362600
O	-5.06180200	-2.85244000	-0.28241700
C	-5.72697200	-0.38589200	-0.97180600
C	-6.40120100	-0.28919200	0.24584100
C	-5.77977900	0.64688800	-1.91399100
C	-7.12606600	0.87024800	0.52594200
H	-6.36836800	-1.11402800	0.94980000
C	-6.50636500	1.79417500	-1.61456600
H	-5.27088400	0.54446100	-2.86668500
C	-7.19247900	1.92478700	-0.39411400
H	-7.65668000	0.94975400	1.47101600
H	-6.55395400	2.59964100	-2.34300200
C	-8.00809300	3.16105400	-0.10289800
H	-7.49922600	4.06796100	-0.44704000
H	-8.97545500	3.11834600	-0.61979200
H	-8.21220900	3.26639500	0.96678800

VCP-**TS4** [X = NTs, R^1 = Ph]

B3LYP SCF energy in gas phase: -2725.859651 a.u.

M06 SCF energy in solution: -2724.865687 a.u.

M06 Free energy in solution: -2723.982064 a.u.

C	-1.51498400	0.87697400	0.39661600
C	-0.36274400	1.49741400	0.49743600
C	-1.93327800	-0.64550500	-0.79664900
C	-1.04917500	-1.81745100	-1.00122600
C	-0.06325700	-1.89666400	-1.96738800
C	0.17064300	-0.80040300	-2.99808300
H	-1.19791100	-2.65817100	-0.32575100
H	-2.09653900	-0.05383500	-1.69640200
H	0.48863100	-2.82828400	-2.05490400
H	-0.68248800	-0.71558100	-3.68724000
C	-3.24853100	-0.98054200	-0.11015900
H	-3.90674000	-1.48705200	-0.82411200
H	-3.08710800	-1.65127200	0.74820200
C	-2.84045600	1.00121300	1.09300000
H	-2.75165800	0.56822900	2.10432200
H	-3.11787900	2.05088100	1.20102300
C	4.57326900	-0.15445400	0.45092300
C	4.05793700	-0.76484800	1.54147200
C	2.32676100	-0.29431300	0.13320600
N	2.68476800	-0.85853900	1.33761700
N	3.51472700	0.11573700	-0.41939900
Rh	0.34656400	-0.25139000	-0.26632000
H	4.52760200	-1.14144900	2.43595500
H	5.58746300	0.10475200	0.19335300
C	3.79599000	0.53111100	-1.78879800
C	3.79254000	1.90211500	-2.12113700
C	4.17082600	-0.46947300	-2.71661900
C	4.12192000	2.25045900	-3.43782100
C	4.48610600	-0.05856900	-4.01834600
C	4.45499800	1.28412000	-4.38135900
H	4.12431500	3.29674400	-3.72447000
H	4.77775200	-0.80147000	-4.75415900
H	4.70779100	1.57886700	-5.39585900
C	1.78343600	-1.61345000	2.19843300
C	1.48674600	-2.95734300	1.84599200
C	1.30176800	-1.03055500	3.39219000
C	0.59351500	-3.65760100	2.66485500
C	0.41655800	-1.78764900	4.17356500
C	0.04676600	-3.07557200	3.80647700
H	0.33940400	-4.68361900	2.42231400
H	0.02489500	-1.36324300	5.09199000
H	-0.64277600	-3.64106500	4.42677900
C	4.33207900	-1.94328800	-2.34779700
H	3.87263200	-2.10549900	-1.36890100
C	5.82788600	-2.30628700	-2.22022700
H	6.33732600	-1.67644600	-1.48369300

H	5.94262900	-3.35079600	-1.90882300
H	6.34549900	-2.18221900	-3.17798300
C	3.64111900	-2.89899000	-3.33869500
H	2.57652700	-2.66965800	-3.45214800
H	4.09706800	-2.85987600	-4.33359100
H	3.73038800	-3.93226800	-2.98452800
C	3.49562200	2.99561200	-1.10360900
H	2.97746800	2.53428200	-0.26028600
C	4.80727700	3.60800000	-0.56715400
H	5.37836700	4.08288700	-1.37317400
H	4.58858300	4.37327900	0.18613500
H	5.45060900	2.85123700	-0.10408600
C	2.57166400	4.09614000	-1.65557600
H	3.06456600	4.69793700	-2.42702400
H	1.65697700	3.67586900	-2.08705800
H	2.28181200	4.77420100	-0.84717300
C	1.77685600	0.31991800	3.91496900
H	2.27807500	0.84266800	3.09601300
C	2.81958300	0.11658200	5.03687600
H	3.19304900	1.08472400	5.38862900
H	2.37841100	-0.40569800	5.89312600
H	3.67756200	-0.47389200	4.69641900
C	0.62708600	1.21528900	4.41134300
H	1.01079000	2.20745100	4.67043700
H	-0.14546900	1.34360100	3.64712400
H	0.15277100	0.80608000	5.30973100
C	2.19575600	-3.68705600	0.70595600
H	2.45267600	-2.95239900	-0.06242900
C	3.51323400	-4.31325500	1.21905200
H	3.30815900	-5.05870000	1.99558500
H	4.04144100	-4.81533700	0.40026600
H	4.18741800	-3.56307300	1.64304700
C	1.34381100	-4.77730000	0.03102800
H	1.19353200	-5.64350100	0.68417300
H	0.35581800	-4.41017600	-0.26589200
H	1.85515100	-5.14249600	-0.86638200
C	0.01908200	2.84138100	0.92365000
C	1.22590500	3.10591000	1.59210200
C	-0.85609700	3.91926100	0.67071500
C	1.53125800	4.39212500	2.03402900
H	1.91863700	2.29255500	1.77003300
C	-0.54358400	5.20625900	1.10106000
H	-1.77728500	3.74254900	0.12344700
C	0.64700400	5.44677700	1.79255100
H	2.46238600	4.57274800	2.56396900
H	-1.23019300	6.02264800	0.89688300
H	0.88679100	6.44953700	2.13383200
N	-3.84223600	0.29411400	0.28702800
S	-5.38049000	0.17857700	1.06012200
O	-5.40780000	-1.02499100	1.90184900
O	-5.59777700	1.50807000	1.63288600
C	-6.46768800	-0.07359300	-0.33008200
C	-7.02641000	-1.33410800	-0.54498100
C	-6.78099000	1.01053100	-1.15710000
C	-7.90243400	-1.50931900	-1.61681300
H	-6.79133000	-2.15286000	0.12675100
C	-7.65586200	0.81383600	-2.21972100
H	-6.35616000	1.98895100	-0.95912800
C	-8.23160800	-0.44487900	-2.46653900
H	-8.34443200	-2.48721100	-1.78784300
H	-7.90670300	1.65169600	-2.86522800
C	-9.20546500	-0.63022400	-3.60452600
H	-9.35807000	-1.68845400	-3.83570600
H	-10.18406000	-0.20219500	-3.35198600
H	-8.85896100	-0.12701800	-4.51382300
H	1.04432600	-1.05170800	-3.60442600
C	0.42315800	0.48155400	-2.19945400
H	1.38894200	0.93884500	-2.39012000
H	-0.36580800	1.23549400	-2.27314000

1a (M06)

M06 SCF energy in gas phase: -1697.933238 a.u.

M06 SCF energy in solution: -1698.440986 a.u.

M06 Free energy in solution: -1697.699511 a.u.

C	-2.64065600	-0.72024700	-3.71825000
C	-2.15184700	-0.38380800	-2.32500300
C	-0.73796900	0.01728300	-2.10816900
C	0.35063900	-0.72178500	-2.62701300
H	0.09916100	-1.64891100	-3.15964500
H	-0.57905700	1.08837300	-1.94338600
C	-2.56130100	-1.78522100	-2.67697400
C	1.70408500	-0.18486500	-2.98636700
C	2.99843100	-1.97458600	-1.68875600
C	1.75102400	-2.46320100	-1.07791700
C	0.79674800	-3.19774400	-0.69028800
H	-2.86785600	0.15859800	-1.70919500
H	-3.48464700	-2.15081800	-2.23075100
H	-1.78680300	-2.54586100	-2.78079800
H	-3.61676600	-0.34471700	-4.01820500
H	-1.89963100	-0.73687000	-4.51662400
H	3.48125600	-1.26427800	-0.99884000
H	3.69431100	-2.81631100	-1.81949500
H	1.64158200	0.28996500	-3.98104700
H	2.00453400	0.60022400	-2.27544900
Rh	0.21335100	-1.18396000	-0.57102900
C	-0.09530800	0.49674100	0.56314700
N	-1.20900000	0.90272000	1.22980400
C	-0.88691500	1.82010900	2.22156700
C	-2.56585700	0.51849700	0.94960500
N	0.91886300	1.19807300	1.13743400
C	0.44878200	2.00768600	2.16086700
C	2.31247600	1.08036100	0.80190000
C	-2.98776100	-0.78427000	1.27108800
C	-3.40818200	1.48188100	0.37546600
C	-4.31913100	-1.09979800	1.00334600
C	-2.05153600	-1.79557200	1.90908800
C	-5.18669800	-0.15978600	0.45723600

C	-4.73736300	1.11422100	0.14845400
C	-2.93860900	2.86829900	-0.02339100
C	-2.52978300	-3.23408400	1.76977500
C	-1.79117400	-1.46778000	3.38038200
C	-3.23291200	3.17388800	-1.49241700
C	-3.56824400	3.93667900	0.87145000
C	3.06222800	0.07969500	1.43963600
C	2.86027300	2.00011600	-0.10584600
C	4.22404700	1.88193600	-0.38225200
C	2.03856000	3.12639900	-0.70368200
C	4.99608400	0.90488600	0.23391300
C	4.42281400	0.01544200	1.13597100
C	2.44185900	-0.85788200	2.45684800
C	2.42530100	3.47740000	-2.13782900
C	2.15949400	4.37893900	0.16911300
C	2.60670000	-0.29532500	3.87002400
C	2.99087400	-2.27947100	2.39038200
H	-1.64498500	2.23753500	2.87113900
H	1.11626400	2.62756100	2.74509300
H	-4.69652300	-2.09382900	1.23051100
H	-6.22456400	-0.42885100	0.26998500
H	-5.42826000	1.83545500	-0.28652800
H	-1.07676500	-1.73931000	1.37681200
H	-1.36221800	-0.46684000	3.52137900
H	-1.09268400	-2.19492100	3.81749800
H	-2.72945800	-1.51663800	3.95071100
H	-3.43226000	-3.42322300	2.36711600
H	-1.75723100	-3.92139600	2.13840500
H	-2.75010400	-3.49180900	0.72433000
H	-1.84550800	2.92168400	0.10522800
H	-4.66040300	3.95278300	0.75376900
H	-3.19225700	4.93321700	0.60713600
H	-3.35851500	3.76525200	1.93521600
H	-4.31211900	3.22165900	-1.68975400
H	-2.80450300	2.42173700	-2.16905300
H	-2.81239600	4.15081400	-1.76353400
H	4.69121500	2.57554500	-1.07962800
H	6.06013100	0.83951900	0.01381400
H	5.04503500	-0.73929900	1.61479200
H	0.97951700	2.81433900	-0.70760300
H	1.81825500	4.20788400	1.19761200
H	1.56633000	5.20196900	-0.24996400
H	3.20682100	4.70859500	0.21702800
H	3.41820200	3.94425400	-2.18852700
H	1.71351600	4.20583200	-2.54593600
H	2.43073400	2.60377400	-2.80170500
H	1.36037800	-0.92027900	2.24709300
H	3.67187900	-0.20522400	4.12591500
H	2.13735900	-0.95984700	4.60762900
H	2.15182200	0.69847500	3.97474300
H	4.03034500	-2.33733800	2.74055900
H	2.94887500	-2.68992800	1.37243400
H	2.39857100	-2.93451000	3.04380800
C	0.09437600	-4.45091000	-0.37700100
H	0.62581300	-5.31721500	-0.79053200
H	0.01554700	-4.58678500	0.70965900
H	-0.92644000	-4.44737800	-0.77867700
C	2.75736000	-1.28856900	-3.04074200
H	3.71247600	-0.87927900	-3.39409000
H	2.44672700	-2.04405200	-3.77899600

TS1a (M06)

M06 SCF energy in gas phase: -1697.893509 a.u.

M06 SCF energy in solution: -1698.40329 a.u.

M06 Free energy in solution: -1697.660407 a.u.

C	3.14112900	3.34891500	-1.10736100
C	2.37151200	2.05182000	-0.93714000
C	0.95785300	1.97366300	-1.36678700
C	0.00638100	3.06233000	-1.07611300
H	0.51080100	3.86740800	-0.52034700
H	0.84484200	1.52929600	-2.37007500
C	2.81454600	2.84112000	0.25641400
C	-0.93369000	3.63974300	-2.10315100
C	-2.16715500	4.01181300	-0.00908300
C	-1.15783400	2.96912300	0.36415600
C	-0.73440300	2.22338500	1.35857000
H	2.94181600	1.14591600	-1.14749100
H	3.62139100	2.41428300	0.85072800
H	2.05883500	3.36603000	0.84415800
H	4.16767600	3.28263900	-1.46105500
H	2.59432800	4.21416100	-1.48204800
H	-3.13213500	3.49300000	-0.11415500
H	-2.29198000	4.74984200	0.79398900
H	-0.36532000	4.10652200	-2.92051000
H	-1.55485900	2.84500800	-2.54447600
Rh	-0.44194700	1.03140300	-0.21096500
C	-0.02640300	-0.95873800	0.15411000
N	1.07507600	-1.70976100	0.42053500
C	0.73626500	-3.03302500	0.65239300
C	2.43882900	-1.26145600	0.34119000
N	-1.05858400	-1.84805700	0.23582800
C	-0.61068400	-3.12077300	0.53678300
C	-2.43171600	-1.48529400	-0.00202100
C	3.02285700	-0.66404700	1.46830600
C	3.13209800	-1.48776400	-0.85541400
C	4.36464500	-0.29775100	1.36979500
C	2.24669400	-0.47602600	2.75560700
C	5.08323600	-0.51138400	0.19823000
C	4.47276300	-1.09711200	-0.90184000
C	2.49332000	-2.13725700	-2.06604000
C	2.70929500	0.72686800	3.57001500
C	2.32502600	-1.74158700	3.61281200
C	2.54569200	-1.22731100	-3.29117600
C	3.14603600	-3.48684200	-2.36384300
C	-3.23360100	-1.12843700	1.09310300
C	-2.89392600	-1.47694500	-1.32660500
C	-4.20973200	-1.06804700	-1.54284200

C	-1.99843200	-1.83114600	-2.49455700
C	-5.02763900	-0.70519700	-0.48097200
C	-4.54679900	-0.74214600	0.82162800
C	-2.72510900	-1.19966000	2.51788900
C	-1.50353900	-0.55747300	-3.17907800
C	-2.67691400	-2.75208900	-3.50504500
C	-3.05949600	-2.56101700	3.13131900
C	-3.27581000	-0.08262400	3.40010300
H	1.49067700	-3.78092200	0.86141900
H	-1.28759600	-3.96070800	0.62285900
H	4.86189000	0.16029800	2.22335900
H	6.13175800	-0.22345700	0.14744400
H	5.04740900	-1.26317300	-1.81287000
H	1.19024400	-0.30615600	2.48813700
H	1.90828700	-2.61755900	3.09907200
H	1.77254100	-1.60924400	4.55252600
H	3.37076400	-1.96660900	3.86625500
H	3.70129300	0.56685400	4.01421700
H	2.01637400	0.90082400	4.40409700
H	2.75433200	1.64220800	2.96328500
H	1.43009600	-2.32033500	-1.84630600
H	4.20398400	-3.36447200	-2.63371500
H	2.64485800	-3.98317000	-3.20473600
H	3.10364000	-4.15948200	-1.49706700
H	3.57855100	-0.99066000	-3.58067800
H	2.02103200	-0.27799100	-3.10992600
H	2.06924000	-1.71774300	-4.15041600
H	-4.60306800	-1.03880000	-2.55822900
H	-6.05490000	-0.39863100	-0.66948500
H	-5.20588600	-0.46614400	1.64284200
H	-1.11776400	-2.36560400	-2.10571800
H	-3.08822900	-3.64813800	-3.02436300
H	-1.95558400	-3.07539400	-4.26609500
H	-3.49713200	-2.24833600	-4.03391900
H	-2.34263500	0.00907300	-3.60874800
H	-0.79645000	-0.78650100	-3.98821200
H	-0.99847300	0.11020300	-2.45816800
H	-1.62526400	-1.10238200	2.49403700
H	-4.14735400	-2.71678100	3.14506400
H	-2.69615700	-2.62273500	4.16536800
H	-2.61172800	-3.38856600	2.56619000
H	-4.33997300	-0.23200800	3.62682000
H	-3.16829900	0.90440800	2.92903200
H	-2.74870500	-0.06666800	4.36327600
C	-0.56987400	2.09816900	2.81272900
H	-1.25955200	2.77397300	3.34015100
H	-0.74722700	1.07460400	3.16610600
H	0.45342600	2.37871400	3.10359800
C	-1.77116000	4.66182200	-1.34127900
H	-2.65005600	4.99481300	-1.90329800
H	-1.15719700	5.55414100	-1.15187700

TS4a (M06)

M06 SCF energy in gas phase: -1697.909827 a.u.

M06 SCF energy in solution: -1698.410662 a.u.

M06 Free energy in solution: -1697.666528 a.u.

C	-1.98336800	-2.20367800	-1.37233500
C	-1.82670800	-0.92952300	-1.57522700
C	-0.51555000	-3.43711100	-0.85221600
C	0.56730500	-3.15710300	0.10857600
C	1.75405900	-2.53431700	-0.22015400
C	2.10837400	-2.15963200	-1.64355900
C	1.01441800	-1.21037100	-2.10679400
H	1.35324600	-0.19513400	-2.32960100
H	0.38721800	-1.57593100	-2.93038300
H	0.39278900	-3.46758600	1.14347900
H	-0.14867600	-3.57025200	-1.87782500
H	2.51664900	-2.42438100	0.55040300
H	2.19097600	-3.05555300	-2.27994000
C	-1.43585800	-4.56918000	-0.44548500
H	-0.86105300	-5.50588600	-0.44599900
H	-1.79403000	-4.41125300	0.58508100
C	-3.11660700	-3.18038100	-1.44503000
H	-3.77864900	-3.00719800	-0.57958700
H	-3.71171400	-2.94960600	-2.34025600
H	3.08960100	-1.66931900	-1.65724500
C	1.28352300	2.59824100	0.90181900
C	-0.04040600	2.77572200	1.07250500
C	0.24818000	0.75255100	0.07418900
N	-0.67200200	1.65214400	0.55167900
N	1.45065900	1.36036700	0.29622400
Rh	-0.18523700	-1.15903600	-0.43145300
H	-0.60176700	3.58432400	1.51945500
H	2.13335400	3.21456800	1.16459800
C	2.75560200	0.75210200	0.24336800
C	3.56792800	0.96818700	-0.87765500
C	3.18668200	0.05099300	1.38348900
C	4.85127200	0.41709100	-0.85173500
C	4.47581900	-0.48165000	1.35391100
C	5.29720000	-0.30693300	0.24639500
H	5.51614900	0.56520700	-1.70117700
H	4.85045800	-1.02732500	2.21942500
H	6.30246500	-0.72407500	0.24727800
C	-2.10325900	1.49589300	0.62645900
C	-2.63326000	0.44167700	1.39764500
C	-2.92064000	2.43586800	-0.02559500
C	-4.02021000	0.32055000	1.45799500
C	-4.30472100	2.28360600	0.10081600
C	-4.85162800	1.23259600	0.81799200
H	-4.46461400	-0.48686100	2.03619900
H	-4.96427600	2.99931800	-0.38764800
H	-5.93214600	1.12704300	0.89294600
C	2.33968300	-0.05606100	2.63818700
H	1.29839900	0.18717100	2.37767200
C	2.81401200	0.96763600	3.67199400
H	2.80500700	1.98890400	3.26976800
H	2.17006300	0.94845500	4.56171400

H	3.84101100	0.74699400	3.99533800
C	2.32329000	-1.45195300	3.25480000
H	1.92039000	-2.20255200	2.56159000
H	3.32203600	-1.78178300	3.57039200
H	1.69159400	-1.45507400	4.15321200
C	3.11919200	1.82079800	-2.04636600
H	2.01782300	1.86400700	-2.03556400
C	3.63820900	3.25073700	-1.87841700
H	4.73670200	3.26177800	-1.84891300
H	3.31754100	3.88098800	-2.71795100
H	3.27556800	3.71224500	-0.95056400
C	3.55487000	1.26275200	-3.39904300
H	4.64013000	1.34912000	-3.54372800
H	3.28435900	0.20501400	-3.52164700
H	3.08057800	1.82953700	-4.20997400
C	-2.38865100	3.60731400	-0.83251000
H	-1.31325300	3.45240700	-1.00951800
C	-2.56661100	4.91588400	-0.05617800
H	-2.12051900	5.75505300	-0.60501600
H	-3.63326700	5.13937800	0.08368200
H	-2.11417400	4.88582400	0.94360600
C	-3.05697000	3.74596000	-2.20048300
H	-2.57416000	4.55113700	-2.76844800
H	-2.99101600	2.82738700	-2.79564800
H	-4.11866700	4.01086600	-2.11018900
C	-1.75657900	-0.47819200	2.22843900
H	-0.82789200	-0.71362100	1.66518300
C	-1.32042600	0.23908700	3.50880100
H	-2.20345600	0.50266000	4.10829600
H	-0.67957700	-0.40971400	4.12224100
H	-0.76921000	1.16633700	3.30108200
C	-2.39485500	-1.81897000	2.56737400
H	-3.21038000	-1.71520700	3.29587300
H	-2.79516700	-2.31749600	1.67332400
H	-1.64385600	-2.48047000	3.02139900
C	-2.47566200	0.14308300	-2.35666400
H	-1.76686900	0.95018300	-2.58751800
H	-3.31190800	0.58571500	-1.79853300
H	-2.87208600	-0.25042200	-3.30299800
C	-2.59505400	-4.60395600	-1.42023000
H	-3.36906200	-5.32106700	-1.12606700
H	-2.23316500	-4.90069700	-2.41569100

1b (M06)

M06 SCF energy in gas phase: -1733.835305 a.u.

M06 SCF energy in solution: -1734.348877 a.u.

M06 Free energy in solution: -1733.63098 a.u.

C	2.88561100	-1.11866100	3.41967700
C	2.31101500	-0.76259600	2.11511900
C	1.07637200	0.06736800	2.01013200
C	-0.05250200	-0.27524000	2.78524100
H	0.05844900	-1.18895000	3.38177400
H	1.22786900	1.10969300	1.71776900
C	-1.15383900	0.62803700	3.24642600
C	-3.00431000	-0.95567500	2.41490000
C	-2.00070100	-1.80626800	1.75344500
C	-1.23977600	-2.75007900	1.40485600
H	2.98914100	-0.71883300	1.26222900
H	3.95627400	-1.31176200	3.50649500
H	2.39250100	-0.77363500	4.33256900
H	-3.42921300	-0.25634400	1.67798700
H	-3.83447600	-1.58244600	2.77200100
H	-0.81960500	1.15760200	4.15530300
H	-1.36034700	1.40253400	2.49143800
Rh	-0.38102100	-0.92441100	0.79588000
C	0.11844300	0.47462700	-0.64261500
N	1.23888900	0.88870400	-1.29344300
C	0.91665900	1.64916800	-2.40715600
C	2.60454500	0.55918800	-0.97774900
N	-0.90443100	1.01691800	-1.36220800
C	-0.43238800	1.72865100	-2.45055600
C	-2.30323500	0.76010800	-1.12945500
C	3.11258500	-0.66945100	-1.42540800
C	3.37884700	1.51056300	-0.29574100
C	4.44662300	-0.95303500	-1.12733700
C	2.26627900	-1.67264200	-2.18202200
C	5.23831200	-0.03717200	-0.44646700
C	4.71138300	1.18288100	-0.04209800
C	2.82760700	2.85514800	0.13478600
C	1.78619100	-2.78701800	-1.25167200
C	2.99287300	-2.26021100	-3.38972400
C	3.22861100	3.22686300	1.56151900
C	3.27410900	3.95041000	-0.83583300
C	-2.86413000	-0.38870400	-1.71070300
C	-3.04812100	1.68888500	-0.38403400
C	-4.41342600	1.43886400	-0.24136200
C	-2.41850400	2.93592100	0.20295100
C	-4.99922700	0.31043800	-0.80427400
C	-4.23215000	-0.59529600	-1.52403900
C	-2.05548000	-1.34766200	-2.56246100
C	-3.06837000	3.38131600	1.51069800
C	-2.47192400	4.08943000	-0.80260300
C	-2.31180800	-1.07803600	-4.04616900
C	-2.32881000	-2.81258500	-2.23153700
H	1.68382800	2.03974800	-3.06267900
H	-1.10353200	2.20669300	-3.15219800
H	4.87608900	-1.90171100	-1.44578300
H	6.27962200	-0.27342200	-0.23539600
H	5.34870800	1.89528500	0.47960500
H	1.37428900	-1.15017300	-2.56402200
H	3.40054300	-1.47748800	-4.04130500
H	2.30117700	-2.87096400	-3.98373000
H	3.82131400	-2.91630900	-3.09161800
H	2.63526200	-3.33510700	-0.81745900
H	1.16033200	-3.50509800	-1.80118200
H	1.19453800	-2.38868600	-0.40634000
H	1.72589900	2.80613100	0.09808600

H	4.36961700	4.03497400	-0.84579400
H	2.86522800	4.92411800	-0.53675600
H	2.94861100	3.74763600	-1.86446500
H	4.29972600	3.45711200	1.63449600
H	3.01389200	2.42326900	2.27975600
H	2.68724300	4.12559900	1.88266400
H	-5.03132400	2.13813800	0.31929600
H	-6.06713900	0.13884900	-0.68221600
H	-4.70738600	-1.47092600	-1.96411500
H	-1.35717300	2.71223100	0.41137800
H	-1.93570100	3.86094400	-1.73189000
H	-2.02757000	4.99731900	-0.37440000
H	-3.51506500	4.31669000	-1.06408500
H	-4.06301500	3.81558600	1.34153500
H	-2.45970100	4.16126000	1.98517700
H	-3.18304400	2.55666400	2.22743700
H	-0.98411900	-1.16685100	-2.37192100
H	-3.36753100	-1.25564000	-4.29483700
H	-1.70318800	-1.74254500	-4.67322000
H	-2.07634800	-0.04171400	-4.32170500
H	-3.33493100	-3.12339000	-2.54384400
H	-2.23961000	-3.00960700	-1.15394300
H	-1.61547600	-3.45675400	-2.76275400
C	-0.68168500	-4.10282500	1.28573400
H	-1.35973600	-4.84686400	1.72231500
H	-0.50005200	-4.37135600	0.23730200
H	0.28118600	-4.15636100	1.81119700
O	2.15428700	-2.05997300	2.65833900
C	-2.41112900	-0.16875300	3.59453800
H	-3.18711100	0.50035300	3.98936500
H	-2.16578300	-0.87230900	4.40466900

TS1b (M06)

M06 SCF energy in gas phase: -1733.795962 a.u.

M06 SCF energy in solution: -1734.31123 a.u.

M06 Free energy in solution: -1733.593789 a.u.

C	2.94996100	3.26820800	-1.24190800
C	2.21417800	2.01044400	-1.05632900
C	0.84722100	1.78508000	-1.58992900
C	-0.15402300	2.86024600	-1.48490300
H	0.31708800	3.75368800	-1.04521400
H	0.84483600	1.20729400	-2.52690900
C	-1.13420200	3.21709500	-2.57269400
C	-2.38373700	3.81976400	-0.54541800
C	-1.30195700	2.91761800	-0.03637300
C	-0.80818600	2.36792500	1.04964200
H	2.80489200	1.09874100	-0.93410300
H	4.04160100	3.25226900	-1.24289300
H	2.49107800	4.09294500	-1.79435700
H	-3.30748900	3.22079200	-0.57056200
H	-2.56426000	4.65426800	0.14417400
H	-0.60429200	3.58287800	-3.46358100
H	-1.71345000	2.32930400	-2.87136800
Rh	-0.50994800	0.95037600	-0.32069100
C	0.03733800	-0.94533000	0.27130600
N	1.17200000	-1.60700500	0.62003100
C	0.88771000	-2.89218900	1.05260800
C	2.51327800	-1.12393800	0.42960500
N	-0.95814800	-1.84886700	0.50535700
C	-0.45700200	-3.04519800	0.98179400
C	-2.34162900	-1.54593500	0.24528800
C	3.09606300	-0.32208900	1.42332300
C	3.18018700	-1.50004500	-0.74517500
C	4.40488100	0.10871900	1.20511800
C	2.35696100	0.02014400	2.69895600
C	5.09735500	-0.25295400	0.05512700
C	4.49184300	-1.04786600	-0.90801900
C	2.54130200	-2.35854100	-1.81769600
C	2.78081000	1.35719200	3.29552200
C	2.54022400	-1.09440300	3.73183000
C	2.50799400	-1.63860100	-3.16441800
C	3.25682500	-3.70292900	-1.93838900
C	-3.12268000	-1.01931000	1.28757600
C	-2.82687600	-1.73598900	-1.05695500
C	-4.14485300	-1.35410500	-1.31078800
C	-1.95888100	-2.27567700	-2.17540700
C	-4.93909000	-0.81878600	-0.30563100
C	-4.43568000	-0.66113900	0.97972100
C	-2.59205800	-0.89347200	2.70046600
C	-1.48277400	-1.13173900	-3.07044900
C	-2.66823700	-3.34383000	-3.00340900
C	-2.91589600	-2.15920200	3.49751400
C	-3.13250400	0.33143100	3.43266700
H	1.67390100	-3.57337000	1.35282500
H	-1.09676300	-3.88780700	1.20923100
H	4.89450300	0.73655100	1.94639100
H	6.12099600	0.08831000	-0.08872500
H	5.04731600	-1.32496100	-1.80366200
H	1.28445400	0.08841000	2.45130000
H	2.16747700	-2.06237400	3.37203100
H	2.00718900	-0.85301000	4.66101200
H	3.60502800	-1.21521500	3.97678700
H	3.79053400	1.30888900	3.72623000
H	2.10552500	1.63239800	4.11668100
H	2.76926500	2.15733400	2.54373900
H	1.49723000	-2.56085300	-1.53111600
H	4.30201800	-3.56947900	-2.24934000
H	2.76643700	-4.33729700	-2.68781500
H	3.26326800	-4.24582000	-0.98403000
H	3.51870700	-1.43457100	-3.54282400
H	1.97741200	-0.67758200	-3.09580700
H	1.99638000	-2.25418000	-3.91598000
H	-4.55701500	-1.47961800	-2.31104800
H	-5.96652600	-0.53218800	-0.52262000
H	-5.07806400	-0.25487800	1.75896800
H	-1.06641200	-2.74266500	-1.72941900
H	-3.05882600	-4.15195000	-2.37305900

H	-1.97309000	-3.78317300	-3.72984700
H	-3.50890900	-2.92630700	-3.57353900
H	-2.33530400	-0.60985300	-3.52913200
H	-0.83650800	-1.50220200	-3.87778300
H	-0.90982500	-0.38674900	-2.49093300
H	-1.49335700	-0.79761200	2.64734200
H	-4.00384500	-2.30290300	3.55861800
H	-2.52675300	-2.08494600	4.52123800
H	-2.48795600	-3.05919000	3.03767000
H	-4.19535100	0.21728900	3.68513600
H	-3.02670400	1.24754800	2.83523400
H	-2.59737000	0.47234200	4.38101200
C	-0.53105500	2.49425900	2.48347000
H	-1.22238500	3.21537100	2.94488000
H	-0.61716100	1.53779700	3.01436400
H	0.49019900	2.87727000	2.62862700
O	2.33675600	2.94986500	-0.00595500
C	-2.02302700	4.29377700	-1.95916400
H	-2.91800400	4.49974600	-2.55568900
H	-1.45378300	5.23275900	-1.90200300

TS4b (M06)

M06 SCF energy in gas phase: -1733.796247 a.u.

M06 SCF energy in solution: -1734.306122 a.u.

M06 Free energy in solution: -1733.584257 a.u.

C	-1.93661800	-2.20386400	-1.34342800
C	-1.75176900	-0.94088300	-1.52620100
C	-0.43050600	-3.45959800	-0.77813500
C	0.61722500	-3.20854500	0.21738700
C	1.79056100	-2.54345500	-0.06794000
C	2.09261800	-2.04961300	-1.46261100
H	0.43761100	-3.57320400	1.23359000
H	-0.04419900	-3.49035400	-1.80364500
H	2.55727500	-2.44844300	0.69985800
H	2.19914700	-2.89948600	-2.16364700
C	-1.35817800	-4.60885100	-0.46021800
H	-0.77648100	-5.54168700	-0.47152800
H	-1.76598800	-4.49577300	0.55820900
C	-3.03117100	-3.21096500	-1.47180300
H	-3.71841200	-3.09160000	-0.61676000
H	-3.61315500	-2.96504100	-2.37161200
H	3.04644200	-1.49980700	-1.46089600
C	1.22816700	2.61364300	1.00094900
C	-0.09510300	2.75754200	1.21350400
C	0.22063800	0.74898900	0.21066700
N	-0.71451400	1.61883900	0.70788000
N	1.40649900	1.38164800	0.39143300
Rh	-0.15783400	-1.16521500	-0.27655000
H	-0.66190500	3.55205900	1.67801700
H	2.06985900	3.25356600	1.23089900
C	2.71836500	0.84390700	0.15184500
C	3.29930800	1.03195500	-1.10936600
C	3.37570700	0.22453800	1.22688500
C	4.60046000	0.55717200	-1.28231600
C	4.66715200	-0.25105500	0.99031300
C	5.27225600	-0.08614800	-0.24984400
H	5.09491300	0.69087100	-2.24354100
H	5.21898200	-0.73620700	1.79543000
H	6.28483100	-0.45243500	-0.40924800
C	-2.14533500	1.45548800	0.73045000
C	-2.70134100	0.33936000	1.38886000
C	-2.94259500	2.42508000	0.09693000
C	-4.08830200	0.21311400	1.39398100
C	-4.33022000	2.26184500	0.16380100
C	-4.89985800	1.17027400	0.79550800
H	-4.55127600	-0.63721200	1.88900300
H	-4.97366900	3.00266900	-0.30809300
H	-5.98181400	1.05975700	0.82606800
C	2.77874400	0.15302700	2.62166600
H	1.72895400	0.48257500	2.57140400
C	3.52413000	1.11821700	3.54659000
H	3.54795600	2.13736900	3.13893800
H	3.04731400	1.15652300	4.53451700
H	4.56554200	0.79919100	3.69091700
C	2.77057800	-1.25128500	3.22138400
H	2.08992300	-1.92254300	2.67899300
H	3.76959700	-1.70736100	3.22678700
H	2.43021200	-1.21038200	4.26449100
C	2.58953900	1.77305800	-2.22216100
H	1.51563000	1.80103400	-1.98235100
C	3.09931800	3.21447400	-2.28481000
H	4.17236200	3.23922200	-2.52164600
H	2.57204800	3.77892000	-3.06490100
H	2.95918600	3.74045400	-1.33029800
C	2.72719800	1.08780500	-3.57718300
H	3.76701600	1.07895600	-3.93169800
H	2.35537800	0.05638000	-3.53684500
H	2.14011900	1.63068600	-4.32924200
C	-2.39139100	3.62750600	-0.65101000
H	-1.30953400	3.48650200	-0.79588900
C	-2.61164400	4.91151300	0.15418000
H	-2.14374700	5.76737800	-0.34854300
H	-3.68450700	5.12871800	0.24908300
H	-2.20770600	4.85381000	1.17347200
C	-3.00602500	3.79538800	-2.04074000
H	-2.51757800	4.62867600	-2.56130900
H	-2.88898000	2.89906100	-2.66138800
H	-4.07659400	4.03322900	-1.99041800
C	-1.84861400	-0.67318300	2.12523300
H	-0.96381700	-0.96312000	1.49017800
C	-1.22739100	-0.07339200	3.38676800
H	-2.02298300	0.17987000	4.10137000
H	-0.55468000	-0.79562100	3.86900300
H	-0.65770800	0.84147500	3.18142000
C	-2.54520500	-1.98514700	2.45139900
H	-3.32299900	-1.84833600	3.21465100
H	-3.00735700	-2.43991200	1.56471500

H	-1.81585700	-2.69618000	2.86202400
C	-2.22775000	0.18125400	-2.35509400
H	-1.40356700	0.86782500	-2.59572300
H	-3.01007500	0.75114500	-1.83735600
H	-2.64452300	-0.19284100	-3.29976900
O	1.03790900	-1.20924900	-1.86075700
C	-2.47008200	-4.61955400	-1.48907000
H	-3.23885600	-5.36833700	-1.26966100
H	-2.05415600	-4.85446300	-2.47962600

1c (M06)

M06 SCF energy in gas phase: -2611.812971 a.u.

M06 SCF energy in solution: -2612.570625 a.u.

M06 Free energy in solution: -2611.651865 a.u.

C	2.64247500	2.44231800	-1.12049800
C	2.03486800	1.18938300	-0.62267100
C	0.73415000	0.67076100	-1.12362900
C	-0.41905700	1.47962200	-1.00159100
H	-0.25401700	2.42687800	-0.47326500
H	0.79265100	-0.06849700	-1.92646800
C	-1.62426100	1.42991100	-1.89051200
C	-3.31465000	1.14651800	0.00840300
C	-2.20019600	0.97344700	0.94798700
C	-1.40720100	1.16435600	1.92520500
H	2.74182700	0.44826900	-0.24834700
H	2.08180500	3.00120000	-1.87916900
H	-3.65050200	0.16424600	-0.36174500
H	-4.16028200	1.63803400	0.50791700
H	-1.42891900	2.02543000	-2.79637400
H	-1.82770100	0.40498200	-2.23171900
Rh	-0.48994500	-0.01868000	0.49764400
C	0.22279200	-1.92448200	0.08628300
N	1.41719800	-2.57364300	0.04431800
C	1.24568900	-3.94169900	0.17917600
C	2.70614600	-2.01338200	-0.26746200
N	-0.69592100	-2.92464200	0.20292500
C	-0.08576400	-4.16278000	0.27606800
C	-2.12526300	-2.74009800	0.23500000
C	3.53516500	-1.57618500	0.77168800
C	3.08132700	-1.97493200	-1.62153100
C	4.79591800	-1.08890500	0.41780500
C	3.10168400	-1.56371400	2.22116000
C	5.19658700	-1.03155700	-0.90929600
C	4.34526200	-1.46658800	-1.91823500
C	2.17707600	-2.48339100	-2.72686500
C	3.12283300	-0.13895400	2.77569300
C	3.96669500	-2.50069000	3.06127500
C	2.17133100	-1.57858700	-3.95737900
C	2.56798300	-3.90758000	-3.12657800
C	-2.76553600	-2.72655600	1.48186200
C	-2.80760400	-2.61812900	-0.99003700
C	-4.19640400	-2.50298800	-0.92885800
C	-2.07722400	-2.63509300	-2.32084800
C	-4.86424700	-2.50541500	0.29228700
C	-4.15741700	-2.60681100	1.48181700
C	-2.00532900	-2.87060200	2.78508000
C	-2.84852700	-1.95862000	-3.44907200
C	-1.72264700	-4.06348300	-2.74480000
C	-2.08840300	-4.31226900	3.29012500
C	-2.49531400	-1.90708100	3.86310500
H	2.09341700	-4.61465200	0.18746900
H	-0.66147200	-5.07400200	0.37533800
H	5.47027300	-0.73242700	1.19619900
H	6.17931500	-0.63876600	-1.16335700
H	4.67157200	-1.41110200	-2.95590200
H	2.06228700	-1.92727200	2.27838900
H	3.93060700	-3.53113000	2.68301500
H	3.62816400	-2.50878000	4.10538700
H	5.01826600	-2.18256400	3.05664300
H	4.14216400	0.27246600	2.78035200
H	2.76529200	-0.12529900	3.81432200
H	2.48871000	0.54175000	2.18592400
H	1.14533000	-2.51866300	-2.34026600
H	3.60425900	-3.93449300	-3.49160200
H	1.91924900	-4.27718300	-3.93165600
H	2.49256800	-4.60699900	-2.28355700
H	3.10661100	-1.66015400	-4.52731300
H	2.03598200	-0.51896200	-3.69825200
H	1.35717600	-1.87251800	-4.63352200
H	-4.76741700	-2.41193500	-1.85077200
H	-5.94956100	-2.42439600	0.31381100
H	-4.69407600	-2.59976400	2.42943200
H	-1.13291200	-2.07872000	-2.18607000
H	-1.05173000	-4.56586100	-2.03637500
H	-1.22376700	-4.05365700	-3.72372100
H	-2.63444900	-4.66983300	-2.84032800
H	-3.70848500	-2.56432900	-3.76814800
H	-2.19657600	-1.85094300	-4.32559200
H	-3.22283900	-0.96035700	-3.18480700
H	-0.94266600	-2.63977500	2.59206000
H	-3.13297500	-4.58926900	3.49016600
H	-1.52528300	-4.43007700	4.22487500
H	-1.68953000	-5.02967900	2.56113200
H	-3.50988100	-2.15718400	4.20091000
H	-2.50303100	-0.86579000	3.51281200
H	-1.84314200	-1.96541400	4.74419900
C	-2.88191200	1.99653500	-1.21146400
O	2.00123800	2.37880200	0.14338700
C	-2.64264100	3.43738800	-0.76069900
O	-2.73777100	3.83458800	0.37458800
O	-2.29041000	4.19756500	-1.79919100
C	-4.04479500	1.97301900	-2.20158000
O	-4.08423800	1.29596700	-3.19912100
O	-5.03513600	2.76069700	-1.78079000
C	-6.19704500	2.79258400	-2.61694000
H	-6.88923900	3.48617400	-2.13835800
H	-5.93037500	3.14055600	-3.61953800

H	-6.63815700	1.79363700	-2.69071500
C	-2.05928100	5.57834000	-1.49983500
H	-1.78664100	6.04654200	-2.44644600
H	-2.96788000	6.03172100	-1.09171200
H	-1.24893900	5.67871600	-0.77060100
C	4.11683900	2.59315500	-1.13796700
C	4.77858700	2.77644600	-2.35240700
C	4.85580400	2.49030800	0.04095200
C	6.16666200	2.84848900	-2.38950100
H	4.20173300	2.86272100	-3.27451800
C	6.24331700	2.57375200	0.00329300
H	4.32940700	2.36257400	0.98642400
C	6.90205100	2.74866300	-1.21111400
H	6.67562200	2.99381700	-3.34072400
H	6.81443400	2.51116000	0.92851300
H	7.98788600	2.81835200	-1.23923200
C	-0.88400900	1.78829900	3.10667900
C	-0.01895600	1.09200500	3.96224400
C	-1.23884100	3.11533900	3.39584400
C	0.48407100	1.71300400	5.09536700
H	0.24028700	0.05851300	3.72556800
C	-0.72443500	3.72991000	4.52842800
H	-1.90642700	3.64394800	2.71715600
C	0.13310500	3.03197000	5.37696200
H	1.14902400	1.16938700	5.76420500
H	-0.99445900	4.75940400	4.75450800
H	0.52777900	3.51787400	6.26729400

TS1c (M06)

M06 SCF energy in gas phase: -2611.779869 a.u.

M06 SCF energy in solution: -2612.536141 a.u.

M06 Free energy in solution: -2611.620488 a.u.

C	2.05842000	2.93713000	-0.37269500
C	1.64925100	1.51525300	-0.34908400
C	0.34964400	1.02695600	-0.87699800
C	-0.86584600	1.74913700	-0.53843600
H	-0.66075100	2.61967400	0.10113900
H	0.41996500	0.63378600	-1.90034500
C	-1.98634200	1.95798200	-1.52125200
C	-3.31430500	1.28825900	0.43192600
C	-1.91970600	0.97257000	0.84059500
C	-1.10812800	0.71290100	1.84008000
H	2.46438200	0.78754100	-0.37624500
H	1.34395700	3.65572100	-0.79377000
H	-3.79289700	0.36208100	0.07301300
H	-3.90386900	1.67849700	1.27003800
H	-1.73121900	2.76704800	-2.22105900
H	-2.17100200	1.05544400	-2.11891000
Rh	-0.54523100	-0.45869400	0.25208100
C	0.52022100	-2.17490600	-0.28448300
N	1.74814200	-2.57074700	-0.70560500
C	1.83234000	-3.95090500	-0.78352200
C	2.81382200	-1.68463900	-1.08526200
N	-0.16310400	-3.34275000	-0.12081100
C	0.62081800	-4.44011800	-0.41830900
C	-1.55427300	-3.33834500	0.24998700
C	3.75899500	-1.31743300	-0.11994100
C	2.84820300	-1.22504000	-2.41225000
C	4.79641400	-0.47647900	-0.53001100
C	3.66459200	-1.77178600	1.32062100
C	4.86336700	-0.00634900	-1.83430200
C	3.89596900	-0.37348500	-2.76309800
C	1.81585000	-1.65676700	-3.43481900
C	3.65516400	-0.58335200	2.28124200
C	4.78809800	-2.75039300	1.65784500
C	1.45828300	-0.55600700	-4.42877300
C	2.29444400	-2.90213800	-4.18328000
C	-1.88878900	-3.36418700	1.61501500
C	-2.50883500	-3.24136100	-0.77539400
C	-3.84642500	-3.13408300	-0.39282300
C	-2.12756700	-3.21507200	-2.24191800
C	-4.20895100	-3.14164900	0.94779000
C	-3.24304400	-3.26557700	1.93867300
C	-0.84030500	-3.55616900	2.69071900
C	-2.19457400	-1.79084700	-2.79551700
C	-2.98629500	-4.16001200	-3.07909500
C	-0.64153700	-5.04958000	2.96059900
C	-1.17461100	-2.83081400	3.98994900
H	2.74460400	-4.44697600	-1.09021500
H	0.24392500	-5.45277300	-0.35545600
H	5.55143700	-0.16424200	0.19104600
H	5.66847700	0.66615400	-2.12604100
H	3.95665900	0.00986100	-3.78044400
H	2.70669900	-2.30017500	1.45083500
H	4.77068700	-3.62699200	0.99632600
H	4.69892100	-3.10387500	2.69337200
H	5.77353300	-2.27547500	1.55230500
H	4.61022400	-0.03820600	2.26354000
H	3.50077400	-0.93020100	3.31254600
H	2.85431600	0.13122000	2.03716700
H	0.89288600	-1.92318900	-2.89425300
H	3.22309300	-2.68793900	-4.73107900
H	1.54086700	-3.23234300	-4.91074100
H	2.49416400	-3.73889700	-3.50149100
H	2.28596300	-0.34116800	-5.11854000
H	1.19173500	0.38606900	-3.92872500
H	0.60395900	-0.86706200	-5.04372600
H	-4.61638100	-3.04475000	-1.15818000
H	-5.25888900	-3.06436600	1.22496600
H	-3.54890300	-3.28602500	2.98305500
H	-1.08275700	-3.55337300	-2.33501400
H	-2.98585800	-5.17862700	-2.67151800
H	-2.60567300	-4.20418800	-4.10726600
H	-4.02943600	-3.82146700	-3.13753400
H	-3.20893200	-1.37228100	-2.70776000
H	-1.91369300	-1.77202500	-3.85796700
H	-1.50943500	-1.12580400	-2.24467200

H	0.11325200	-3.14956100	2.31338700
H	-1.57754000	-5.49999800	3.32041300
H	0.12640600	-5.20803300	3.72897700
H	-0.33543200	-5.59530500	2.05842700
H	-2.01614500	-3.30333500	4.51476300
H	-1.43030300	-1.77580500	3.81945900
H	-0.31548800	-2.86631600	4.67288600
O	1.61534100	2.31069300	0.82195200
C	-3.25055700	2.30236100	-0.72536500
C	-3.11945800	3.71156000	-0.15921300
O	-2.85427800	3.97172000	0.99127100
O	-3.27465900	4.62098100	-1.12046900
C	-4.49774600	2.17199500	-1.58442200
O	-4.53689100	1.63479400	-2.66311100
O	-5.55459300	2.66715700	-0.93746800
C	-6.80419200	2.56664600	-1.62775400
H	-7.55212900	2.97957900	-0.94961100
H	-6.76863000	3.14067700	-2.55897500
H	-7.02804200	1.52079300	-1.86051100
C	-3.16503500	5.98649400	-0.70417100
H	-3.34267500	6.58499100	-1.59832000
H	-3.91285100	6.20627100	0.06384000
H	-2.16718600	6.18091500	-0.29820300
C	3.48845800	3.30938300	-0.47157100
C	4.41463200	2.84127200	0.46105200
C	3.92491500	4.08597000	-1.54508500
C	5.76423600	3.13966100	0.31230700
H	4.06271600	2.24895500	1.30546200
C	5.27577000	4.37818100	-1.69608200
H	3.20065700	4.46307200	-2.26871000
C	6.19898800	3.90267500	-0.76866300
H	6.48196800	2.77874700	1.04813200
H	5.60786000	4.98484700	-2.53659500
H	7.25584200	4.13688400	-0.88240300
C	-0.54198200	1.12607300	3.07113300
C	0.40128500	0.33265500	3.74869500
C	-0.90038100	2.38964800	3.58527800
C	0.96795400	0.78979100	4.92563800
H	0.67583600	-0.63411600	3.32470600
C	-0.33434100	2.83189800	4.76927300
H	-1.61150500	3.00180600	3.02846700
C	0.59638500	2.03464100	5.43662200
H	1.70023100	0.18169200	5.45324900
H	-0.60780200	3.80424000	5.17306900
H	1.04042600	2.38967100	6.36488800

TS4c (M06)

M06 SCF energy in gas phase: -2611.775401 a.u.

M06 SCF energy in solution: -2612.529455 a.u.

M06 Free energy in solution: -2611.609197 a.u.

C	-2.18133800	0.24217000	0.22063300
C	-1.46720400	-0.52351600	1.03201800
C	-1.60276200	2.09538900	-0.62166700
C	-0.55052500	1.98549000	-1.63036300
C	0.78628900	2.22198600	-1.43067900
C	1.34847200	2.64003000	-0.09244400
H	-0.87928100	1.64515400	-2.61663800
H	-1.35307400	2.67801300	0.27231000
H	1.47529600	2.07559600	-2.26475800
H	0.66510300	3.40132700	0.34216500
C	-2.97371800	2.37415700	-1.17943200
H	-3.11361400	3.46182300	-1.25027300
H	-3.06625500	1.97335300	-2.19864500
C	-3.61375300	0.28772000	-0.18394100
H	-3.73083300	-0.21736100	-1.15728700
H	-4.22093500	-0.25044100	0.55557700
C	2.62740200	-2.89415700	0.18079300
C	1.74086000	-3.34343400	-0.73375000
C	1.14949000	-1.23496800	-0.17187900
N	0.83999900	-2.31037600	-0.95359200
N	2.27249800	-1.58682800	0.50336700
Rh	-0.11669500	0.31487400	-0.11858600
H	1.65965200	-4.28661900	-1.25858400
H	3.49959600	-3.35473200	0.62630200
C	3.23030700	-0.75199000	1.20690800
C	3.03701000	-0.44330300	2.55675600
C	4.38623600	-0.39056700	0.49870100
C	4.07756900	0.20422400	3.22324000
C	5.39628600	0.25477900	1.21258800
C	5.25508300	0.53315300	2.56482400
H	3.96530900	0.44077800	4.28089900
H	6.30814400	0.54851700	0.69241300
H	6.06250400	1.02432400	3.10602800
C	-0.14296100	-2.27934900	-2.01287300
C	0.16071200	-1.52500000	-3.16681100
C	-1.33759000	-3.00031400	-1.87181000
C	-0.82010400	-1.45161300	-4.15516100
C	-2.28039200	-2.89224200	-2.89832900
C	-2.03552700	-2.11303700	-4.01739700
H	-0.62772400	-0.87871600	-5.05980100
H	-3.21811300	-3.44092200	-2.82036000
H	-2.78403200	-2.03903400	-4.80426400
C	4.57402200	-0.65171800	-0.98242600
H	3.67143600	-1.14356200	-1.37454600
C	5.75180600	-1.58821600	-1.24406300
H	5.63818600	-2.54491400	-0.71649500
H	5.84497800	-1.80224600	-2.31736700
H	6.69874300	-1.13975100	-0.91354500
C	4.73062600	0.65572800	-1.75656300
H	3.87993500	1.33031200	-1.58101700
H	5.63782800	1.20049400	-1.46037600
H	4.80739100	0.45241800	-2.83458400
C	1.77680700	-0.82624500	3.28893200
H	1.03008900	-1.09159400	2.53222500
C	2.01898700	-2.05190400	4.16638300
H	2.78982200	-1.85009900	4.92352100
H	1.09830400	-2.34037700	4.69218700

H	2.35745100	-2.91386600	3.57103500
C	1.17936700	0.32664100	4.08718900
H	1.81173400	0.61864600	4.93716500
H	1.03012800	1.20637700	3.44679800
H	0.20437300	0.02495400	4.49715500
C	-1.60379400	-3.94247300	-0.71811200
H	-0.87518900	-3.73039000	0.07587100
C	-1.39015200	-5.38894500	-1.17107900
H	-1.53029300	-6.08229300	-0.33179600
H	-2.10868300	-5.66366000	-1.95578700
H	-0.38396100	-5.54957100	-1.58143800
C	-2.99697300	-3.78108400	-0.11596900
H	-3.08756400	-4.39292200	0.79155800
H	-3.20321200	-2.73951200	0.16473100
H	-3.78293500	-4.10997400	-0.80938700
C	1.52091600	-0.88591000	-3.38631000
H	1.87203700	-0.47086900	-2.42740600
C	2.53175500	-1.94362300	-3.84203900
H	2.20200500	-2.40438700	-4.78399100
H	3.51430100	-1.48365500	-4.02000100
H	2.66678800	-2.74339600	-3.10209800
C	1.51274900	0.25948600	-4.39361400
H	1.36703300	-0.09977300	-5.42144400
H	0.72845900	1.00154200	-4.18674500
H	2.48178300	0.77590400	-4.37424900
O	1.33588800	1.47264500	0.68442700
C	-4.06547800	1.73449500	-0.33494100
C	-4.19350400	2.39898900	1.03030900
O	-4.01178800	1.84810000	2.09022700
O	-4.51693100	3.68358500	0.89286200
C	-5.40198600	1.78005200	-1.06690200
O	-5.52372500	1.96842200	-2.25063600
O	-6.40036900	1.51501200	-0.22401700
C	-7.70993600	1.49897800	-0.80524800
H	-8.39836200	1.30393200	0.01772400
H	-7.92609000	2.46474100	-1.27198600
H	-7.77908300	0.71153100	-1.56217600
C	-4.72295200	4.40489200	2.11347300
H	-4.99875900	5.41749100	1.81717300
H	-5.52559900	3.93837000	2.69271600
H	-3.80625700	4.41282000	2.71138300
C	2.71807000	3.26624900	-0.17770900
C	3.64451900	3.05884300	0.84095000
C	3.04492200	4.10808900	-1.24207600
C	4.89199900	3.67171400	0.78305000
H	3.38603900	2.40554200	1.67367300
C	4.29450200	4.71601200	-1.30125200
H	2.31793800	4.30009700	-2.03403200
C	5.22301300	4.49597500	-0.28783800
H	5.61237300	3.49838100	1.58184800
H	4.54206600	5.36476500	-2.13951700
H	6.20078900	4.97223600	-0.33168500
C	-1.71720400	-1.45054100	2.11082700
C	-0.90726000	-2.56621400	2.36705800
C	-2.82914000	-1.20365500	2.93668600
C	-1.21877300	-3.43401400	3.40353400
H	-0.03252200	-2.75463300	1.74583900
C	-3.12469100	-2.06752000	3.98157000
H	-3.43068900	-0.31119100	2.76358200
C	-2.32747900	-3.18632100	4.21169100
H	-0.58811400	-4.30129000	3.59077900
H	-3.98051900	-1.86522300	4.62214600
H	-2.56418800	-3.86364500	5.02992700

1c (M06-solvent)

M06 SCF energy in gas phase: -2611.908715 a.u.

M06 SCF energy in solution: -2612.572351 a.u.

M06 Free energy in solution: -2611.651231 a.u.

C	2.56672400	2.48191500	-1.08056000
C	1.98456500	1.23489000	-0.54129400
C	0.68398300	0.70777700	-1.03124600
C	-0.48180600	1.49022900	-0.88915700
H	-0.33929300	2.43172800	-0.34418100
H	0.74999800	-0.01152500	-1.85089600
C	-1.66858300	1.45053600	-1.80305900
C	-3.36282100	1.12649700	0.07931400
C	-2.24551300	0.97314300	1.01960300
C	-1.43379800	1.19057400	1.96731500
H	2.69987600	0.50095600	-0.16766100
H	1.97578500	3.02028500	-1.82968500
H	-3.68451100	0.14239400	-0.29845300
H	-4.21994800	1.59244500	0.58268600
H	-1.45698000	2.06310400	-2.69315600
H	-1.85442100	0.42974300	-2.16442700
Rh	-0.52395000	-0.05592700	0.55977300
C	0.25490700	-1.93722400	0.07343900
N	1.45781100	-2.56588700	-0.01932900
C	1.31184600	-3.94275000	0.05203700
C	2.73530200	-1.98075000	-0.32317200
N	-0.64129100	-2.95860100	0.16444100
C	-0.01250200	-4.19068000	0.16714000
C	-2.06991900	-2.80608400	0.23073100
C	3.57430100	-1.58312700	0.72514200
C	3.09942800	-1.89346500	-1.67748800
C	4.83106900	-1.07823800	0.37991300
C	3.16474500	-1.68246400	2.17908800
C	5.21966100	-0.97327500	-0.94931600
C	4.36141900	-1.37356300	-1.96747800
C	2.18569000	-2.36613500	-2.79063800
C	3.33811100	-0.35134400	2.90590600
C	3.94368800	-2.79424200	2.87914800
C	2.12044900	-1.38959000	-3.96213800
C	2.61296100	-3.74916700	-3.28232300
C	-2.68566800	-2.81759200	1.49084100
C	-2.78329500	-2.69087700	-0.97661100
C	-4.17377800	-2.61639600	-0.88715000
C	-2.07887800	-2.65139900	-2.31987000

C	-4.81558300	-2.64377200	0.34764400
C	-4.08051700	-2.73198600	1.52235300
C	-1.89051800	-2.94905600	2.77378500
C	-2.86780100	-1.91037200	-3.39342000
C	-1.74694700	-4.05796800	-2.82136300
C	-1.92438000	-4.39559200	3.26691100
C	-2.38156400	-2.00962800	3.87150700
H	2.16717600	-4.60467100	0.00295300
H	-0.57136400	-5.11524700	0.23950300
H	5.51436500	-0.75740900	1.16626100
H	6.20279200	-0.57575900	-1.19762600
H	4.68096700	-1.28395800	-3.00537500
H	2.09562400	-1.94726900	2.22165900
H	3.79838200	-3.76282900	2.38101200
H	3.61773000	-2.89651500	3.92317600
H	5.02172400	-2.57781200	2.88437700
H	4.38958000	-0.03193800	2.92351900
H	3.01252300	-0.44681700	3.95105700
H	2.75056300	0.45149900	2.43507600
H	1.16627700	-2.46026400	-2.38174500
H	3.63575500	-3.71827700	-3.68517600
H	1.94614300	-4.09675100	-4.08358700
H	2.59122800	-4.49447400	-2.47594000
H	3.04516000	-1.40149900	-4.55579100
H	1.95072200	-0.35366200	-3.63371500
H	1.29904600	-1.67174700	-4.63588200
H	-4.76668400	-2.53358500	-1.79654000
H	-5.90216600	-2.58878500	0.39272300
H	-4.59661500	-2.74344300	2.48183400
H	-1.12463100	-2.11607800	-2.17827600
H	-1.10372700	-4.61316100	-2.12676300
H	-1.22542900	-4.00151000	-3.78774200
H	-2.66942200	-4.63873700	-2.96874700
H	-3.73351600	-2.49611200	-3.73440300
H	-2.22871800	-1.74206800	-4.27076100
H	-3.23880000	-0.93247100	-3.05514600
H	-0.83954400	-2.68964300	2.55770700
H	-2.95708900	-4.69631700	3.49647000
H	-1.32962200	-4.50677100	4.18378600
H	-1.53012200	-5.09479100	2.51738600
H	-3.37414400	-2.30190300	4.24091000
H	-2.44659500	-0.96782100	3.52560000
H	-1.69524600	-2.04226500	4.72844500
C	-2.94434400	1.98717300	-1.13551600
O	1.96868400	2.43797700	0.20812800
C	-2.75699100	3.43993700	-0.69516400
O	-2.88364700	3.85159900	0.43376200
O	-2.43898900	4.20091800	-1.74207600
C	-4.09427400	1.96308600	-2.14035300
O	-4.06386700	1.42373200	-3.22112400
O	-5.15462200	2.60128700	-1.64606700
C	-6.31782900	2.62159200	-2.48229800
H	-7.08795100	3.14252200	-1.91089500
H	-6.10820200	3.15895900	-3.41305000
H	-6.63918400	1.60072300	-2.71210000
C	-2.25697700	5.59546300	-1.46696100
H	-1.99508100	6.05554500	-2.42133000
H	-3.18342700	6.02945200	-1.07692200
H	-1.44964000	5.73893100	-0.74137900
C	4.03696400	2.65664000	-1.15227000
C	4.64539900	2.85680500	-2.39321800
C	4.82845900	2.56602500	-0.00583300
C	6.03001600	2.95808300	-2.48670600
H	4.02830400	2.92734300	-3.29013700
C	6.21217500	2.68026200	-0.09933800
H	4.34857000	2.41983000	0.96180500
C	6.81649900	2.87360100	-1.33965800
H	6.49691700	3.11032000	-3.45879200
H	6.82122300	2.62031500	0.80172200
H	7.89930000	2.96210700	-1.41301500
C	-0.84231300	1.84168400	3.10486100
C	0.09263500	1.17670300	3.91189000
C	-1.17907700	3.17574500	3.38314200
C	0.68434000	1.83868000	4.97928900
H	0.34428100	0.13743200	3.69063400
C	-0.58057200	3.83012400	4.45180400
H	-1.90042800	3.68297900	2.74347600
C	0.35001600	3.16479100	5.24853800
H	1.41021800	1.32000300	5.60333600
H	-0.83864500	4.86602500	4.66465800
H	0.81792300	3.68196200	6.08449800

TS1c (M06-solvent)

M06 SCF energy in gas phase: -2611.878457 a.u.

M06 SCF energy in solution: -2612.540647 a.u.

M06 Free energy in solution: -2611.61995 a.u.

C	2.05245400	3.04972200	-0.05210600
C	1.65784100	1.62911800	-0.15943500
C	0.39591200	1.20411900	-0.81747700
C	-0.85746700	1.83614500	-0.39831800
H	-0.65864800	2.59439500	0.37264200
H	0.52203700	1.01864900	-1.89336000
C	-1.95170000	2.23990700	-1.34666500
C	-3.26192300	1.50029400	0.61648100
C	-1.89893700	0.95323700	0.87046800
C	-1.13400500	0.34754100	1.75995600
H	2.47552800	0.90421000	-0.19398300
H	1.35088700	3.79113800	-0.45142800
H	-3.89361900	0.67461000	0.25115000
H	-3.72497200	1.89231900	1.52968700
H	-1.64057500	3.10185200	-1.95381900
H	-2.20646800	1.42420100	-2.03623500
Rh	-0.60998000	-0.39953700	-0.05061500
C	0.55604600	-2.09772400	-0.41101700
N	1.83269700	-2.42991600	-0.73634200
C	1.97194300	-3.80057400	-0.90037200
C	2.90675900	-1.50830000	-0.98698400

N	-0.09973300	-3.29565400	-0.40104100
C	0.75007600	-4.34722800	-0.69412000
C	-1.53193500	-3.36984300	-0.28383600
C	3.81682800	-1.24165800	0.04296000
C	3.01016900	-0.93553300	-2.26891600
C	4.87950200	-0.37892400	-0.24365800
C	3.66223600	-1.80366100	1.43950400
C	5.01448000	0.19487900	-1.49958200
C	4.08554300	-0.07672900	-2.49918800
C	2.00581200	-1.23990600	-3.36335500
C	3.47634800	-0.67408800	2.45173100
C	4.85104500	-2.68482600	1.81432400
C	1.79815600	-0.08491500	-4.33710300
C	2.39733900	-2.49692300	-4.14088100
C	-2.10614300	-3.66267400	0.96464700
C	-2.29409600	-3.08053600	-1.42858800
C	-3.68231600	-3.03010300	-1.27988400
C	-1.66565600	-2.82931300	-2.78637100
C	-4.27723800	-3.28750500	-0.05132200
C	-3.49911600	-3.61621800	1.05302200
C	-1.26393600	-4.06331800	2.15689800
C	-1.75667400	-1.35842100	-3.18689200
C	-2.28618500	-3.71456400	-3.86475200
C	-1.09598600	-5.58408900	2.18882900
C	-1.83522300	-3.58317000	3.48652000
H	2.92638500	-4.24707100	-1.15078200
H	0.40266700	-5.37123500	-0.74096700
H	5.60361500	-0.14458100	0.53726100
H	5.84164200	0.87518500	-1.69935800
H	4.20261300	0.39032200	-3.47581500
H	2.75740800	-2.43069600	1.46840000
H	4.98547800	-3.50833800	1.09956000
H	4.70948800	-3.12132200	2.81234400
H	5.78459700	-2.10454600	1.83503400
H	4.36854400	-0.03167900	2.49640200
H	3.31877700	-1.08534200	3.45849100
H	2.61226600	-0.03955900	2.19878500
H	1.03680000	-1.43796600	-2.87909700
H	3.36003800	-2.34990600	-4.65265900
H	1.63907900	-2.72177700	-4.90531700
H	2.49190500	-3.37761500	-3.49245800
H	2.67235500	0.06769200	-4.98529500
H	1.59177100	0.86592200	-3.82490000
H	0.94822800	-0.30552600	-4.99695000
H	-4.30574400	-2.79109100	-2.14123100
H	-5.36112100	-3.24704400	0.04483200
H	-3.98545100	-3.83713900	2.00189000
H	-0.59737600	-3.09177000	-2.73126800
H	-2.25503200	-4.77557500	-3.58432300
H	-1.73627400	-3.59751700	-4.80847100
H	-3.33386000	-3.44869800	-4.06223900
H	-2.80072800	-1.00904800	-3.20254300
H	-1.33771300	-1.20799300	-4.19304000
H	-1.19497100	-0.70995400	-2.49197100
H	-0.26443800	-3.61401800	2.03320400
H	-2.07532600	-6.07339200	2.29636900
H	-0.47309200	-5.88538800	3.04218600
H	-0.62840300	-5.97193800	1.27407300
H	-2.74122400	-4.14058400	3.76318600
H	-2.08745900	-2.51402300	3.46899800
H	-1.10233700	-3.74384500	4.28895600
O	1.55877400	2.32658700	1.06950700
C	-3.17096600	2.58454000	-0.47675200
C	-2.96021900	3.95118900	0.16868800
O	-2.66414100	4.13492400	1.32712900
O	-3.11074900	4.92024400	-0.73273500
C	-4.45371400	2.60418200	-1.29046100
O	-4.55553200	2.25743800	-2.44333500
O	-5.46914400	3.01598900	-0.53056900
C	-6.75069900	3.05699500	-1.16771500
H	-7.44500300	3.44397200	-0.41952600
H	-6.72405600	3.72106000	-2.03769200
H	-7.05457100	2.05283400	-1.48169100
C	-2.93775600	6.25779000	-0.24899300
H	-3.11300700	6.90968500	-1.10637600
H	-3.66153800	6.47101700	0.54415300
H	-1.92226800	6.39732900	0.13577700
C	3.48019100	3.44629400	-0.04582100
C	4.36720000	2.93337700	0.90238900
C	3.95651100	4.30959600	-1.03495000
C	5.71550800	3.27356500	0.85479900
H	3.98936800	2.27101700	1.68112200
C	5.30607600	4.64285800	-1.08577100
H	3.26200900	4.72029500	-1.76917400
C	6.18978900	4.12437700	-0.14143100
H	6.40051200	2.87181100	1.60069700
H	5.66856300	5.31573400	-1.86149300
H	7.24513900	4.38983600	-0.17732400
C	-0.73656900	0.31280000	3.13214300
C	0.02352200	-0.74226600	3.66230700
C	-1.11069600	1.38296700	3.96950200
C	0.38243000	-0.73772800	5.00249800
H	0.32026800	-1.56445100	3.00930500
C	-0.75477600	1.37553600	5.30938600
H	-1.67495100	2.21310000	3.54331900
C	-0.00856000	0.31648400	5.82764200
H	0.96787900	-1.56071700	5.40950700
H	-1.04867700	2.20333200	5.95213800
H	0.27437800	0.31589600	6.87881500

TS4c (M06-solvent)

M06 SCF energy in gas phase: -2611.868301 a.u.

M06 SCF energy in solution: -2612.530788 a.u.

M06 Free energy in solution: -2611.608529 a.u.

C	-2.21213600	0.20180600	0.28285600
C	-1.43912800	-0.54084500	1.04541600
C	-1.66370700	2.02932900	-0.67833400

C	-0.60815700	1.95377300	-1.68151600
C	0.72260500	2.20791500	-1.45815000
C	1.24765100	2.63507100	-0.10622600
H	-0.91994400	1.62350500	-2.67626800
H	-1.44243800	2.63444500	0.20769000
H	1.42583600	2.09508200	-2.28607100
H	0.52182200	3.35570100	0.32539900
C	-3.04357300	2.23858200	-1.23638600
H	-3.18850300	3.31417200	-1.41046800
H	-3.14226400	1.73405400	-2.20780900
C	-3.66318300	0.24577800	-0.04549900
H	-3.84447000	-0.34320600	-0.95953400
H	-4.23224700	-0.22218200	0.76803400
C	2.67754800	-2.89189500	0.14673000
C	1.78016600	-3.35832800	-0.74761200
C	1.18015000	-1.24376700	-0.20422300
N	0.87105300	-2.33203400	-0.96818000
N	2.31466900	-1.58181900	0.46316700
Rh	-0.11616900	0.27963500	-0.18548300
H	1.69245400	-4.31127100	-1.25500900
H	3.55969900	-3.34360600	0.58227700
C	3.27607800	-0.73613900	1.14599800
C	3.14359100	-0.47375300	2.51518300
C	4.39175600	-0.31846200	0.40200700
C	4.18852300	0.20022900	3.15057900
C	5.40879500	0.35192900	1.08424500
C	5.31898100	0.59719200	2.44768300
H	4.11714200	0.40285500	4.21908000
H	6.28439400	0.69117900	0.52964500
H	6.12916400	1.11155100	2.96321200
C	-0.13672700	-2.32807300	-2.00369200
C	0.13591400	-1.60935200	-3.18779200
C	-1.33205300	-3.03804400	-1.81401300
C	-0.87096600	-1.55456100	-4.15183400
C	-2.30640600	-2.94655300	-2.81290000
C	-2.08824300	-2.19985600	-3.96081800
H	-0.69660500	-1.00730500	-5.07598000
H	-3.24647500	-3.48293600	-2.68879900
H	-2.86013500	-2.13866000	-4.72649900
C	4.52778100	-0.53830700	-1.09156600
H	3.65831700	-1.11018700	-1.44441500
C	5.77273000	-1.35213700	-1.43424200
H	5.78691100	-2.31550100	-0.90612500
H	5.81129900	-1.55659400	-2.51320600
H	6.69201100	-0.81115000	-1.16837800
C	4.52386500	0.79296100	-1.84175700
H	3.61329000	1.37368400	-1.63227700
H	5.38353100	1.41798700	-1.55768400
H	4.58187200	0.62207200	-2.92683600
C	1.94321200	-0.93014900	3.30540800
H	1.15993600	-1.18945900	2.58627700
C	2.27243100	-2.18328200	4.11266400
H	3.08743800	-1.98785300	4.82518900
H	1.39484100	-2.51105500	4.68780200
H	2.58578400	-3.01806000	3.46798300
C	1.36796000	0.15585800	4.20708500
H	2.04106200	0.40573500	5.03970000
H	1.16046300	1.07773400	3.64619500
H	0.42288000	-0.19400500	4.64861200
C	-1.56550400	-3.95562600	-0.63429700
H	-0.81648900	-3.72554700	0.13361700
C	-1.34730500	-5.40711800	-1.06441200
H	-1.46493600	-6.08549600	-0.20851800
H	-2.07838200	-5.70319400	-1.83074200
H	-0.34347300	-5.55944500	-1.48480800
C	-2.94584500	-3.78902300	-0.00764200
H	-3.01533600	-4.38012500	0.91637800
H	-3.15543300	-2.74094800	0.24887800
H	-3.74204900	-4.14087600	-0.67854300
C	1.49327100	-0.99027700	-3.46468000
H	1.89371500	-0.59887200	-2.51688900
C	2.45357700	-2.06654600	-3.97783300
H	2.07321500	-2.49948100	-4.91497000
H	3.44322500	-1.63553700	-4.18588300
H	2.58728100	-2.88526700	-3.25799600
C	1.45713600	0.17070700	-4.45185600
H	1.24655000	-0.16737500	-5.47630200
H	0.70378000	0.92492100	-4.18475400
H	2.43796300	0.66566200	-4.47414300
O	1.29119000	1.46292400	0.66302800
C	-4.10655200	1.67927700	-0.30218800
C	-4.17118600	2.46462000	1.00314500
O	-3.87509100	2.03177200	2.09314200
O	-4.58488500	3.70841600	0.77263500
C	-5.47896800	1.70319700	-0.95865200
O	-5.69612900	2.00639500	-2.10695900
O	-6.40579200	1.30366500	-0.08855300
C	-7.74775200	1.24028400	-0.58710000
H	-8.35749900	0.88299800	0.24438600
H	-8.08453500	2.23239100	-0.90515700
H	-7.80749100	0.54477600	-1.43041600
C	-4.67495400	4.56497700	1.91860600
H	-5.03238000	5.52556400	1.54356300
H	-5.38195800	4.15520200	2.64709400
H	-3.69112800	4.68179700	2.38495500
C	2.57853200	3.34504700	-0.16311700
C	3.53238500	3.14639400	0.83297300
C	2.84058600	4.25986000	-1.18601700
C	4.73771400	3.84314500	0.79902200
H	3.33357600	2.43077500	1.63053100
C	4.04640800	4.95294200	-1.22200900
H	2.09559600	4.43397900	-1.96497300
C	5.00051700	4.74550200	-0.22785600
H	5.47895800	3.67410900	1.57991300
H	4.24051400	5.65836100	-2.02878400
H	5.94476300	5.28727600	-0.25422500
C	-1.61667200	-1.42804300	2.17708400
C	-0.80511500	-2.54576000	2.41433700

C	-2.66648800	-1.14628100	3.06947700
C	-1.05764000	-3.38080600	3.49530500
H	0.02462200	-2.76597600	1.74409100
C	-2.90568400	-1.97598000	4.15637900
H	-3.27526700	-0.25723800	2.90596400
C	-2.10833800	-3.09926600	4.36715200
H	-0.42675400	-4.25236200	3.66214000
H	-3.71872500	-1.74525500	4.84232400
H	-2.30126900	-3.75240200	5.21631300