Supplementary Information for

Theoretical Study on Thermal Curing Mechanism of Arylethynyl-Containing Resins

Zuowei Chen, Liquan Wang*, Jiaping Lin* and Lei Du

Shanghai Key Laboratory of Advanced Polymeric Materials, Key Laboratory for Ultrafine Materials of Ministry of Education, School of Materials Science and Engineering, East China University of Science and Technology, Shanghai 200237, China

Contents

Corresponding Author

* Tel: +86-21-64253370; E-mail: jlin@ecust.edu.cn (J. Lin) and lq_wang@ecust.edu.cn (L. Wang)

1. Computational Results

1.1 Transition states for the formation of Dewar benzenes (for phenylacetylene)

The diphenylcyclobutadiene **INT3** reacts with a phenylacetylene molecule to generate Dewar benzene **INT5** *via* a concerted or diradical mechanism. The stepwise pathway through **TS7** generating diradical intermediate **INT4** is the most favored according to the activation free energies. As such, the main product could be 1,2,4-triphenylbenzene generated by further isomerization of Dewar benzene.

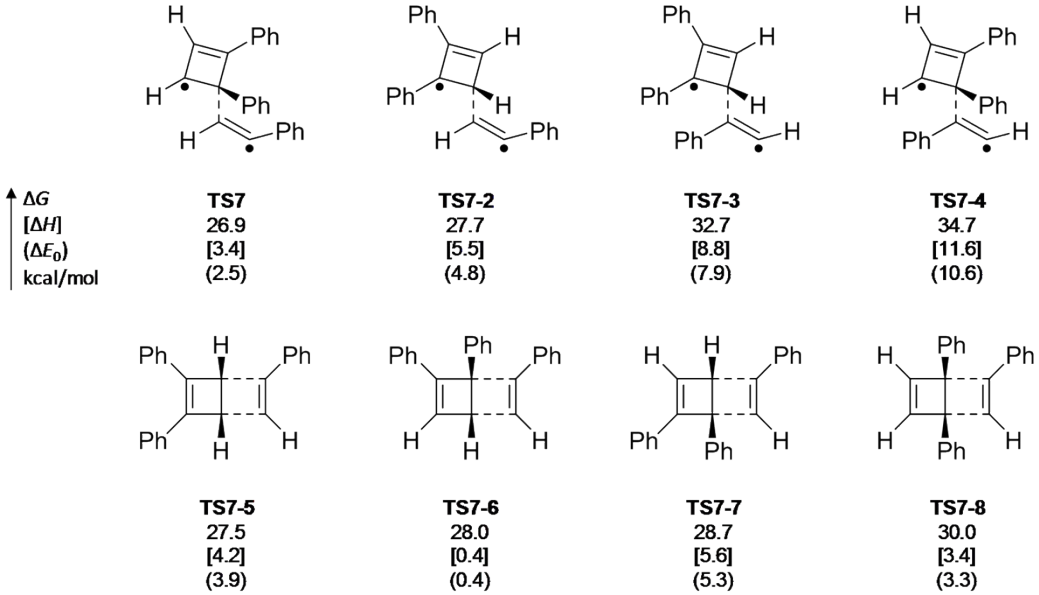

Figure S1. Transition states for the reaction of diphenylcyclobutadiene **INT3** with a phenylacetylene molecule. The energies of the transition states are relative to the energies of diphenylcyclobutadiene **INT3** and phenylacetylene.

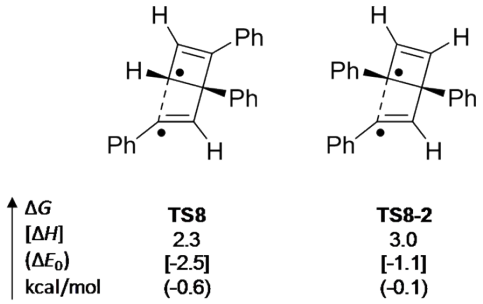

Figure S2. Transition states for the intramolecular coupling of diradical intermediate **INT4** to Dewar benzene **INT5**. The energies of the transition states are relative to the energies of diradical intermediate **INT4**.

1.2 Transition states for the diradical growth of INT1

The diradical intermediate **INT1** reacts with a phenylacetylene molecule to initiate diradical polymerization. The reaction pathway through **TS4** is the most favored according to the activation free energies.

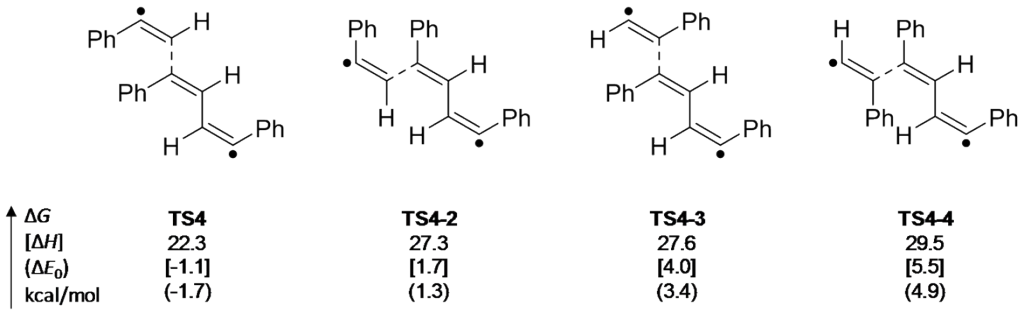

Figure S3. Transition states for the diradical growth of **INT1**. The energies of the transition states are relative to the energies of diradical **INT1** and phenylacetylene.

1.3 Transition states for the formation of Dewar benzenes (for diphenylacetylene)

The tetraphenylcyclobutadiene **INT3-Ph** reacts with a diphenylacetylene molecule to generate Dewar benzene **INT5-Ph** *via* a concerted or diradical mechanism. The stepwise reaction pathway generating diradical intermediate **INT4-Ph** through **TS7-Ph** is the most favored according to the activation free energies.

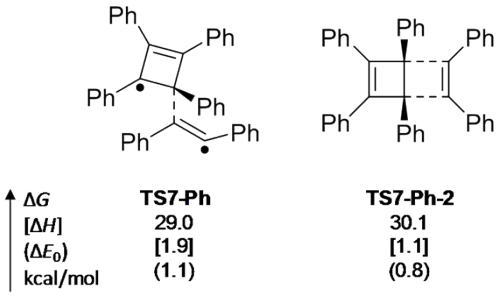

Figure S4. Transition states for the reaction of tetraphenylcyclobutadiene **INT3-Ph** with a diphenylacetylene molecule. Transition states for the formation of Dewar benzenes. The energies of the transition states are relative to the energies of tetraphenylcyclobutadiene **INT3-Ph** and diphenylacetylene.

1.4 Transition states for the diradical growth of INT1-Ph

The diradical intermediate **INT1-Ph** reacts with a diphenylacetylene molecule to initiate diradical polymerization. The reaction pathway through **TS4-Ph** is the most favored according to the activation free energies.

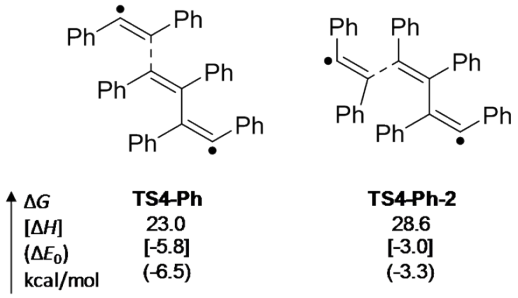

Figure S5. Transition states for the diradical growth of **INT1-Ph**. The energies of the transition states are relative to the energies of diradical **INT1-Ph** and diphenylacetylene.

1.5 Transition states for the dimerization of various arylacetylenes

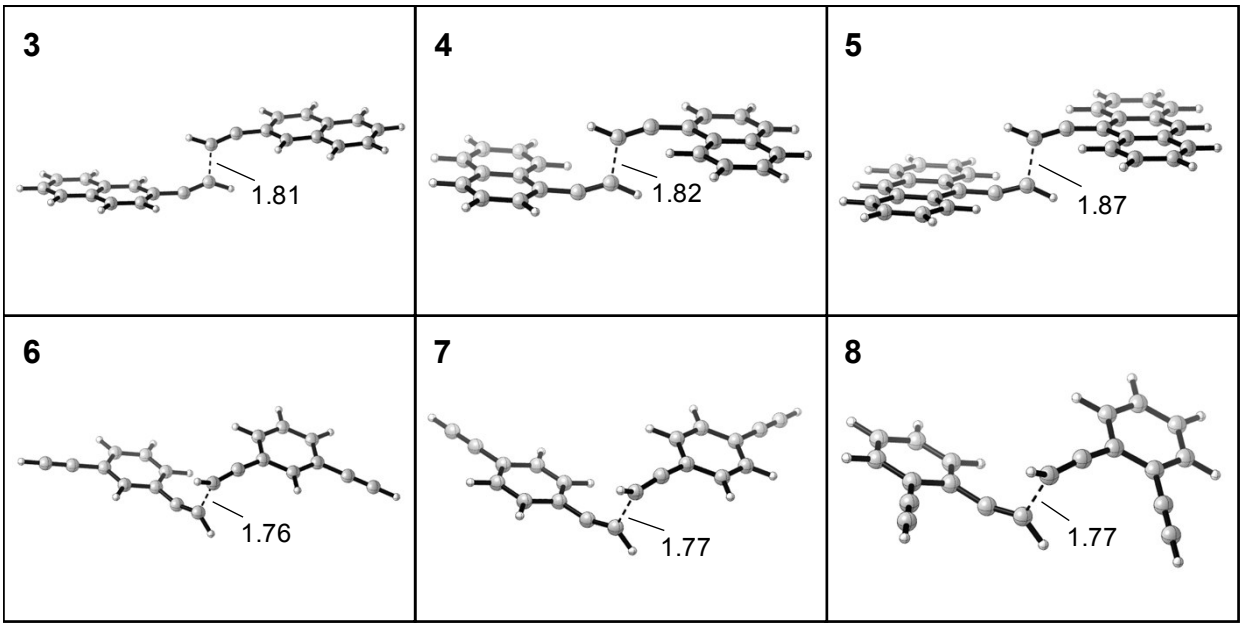

Figure S6. Transition states for the dimerization of various arylacetylenes in **Table 1 (**compounds **3**-**8)**. Bond lengths are given in Å.

1.6 Energy surfaces of the favored reaction pathways calculated by (U)M06-2X/6-311G(d,p)

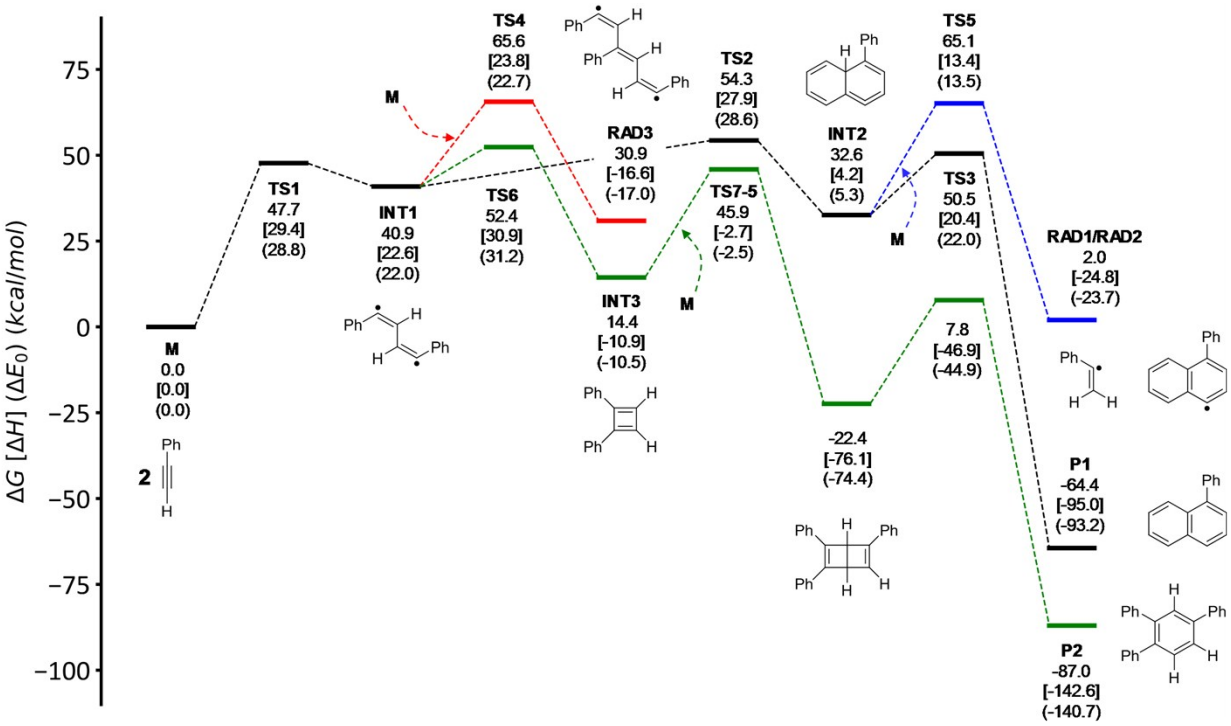

Figure S7. The (U)M06-2X/6-311G(d,p) computed energy surfaces of the favored reaction pathways of phenylacetylene. Gibbs free energies and enthalpies [in brackets] are calculated at 573.15 K in the gas phase. Electronic energies with zero-point energy correction (in parenthesis) are also given.

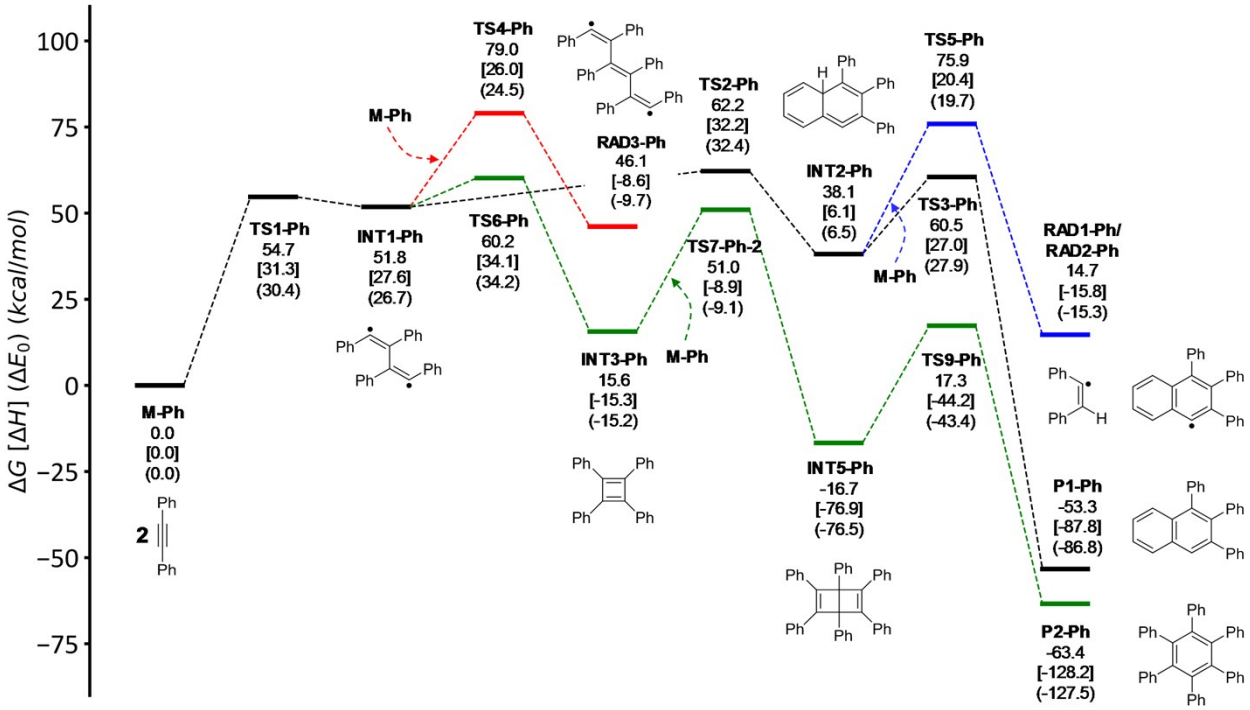

Figure S8. The (U)M06-2X/6-311G(d,p) computed energy surfaces of the favored reaction pathways of diphenylacetylene.

The energy surfaces calculated by (U)B3LYP-D3BJ/6-311G(d,p)//(U)M06-2X/6-311G(d,p) are generally identical with those calculated by (U)M06-2X/6-311G(d,p). There are two main differences between the energy surfaces calculated by (U)B3LYP and (U)M06-2X, since the UM06-2X functional overestimates the energies of diradical transition states. One is that the cyclobutadiene **INT3** reacts with a molecule of phenylacetylene is favored *via* a stepwise pathway generating a diradical intermediate first instead of a concerted pathway. (Note that the computational results show that the activation free energies for the competitive reactions are slightly different.) The other is that the formation of polyene is preferred by monoradical initiation instead of diradical growth. The reason is that the UB3LYP calculation shows the transition state **TS5** for intermolecular hydrogen abstraction is a singlet diradical, of which activation barrier was previously overestimated. Such a conclusion is consistent with most studies of the polymerization involving diradicals.

2. Cartesian Coordinates and Associated Energies

All calculations were implemented with Gaussian 09 program package. The molecular structures in the gas phase were optimized using (U)M06-2X/6-311G(d,p). Electronic energies were calculated using (U)B3LYP/6-311G(d,p) with a D3 dispersion correction damped according to the scheme of Becke and Johnson. All thermal dynamic contributions were computed at 300 °C. Scaling factor of frequencies is 0.946. The $\langle S^2 \rangle$ values of open shell species are also given.

M

C	-1.50677200	-1.20449600	-0.00001000
C	-0.11895500	-1.20848200	0.00001200
C	0.58577800	-0.00002100	0.00001900
C	-0.11893900	1.20847400	0.00001100
C	-1.50673700	1.20451700	-0.00000900
C	-2.20300600	0.00001000	-0.00002200
H	-2.04670000	-2.14360100	-0.00001800
H	0.43228100	-2.14060800	0.00002000
H	0.43234200	2.14057300	0.00001900
H	-2.04666800	2.14362100	-0.00001700
H	-3.28625500	0.00003400	-0.00003900
C	2.01974800	-0.00001300	0.00004800
C	3.22069500	0.00000500	0.00002600
H	4.28412900	0.00001500	-0.00042000

SCF Done: E(RM062X) = -308.334329570 A.U.

Zero-point correction= 0.104523 (Hartree/Particle)
Thermal correction to Energy= 0.127271
Thermal correction to Enthalpy= 0.129086
Thermal correction to Gibbs Free Energy= 0.033224

SCF Done: E(RB3LYP) = -308.497988944 A.U.

TS1

C	4.24623700	1.56666400	-0.24100500
C	3.02719900	1.89631100	0.34891200
C	4.55072900	0.23122400	-0.49954800

H	4.95521900	2.34505500	-0.49465600
C	2.11469200	0.90776700	0.67445200
H	2.78794100	2.93344000	0.55269500
C	3.65275900	-0.76972700	-0.17141600
H	5.49794000	-0.02871200	-0.95692100
C	2.41187200	-0.44719200	0.41520100
H	1.16310500	1.15631000	1.12857400
H	3.88877500	-1.80951800	-0.36176900
C	1.48636800	-1.44958000	0.74824000
C	0.49260500	-2.21361600	0.73051400
C	-0.49260600	-2.21361600	-0.73051500
C	-1.48636900	-1.44958000	-0.74824000
C	-2.41187200	-0.44719200	-0.41520200
C	-2.11469300	0.90776600	-0.67445400
C	-3.65275900	-0.76972700	0.17141800
C	-3.02719900	1.89631100	-0.34891300
H	-1.16310600	1.15630900	-1.12857800
C	-4.55072800	0.23122400	0.49955000
H	-3.88877500	-1.80951700	0.36177200
C	-4.24623600	1.56666400	0.24100600
H	-2.78794100	2.93344000	-0.55269700
H	-5.49793800	-0.02871100	0.95692500
H	-4.95521800	2.34505600	0.49465800
H	0.04765700	-2.92767900	1.40515800
H	-0.04765800	-2.92768000	-1.40515800

SCF Done: E(UM062X) = -616.621179090 A.U.
<S**2> = 0.3225
Zero-point correction= 0.207514 (Hartree/Particle)
Thermal correction to Energy= 0.255751
Thermal correction to Enthalpy= 0.257566
Thermal correction to Gibbs Free Energy= 0.095056

SCF Done: E(UB3LYP) = -616.962651218 A.U.
<S**2> = 0.2183

INT1

C	-5.57278600	0.00010600	0.38230500
C	-4.90658200	1.20641000	0.16806600
C	-4.90673200	-1.20627400	0.16802700
H	-6.60437300	0.00016400	0.71224200
C	-3.59009600	1.21515000	-0.25619100
H	-5.42102700	2.14539700	0.33458200
C	-3.59024700	-1.21516400	-0.25623200

H	-5.42129100	-2.14520300	0.33451600
C	-2.89910000	-0.00004700	-0.46930600
H	-3.06897400	2.14927900	-0.42658500
H	-3.06924000	-2.14935300	-0.42665400
C	-1.56993000	-0.00011400	-0.92083000
C	-0.28394800	-0.00010100	-0.69364200
C	0.28397200	-0.00009200	0.69373100
C	1.56995600	-0.00010500	0.92091300
C	2.89911200	-0.00004300	0.46933800
C	3.59010100	1.21515100	0.25619100
C	3.59024600	-1.21516200	0.25623800
C	4.90656900	1.20640800	-0.16812300
H	3.06898700	2.14928200	0.42660600
C	4.90671300	-1.20627700	-0.16807800
H	3.06924400	-2.14934900	0.42668500
C	5.57276000	0.00010100	-0.38238800
H	5.42100900	2.14539300	-0.33466300
H	5.42126300	-2.14520700	-0.33458700
H	6.60433300	0.00015700	-0.71236900
H	0.44182700	-0.00011800	-1.50350900
H	-0.44180100	-0.00011500	1.50359900

SCF Done: E(UM062X) = -616.634451174 A.U.
<S**2> = 1.0096
Zero-point correction= 0.209956 (Hartree/Particle)
Thermal correction to Energy= 0.258211
Thermal correction to Enthalpy= 0.260027
Thermal correction to Gibbs Free Energy= 0.097478

SCF Done: E(UB3LYP) = -616.974949535 A.U.
<S**2> = 0.9393

TS2

C	0.98341600	-2.42140000	0.44784100
C	2.03121300	-2.28122900	-0.48914800
C	2.73471700	-1.10490700	-0.58076500
C	2.39794400	-0.00883300	0.25152400
C	1.30891000	-0.14073900	1.15380300
C	0.64394800	-1.37583200	1.27455900
C	2.91317100	1.28051600	0.08769100
C	2.26850400	2.37983900	-0.22023000
H	0.45705900	-3.36556600	0.52312200
H	3.54388500	-0.99025700	-1.29166800
H	1.12928200	0.64481800	1.87777200

H	-0.15208800	-1.48803600	2.00126600
C	-3.79940800	-0.53356300	-0.13016900
C	-3.53134000	0.55595700	0.69635700
C	-2.29497400	1.17967600	0.65496900
C	-1.29746600	0.72274500	-0.22805400
C	-1.57198500	-0.39301300	-1.04385200
C	-2.81545600	-1.00208100	-0.99863900
C	-0.00826100	1.30706500	-0.23667900
C	0.79900000	2.26140100	-0.59446500
H	-4.76814800	-1.01681500	-0.09459700
H	-4.29374100	0.92240600	1.37369800
H	-2.08070800	2.02758300	1.29471600
H	-0.79325300	-0.76261500	-1.70095100
H	-3.01994100	-1.85160400	-1.63963100
H	2.28435000	-3.11320300	-1.13556800
H	0.43274400	3.06193900	-1.23611300
H	2.68897000	3.37775500	-0.24050100

SCF Done: E(UM062X) = -616.624003581 A.U.
<S**2> = 0.6030
Zero-point correction= 0.210009 (Hartree/Particle)
Thermal correction to Energy= 0.256176
Thermal correction to Enthalpy= 0.257991
Thermal correction to Gibbs Free Energy= 0.108398

SCF Done: E(UB3LYP) = -616.966457487 A.U.
<S**2> = 0.4758

INT2

C	1.64321000	-2.31612100	0.45090800
C	2.78717600	-1.95767700	-0.37529400
C	3.17897100	-0.67324200	-0.50131500
C	2.44304200	0.38109100	0.14811200
C	1.11590000	0.08177800	0.81420500
C	0.86568400	-1.38310700	1.01437800
C	2.60604000	1.69655200	-0.03922000
C	1.70260300	2.63202700	-0.25928100
H	1.44183700	-3.36678700	0.62652500
H	4.04893300	-0.39949700	-1.08662600
H	1.03954600	0.56182200	1.80109500
H	0.04576000	-1.66799600	1.66439200
C	-3.97325400	-0.63986500	-0.17737800
C	-3.70789200	0.56766300	0.45699600
C	-2.40642800	1.05559300	0.51091800

C	-1.35382900	0.34056800	-0.06451500
C	-1.63118000	-0.87547600	-0.69830200
C	-2.93190500	-1.35774300	-0.75872500
C	0.03061300	0.87163300	-0.01823200
C	0.35098400	2.05986700	-0.54643700
H	-4.98676300	-1.02023200	-0.22168400
H	-4.51367800	1.13153800	0.91202400
H	-2.19408500	1.99506100	1.00863700
H	-0.82095700	-1.42927100	-1.15829200
H	-3.13478100	-2.29409500	-1.26494900
H	3.33862900	-2.74773100	-0.87125400
H	-0.39493100	2.64149300	-1.07695100
H	1.81208300	3.69444500	-0.07382500

SCF Done: E(RM062X) = -616.665430709 A.U.

Zero-point correction= 0.214258 (Hartree/Particle)
Thermal correction to Energy= 0.259896
Thermal correction to Enthalpy= 0.261711
Thermal correction to Gibbs Free Energy= 0.115149

SCF Done: E(RB3LYP) = -616.996242205 A.U.

TS3

C	2.03686400	-2.31907800	-0.39004800
C	3.34847300	-1.77002700	-0.20759300
C	3.51630400	-0.44049100	-0.01320700
C	2.40619000	0.49418100	0.05097800
C	1.02900600	-0.12570900	-0.03077200
C	0.93012200	-1.54157700	-0.32136300
C	2.64756200	1.90519500	0.14656400
C	1.46854700	2.64224900	0.22789100
H	1.93303200	-3.37430500	-0.61345000
H	4.49423800	0.01932400	0.05956900
H	1.70294400	0.05679900	1.04980900
H	-0.05144700	-1.95521200	-0.51570200
C	-4.13974200	-0.64680100	0.00033600
C	-3.22454900	-1.22007400	0.87775500
C	-1.90859100	-0.77683600	0.90044600
C	-1.48565800	0.24563700	0.04521000
C	-2.41399300	0.81658600	-0.82858200
C	-3.73129000	0.37362200	-0.85062500
C	-0.09244700	0.75562500	0.08467000

C	0.16387500	2.10315800	0.23557100
H	-5.16595900	-0.99325500	-0.01801300
H	-3.53894600	-2.00770200	1.55209700
H	-1.20280500	-1.21248100	1.60019300
H	-2.09024500	1.60234500	-1.50201000
H	-4.43794700	0.82222100	-1.53872500
H	4.20879200	-2.42563800	-0.26400400
H	-0.69025900	2.76571100	0.35410800
H	1.53457000	3.72823400	0.27274100

SCF Done: E(RM062X) = -616.634965760 A.U.

Zero-point correction= 0.210477 (Hartree/Particle)
Thermal correction to Energy= 0.255155
Thermal correction to Enthalpy= 0.256970
Thermal correction to Gibbs Free Energy= 0.113254

SCF Done: E(RB3LYP) = -616.963332847 A.U.

P1

C	3.30140500	-1.82697700	-0.22221200
C	3.47375900	-0.48284300	-0.03706300
C	2.35899200	0.39047100	0.04993900
C	1.04398100	-0.14803600	-0.03663900
C	0.90087800	-1.54550500	-0.25239200
C	1.99795300	-2.36047300	-0.34155000
H	3.54449800	2.18216800	0.27176100
H	4.16012100	-2.48428800	-0.28849700
H	4.46945300	-0.05928100	0.04018800
C	2.53594500	1.78884200	0.20541100
C	-0.07410900	0.74166000	0.05818900
H	-0.09184900	-1.96321900	-0.36345800
H	1.86734800	-3.42248300	-0.51226800
C	0.14752400	2.09273000	0.18939800
C	1.45428000	2.62255700	0.26191000
C	-1.47517100	0.24232800	0.02870200
C	-2.37654000	0.73772600	-0.91583800
C	-1.92954300	-0.68578300	0.97029000
C	-3.70045000	0.31318900	-0.92338100
H	-2.02649900	1.45084300	-1.65408100
C	-3.25293700	-1.10781700	0.96472500
H	-1.23921700	-1.06355000	1.71687700
C	-4.14200600	-0.61057900	0.01646000

H	-4.38661400	0.70272100	-1.66619200
H	-3.59374500	-1.82075900	1.70629500
H	-5.17376600	-0.94126100	0.01231300
H	-0.70467700	2.75888000	0.26566700
H	1.59119200	3.69128800	0.37569600

SCF Done: E(RM062X) = -616.825383810 A.U.

Zero-point correction= 0.217268 (Hartree/Particle)
Thermal correction to Energy= 0.261661
Thermal correction to Enthalpy= 0.263476
Thermal correction to Gibbs Free Energy= 0.120498

SCF Done: E(RB3LYP) = -617.155235568 A.U.

TS4

C	3.21139300	2.48638400	0.53306100
C	2.89429700	1.45610600	1.41490600
C	2.40916900	2.71648900	-0.58204700
H	4.08335100	3.10406300	0.71167900
C	1.78667300	0.65565200	1.18305800
H	3.52354600	1.26578400	2.27630900
C	1.30075500	1.91767300	-0.82371700
H	2.65194900	3.51939200	-1.26827300
C	0.96792600	0.87834100	0.06220200
H	1.54755900	-0.16373500	1.85113600
H	0.68081900	2.08102100	-1.69762100
C	-0.11246900	-0.01058700	-0.23184800
C	-1.42474300	-0.06206400	-0.18043900
C	-2.24949800	1.05163100	0.37368900
C	-3.55310400	0.99040800	0.43720500
C	-4.77736900	0.33668900	0.24066100
C	-5.33269700	-0.47660000	1.25710000
C	-5.50906200	0.50920400	-0.95833200
C	-6.55484900	-1.09594300	1.06890300
H	-4.78177600	-0.60592500	2.18061300
C	-6.72989800	-0.11778500	-1.12988000
H	-5.09414500	1.13728600	-1.73712300
C	-7.26100900	-0.92179200	-0.12136400
H	-6.96431300	-1.72085300	1.85370500
H	-7.27565000	0.01829700	-2.05602000
H	-8.21872300	-1.40757000	-0.26128200
H	-1.97729900	-0.92958000	-0.53436100

H	-1.70012000	1.92259600	0.72506400
C	5.24766000	-1.67108500	0.98768200
C	3.98341600	-2.09737800	0.61147700
C	3.35412500	-1.53090400	-0.50774000
C	4.02404600	-0.54644500	-1.24908400
C	5.28785100	-0.12717000	-0.86356100
C	5.90237300	-0.68337600	0.25533900
H	5.72556200	-2.10900000	1.85588800
H	3.46286600	-2.85849300	1.17978300
H	3.52761000	-0.10158000	-2.10268600
H	5.79231300	0.64474300	-1.43241900
H	6.88887000	-0.35057500	0.55473700
C	2.02241100	-1.89324700	-0.85224800
C	0.82110300	-1.95159200	-1.04518500
H	-0.12344000	-2.32152900	-1.37815000

SCF Done: E(UM062X) = -924.968685785 A.U.
<S**2> = 1.0178
Zero-point correction= 0.315420 (Hartree/Particle)
Thermal correction to Energy= 0.389144
Thermal correction to Enthalpy= 0.390959
Thermal correction to Gibbs Free Energy= 0.169858

SCF Done: E(UB3LYP) = -925.476501327 A.U.
<S**2> = 0.9510

RAD3

C	-2.34222800	2.65276700	-0.65582500
C	-2.52530000	1.58717200	-1.53230600
C	-1.45949900	2.52621900	0.41026100
H	-2.88553500	3.57820300	-0.80512200
C	-1.83743700	0.39742800	-1.33525800
H	-3.21483600	1.67844600	-2.36316300
C	-0.77576200	1.33172500	0.61010500
H	-1.30941400	3.35313300	1.09428100
C	-0.96389600	0.25325500	-0.25581500
H	-1.99543000	-0.44048700	-2.00551300
H	-0.10331000	1.21912700	1.45387600
C	-0.32027000	-1.05689500	0.03382600
C	1.01570700	-1.22743800	0.07296800
C	2.00206000	-0.19324900	-0.23462700
C	3.29411400	-0.34254600	-0.07834700
C	4.66124200	-0.14117500	-0.02654100
C	5.49689200	-0.49047300	-1.12241900

C	5.27522000	0.38925600	1.14119100
C	6.86292600	-0.30472200	-1.04694600
H	5.04148100	-0.90071500	-2.01512800
C	6.64333400	0.56639900	1.19365900
H	4.64919900	0.65476000	1.98411600
C	7.44861600	0.22270300	0.10573500
H	7.48409400	-0.57216100	-1.89378500
H	7.09306800	0.97806500	2.08956300
H	8.52093600	0.36404100	0.15580400
H	1.41196200	-2.20038700	0.34966000
H	1.61955100	0.75541600	-0.61976700
C	-5.70120700	-0.58028000	-0.70865600
C	-4.61851900	-1.43966800	-0.62970700
C	-3.67363400	-1.30116200	0.40672700
C	-3.87684400	-0.30134100	1.38073200
C	-4.95942200	0.55593600	1.28550300
C	-5.87362700	0.42503600	0.24158100
H	-6.41540500	-0.68979600	-1.51623500
H	-4.47307600	-2.21565100	-1.37212100
H	-3.15119000	-0.19112800	2.17750100
H	-5.08957500	1.33735900	2.02491400
H	-6.71814000	1.09968100	0.17155900
C	-2.52191600	-2.12024100	0.45696600
C	-1.20993300	-2.18801800	0.37159100
H	-0.70808100	-3.13202400	0.58314900

SCF Done: E(UM062X) = -925.035903775 A.U.
<S**2> = 1.0874
Zero-point correction= 0.319446 (Hartree/Particle)
Thermal correction to Energy= 0.391859
Thermal correction to Enthalpy= 0.393674
Thermal correction to Gibbs Free Energy= 0.181830

SCF Done: E(UB3LYP) = -925.540671920 A.U.
<S**2> = 1.0710

TS5

C	-0.10861100	2.90345800	0.06841700
C	1.23526400	2.64550300	0.47232800
C	1.57338800	1.45049200	1.03560400
C	0.62067000	0.40191100	1.23685400
C	-0.71558100	0.61844000	0.64663600
C	-1.06585000	1.94527900	0.17744800
C	0.99567000	-0.80878200	1.84834300

C	0.03919800	-1.80897100	1.82949000
H	-0.36932000	3.88255600	-0.31627700
H	2.57852100	1.25288500	1.39316300
H	-0.07783000	0.13152700	-0.49103800
H	-2.08167300	2.15353800	-0.13378700
C	-5.63049100	-0.17027200	-0.88883100
C	-4.75331200	-1.12910500	-1.38124200
C	-3.46328400	-1.22232100	-0.86970400
C	-3.02813700	-0.35638700	0.13767000
C	-3.92490600	0.59726900	0.63235800
C	-5.21396500	0.68836400	0.12441400
C	-1.65666600	-0.48365700	0.68859500
C	-1.21675900	-1.68949400	1.18007900
H	-6.63518200	-0.09484600	-1.28695600
H	-5.07237100	-1.80536500	-2.16552400
H	-2.77920800	-1.97419200	-1.24978200
H	-3.60937100	1.25362200	1.43604700
H	-5.89885700	1.42644500	0.52511400
H	1.98213100	3.42253400	0.35609100
H	-1.90135800	-2.53382100	1.16018400
H	0.21404500	-2.73582700	2.37534600
C	4.98779500	0.52676500	-1.00023400
C	3.70881200	0.45016100	-1.51170500
C	2.83444600	-0.55779100	-1.05860400
C	3.25302500	-1.46892000	-0.07640800
C	4.54387700	-1.37234900	0.43338100
C	5.40460700	-0.38623200	-0.02509400
H	5.66437900	1.29811200	-1.34655000
H	3.35643800	1.16053600	-2.24954900
H	2.56678100	-2.21880100	0.28704100
H	4.86394700	-2.06209200	1.20375600
H	6.40708800	-0.31548500	0.38031900
C	1.50532000	-0.58161000	-1.53050000
C	0.30710200	-0.46763200	-1.76187500
H	-0.59781900	-0.58602300	-2.32213600

SCF Done: E(RM062X) = -924.981748612 A.U.

Zero-point correction= 0.313829 (Hartree/Particle)
Thermal correction to Energy= 0.385506
Thermal correction to Enthalpy= 0.387321
Thermal correction to Gibbs Free Energy= 0.182202

SCF Done: E(UB3LYP) = -925.486558483 A.U.

<S**2> = 0.0134

RAD1

C	-2.07671600	-2.29976600	-0.33858400
C	-3.37190400	-1.74582200	-0.22042100
C	-3.52671000	-0.39966500	-0.03356800
C	-2.39233800	0.44648100	0.05560900
C	-1.07805900	-0.10783600	-0.03100600
C	-0.96306300	-1.50693200	-0.24815600
C	-2.48071300	1.83562400	0.21077800
C	-1.43760700	2.69036300	0.27525600
H	-1.96514700	-3.36374800	-0.51039000
H	-4.51094100	0.04694500	0.04349000
H	0.02160400	-1.94372500	-0.35911700
C	4.09139600	-0.67264900	0.00714100
C	3.66528000	0.25765000	-0.93324000
C	2.35110400	0.71149900	-0.91999600
C	1.44473800	0.24048600	0.03200900
C	1.88373200	-0.69383900	0.97466900
C	3.19700500	-1.14634500	0.96240500
C	0.05336400	0.76772500	0.06558000
C	-0.13728300	2.12377700	0.20084500
H	5.11527900	-1.02663300	-0.00192800
H	4.35545600	0.62917500	-1.68148500
H	2.01264800	1.42854700	-1.65981200
H	1.19000800	-1.05315500	1.72722500
H	3.52586100	-1.86421600	1.70459400
H	-4.24018800	-2.38999000	-0.28888600
H	0.72877500	2.77240200	0.27782800
H	-1.56670500	3.75990800	0.39254900

SCF Done: E(UM062X) = -616.138862094 A.U.
<S**2> = 0.7657
Zero-point correction= 0.205028 (Hartree/Particle)
Thermal correction to Energy= 0.248785
Thermal correction to Enthalpy= 0.250600
Thermal correction to Gibbs Free Energy= 0.107233

SCF Done: E(UB3LYP) = -616.464225550 A.U.
<S**2> = 0.7593

RAD2

H	-3.78707600	-0.00006300	0.92599400
C	1.56905800	1.20777200	-0.00000700

C	0.19018400	1.22249500	0.00001800
C	-0.54373300	0.00006100	0.00003100
C	0.19010800	-1.22246000	0.00001100
C	1.56895500	-1.20784100	-0.00000400
C	2.27221400	-0.00004400	-0.00001700
H	2.11109300	2.14615200	-0.00001500
H	-0.35599000	2.15746200	0.00003900
H	-0.35617900	-2.15736100	0.00001700
H	2.11095100	-2.14624300	-0.00000200
H	3.35468600	-0.00009900	-0.00003300
C	-1.91624500	0.00006700	-0.00001800
C	-3.21226300	-0.00002400	-0.00001600
H	-3.78715100	-0.00000700	-0.92599200

SCF Done: E(UM062X) = -308.906168087 A.U.
<S**2> = 0.7855
Zero-point correction= 0.112889 (Hartree/Particle)
Thermal correction to Energy= 0.137338
Thermal correction to Enthalpy= 0.139153
Thermal correction to Gibbs Free Energy= 0.037725

SCF Done: E(UB3LYP) = -309.081890370 A.U.
<S**2> = 0.7834

TS6

C	-0.73546500	2.45286200	-0.00002500
C	-1.20506700	1.21814200	0.00026400
C	1.20503700	1.21810900	-0.00022800
C	0.73546700	2.45284100	-0.00026500
H	-1.35817700	3.34689700	-0.00003200
H	1.35820400	3.34686100	-0.00048500
C	2.31213200	0.33534800	-0.00018000
C	2.85475800	-0.13721600	-1.21250900
C	2.85582100	-0.13579300	1.21222400
C	3.91303000	-1.03021200	-1.20592900
H	2.43115000	0.21283200	-2.14613200
C	3.91409200	-1.02879600	1.20575400
H	2.43301000	0.21531700	2.14581000
C	4.44727400	-1.48029700	-0.00005800
H	4.32550500	-1.38051700	-2.14480900
H	4.32738800	-1.37800600	2.14468000
H	5.27362000	-2.18054100	-0.00001000
C	-2.31215800	0.33538400	0.00025300
C	-2.85570200	-0.13591200	-1.21216300

C	-2.85491800	-0.13704600	1.21257300
C	-3.91392900	-1.02896300	-1.20571500
H	-2.43279600	0.21511500	-2.14573400
C	-3.91315300	-1.03008400	1.20596900
H	-2.43145500	0.21314400	2.14620900
C	-4.44723000	-1.48034700	0.00008500
H	-4.32708800	-1.37831400	-2.14465200
H	-4.32574400	-1.38028100	2.14483700
H	-5.27354700	-2.18062500	0.00002700

SCF Done: E(UM062X) = -616.619724435 A.U.
<S**2> = 0.7119
Zero-point correction= 0.209763 (Hartree/Particle)
Thermal correction to Energy= 0.256612
Thermal correction to Enthalpy= 0.258427
Thermal correction to Gibbs Free Energy= 0.101097

SCF Done: E(UB3LYP) = -616.961748044 A.U.
<S**2> = 0.5072

INT3

C	0.76903500	2.69598200	0.02814400
C	0.79457900	1.35762500	0.02978600
C	-0.79446000	1.35757600	-0.02968100
C	-0.76891600	2.69593200	-0.02799300
H	1.52826300	3.46478500	-0.00669800
H	-1.52815600	3.46473800	0.00691300
C	-1.82316100	0.33690400	0.02685700
C	-1.57030800	-0.89648600	0.64141000
C	-3.09924600	0.58157200	-0.50143700
C	-2.57165900	-1.85597100	0.73018300
H	-0.59166600	-1.08732400	1.06679500
C	-4.09411000	-0.37842300	-0.40907300
H	-3.29083100	1.52579100	-0.99884800
C	-3.83365500	-1.60195600	0.20588800
H	-2.36597600	-2.80341000	1.21407800
H	-5.07481400	-0.18011800	-0.82529100
H	-4.61170400	-2.35283400	0.27325400
C	1.82322300	0.33689300	-0.02680300
C	3.09946700	0.58156500	0.50110500
C	1.57011800	-0.89658200	-0.64107100
C	4.09423200	-0.37851400	0.40866100
H	3.29125400	1.52586800	0.99828500
C	2.57137500	-1.85615900	-0.72993300

H	0.59135400	-1.08742400	-1.06617200
C	3.83352300	-1.60214400	-0.20601200
H	5.07505900	-0.18020000	0.82457900
H	2.36550100	-2.80366500	-1.21361500
H	4.61150100	-2.35308900	-0.27346100

SCF Done: E(RM062X) = -616.689371743 A.U.

Zero-point correction= 0.213093 (Hartree/Particle)
Thermal correction to Energy= 0.259661
Thermal correction to Enthalpy= 0.261476
Thermal correction to Gibbs Free Energy= 0.110043

SCF Done: E(RB3LYP) = -617.017529809 A.U.

TS7

C	2.20667900	1.21367300	-0.17041000
C	2.41995500	2.58543100	-0.58846900
H	3.29550700	3.15242300	-0.87424700
C	3.03165300	0.04928000	-0.10475200
C	2.46735800	-1.24251300	-0.09284400
C	4.43550700	0.16676000	-0.09227800
C	3.27919100	-2.36413600	-0.05363800
H	1.38890600	-1.34480100	-0.14486400
C	5.23835900	-0.96014600	-0.04926800
H	4.88228000	1.15472000	-0.10303000
C	4.66623800	-2.23143500	-0.02676000
H	2.83110000	-3.35078600	-0.05299000
H	6.31641500	-0.85155400	-0.03266400
H	5.29691400	-3.11153600	0.00427600
C	-0.24614300	1.05923700	0.87331600
C	-1.53098100	1.61484600	0.80561800
C	0.01576600	0.09617000	1.85611700
C	-2.53014300	1.20809900	1.67657500
H	-1.74480200	2.35085500	0.03719300
C	-0.98636600	-0.30789500	2.72931100
H	1.01260000	-0.31899100	1.94714400
C	-2.26337300	0.23804800	2.63870700
H	-3.52257200	1.63585900	1.59523700
H	-0.76802500	-1.05039600	3.48815100
H	-3.04477300	-0.08764700	3.31481300
C	1.07346200	2.87009100	-0.53501900
H	0.46806800	3.74338900	-0.72793100

C	0.75580200	1.47352900	-0.10291700
C	-1.01136300	0.05290500	-1.86538600
C	-2.24742900	-0.46432500	-1.40817800
C	-2.27257900	-1.60261900	-0.58387500
C	-3.45818600	0.17721300	-1.72447300
C	-3.47308300	-2.06310100	-0.06839100
H	-1.33924200	-2.09315300	-0.33549200
C	-4.65264300	-0.29424100	-1.20520300
H	-3.43914200	1.04973900	-2.36639800
C	-4.66601600	-1.41115900	-0.37176500
H	-3.47904600	-2.93134800	0.57985400
H	-5.57978300	0.21073000	-1.44921600
H	-5.60220300	-1.77416300	0.03499700
C	0.09231400	0.59632400	-1.93733900
H	0.96391400	0.85643800	-2.50689400

SCF Done: E(UM062X) = -925.007946726 A.U.
<S**2> = 1.0408
Zero-point correction= 0.315749 (Hartree/Particle)
Thermal correction to Energy= 0.388260
Thermal correction to Enthalpy= 0.390075
Thermal correction to Gibbs Free Energy= 0.180158

SCF Done: E(UB3LYP) = -925.509634581 A.U.
<S**2> = 1.0457

INT4

C	-2.12754100	-0.71719800	-0.83923500
C	-2.70135300	-1.75461100	-1.61750300
H	-3.71952400	-1.99559700	-1.89663600
C	-2.57444100	0.44698900	-0.15126900
C	-1.65980200	1.24027500	0.57323700
C	-3.93096000	0.83183300	-0.16778900
C	-2.09068900	2.37335300	1.24381600
H	-0.61623500	0.94642400	0.61173600
C	-4.35022000	1.96487900	0.50625900
H	-4.64451000	0.23159100	-0.72135100
C	-3.43397200	2.74370900	1.21396600
H	-1.37629500	2.96974300	1.79968400
H	-5.39593900	2.24863100	0.48291600
H	-3.76598800	3.63000700	1.74073700
C	0.05267000	-1.82546800	0.09106200
C	1.33607000	-2.34452600	-0.10013200
C	-0.50996800	-1.88596800	1.36488800

C	2.04247000	-2.90122900	0.95706200
H	1.78143100	-2.30886500	-1.08831100
C	0.19831200	-2.44240200	2.42600900
H	-1.50614700	-1.49193400	1.53133700
C	1.47610700	-2.94856100	2.22725300
H	3.03765600	-3.29707300	0.79106300
H	-0.25183900	-2.47549800	3.41113700
H	2.02804900	-3.37772000	3.05491200
C	-1.49229300	-2.34022400	-1.88540100
H	-1.16118900	-3.21503300	-2.42740200
C	-0.71650600	-1.27666700	-1.09225300
C	1.09040300	0.39182300	-1.58974300
C	2.11757100	1.05343400	-0.95113400
C	1.88516800	2.30738500	-0.31711600
C	3.43721600	0.52256700	-0.92333000
C	2.91749300	2.97342500	0.31188300
H	0.88639000	2.72705500	-0.34628200
C	4.45194900	1.20697700	-0.28629900
H	3.62762700	-0.42826900	-1.40560700
C	4.20527100	2.43315500	0.33617100
H	2.72426800	3.92670000	0.78990900
H	5.45036100	0.78602800	-0.26945600
H	5.00866400	2.96215600	0.83343800
C	0.07850100	-0.32261200	-1.98012600
H	-0.31550300	-0.22036800	-2.99348100

SCF Done: E(UM062X) = -925.045423526 A.U.
<S**2> = 1.0664
Zero-point correction= 0.319098 (Hartree/Particle)
Thermal correction to Energy= 0.391019
Thermal correction to Enthalpy= 0.392834
Thermal correction to Gibbs Free Energy= 0.183525

SCF Done: E(UB3LYP) = -925.544436915 A.U.
<S**2> = 1.0643

TS8

C	-1.04239100	-0.76149400	0.88444400
C	-0.32216500	-0.74871800	2.08975300
H	-0.28580800	-1.41764300	2.94022500
C	-1.98150100	-1.62018100	0.23074700
C	-2.47595400	-1.27977600	-1.04222300
C	-2.43507300	-2.80965200	0.83246200
C	-3.38197500	-2.10527200	-1.69009800

H	-2.15035800	-0.35519000	-1.50690700
C	-3.34360800	-3.62509200	0.18102400
H	-2.06264900	-3.08312300	1.81343700
C	-3.82056900	-3.27926600	-1.08383300
H	-3.75271100	-1.83031500	-2.67035800
H	-3.68413700	-4.53801000	0.65540500
H	-4.53132400	-3.92079000	-1.59024800
C	-1.20720500	1.73999800	0.16447400
C	-0.67137300	2.84292600	-0.50334900
C	-2.51900600	1.81522300	0.63826500
C	-1.42584100	3.99523600	-0.69081500
H	0.34595300	2.79573600	-0.87608100
C	-3.27366100	2.96665600	0.44993400
H	-2.95044000	0.96292000	1.15166900
C	-2.73036200	4.06073600	-0.21509200
H	-0.99362600	4.84228500	-1.21061100
H	-4.29130900	3.00743600	0.82013400
H	-3.32068200	4.95683900	-0.36468500
C	0.35567500	0.41511800	1.77539900
H	0.99559600	1.10946200	2.30012600
C	-0.35701300	0.51477400	0.40966800
C	1.90802000	0.06015300	-0.16821800
C	3.28945000	-0.17589600	-0.21947300
C	4.20308000	0.89124900	-0.37772000
C	3.80189100	-1.48452900	-0.06433500
C	5.56540000	0.65048200	-0.39198100
H	3.81740200	1.89732900	-0.49056800
C	5.16654100	-1.70844700	-0.08722600
H	3.10590000	-2.30390800	0.06748300
C	6.05640100	-0.64664700	-0.24842000
H	6.25393600	1.47748100	-0.51920100
H	5.54494500	-2.71784700	0.02306600
H	7.12386100	-0.82854800	-0.26111800
C	0.70687100	0.24983200	-0.63764500
H	0.44167000	0.20139500	-1.69621300

SCF Done: E(UM062X) = -925.044290480 A.U.
<S**2> = 0.7680

SCF Done: E(UB3LYP) = -925.544922303 A.U.
<S**2> = 0.6036

INT5

C	0.82849000	-0.83203600	-0.57749300

C	-0.13527100	-0.96993000	-1.49852500
H	-0.39003900	-1.75181100	-2.20354600
C	1.95761200	-1.64014200	-0.12328800
C	2.71319900	-1.23694400	0.98104300
C	2.29547900	-2.82937700	-0.77953500
C	3.77848300	-2.01249800	1.42525400
H	2.46434700	-0.30935600	1.48581500
C	3.35828800	-3.60024900	-0.33662700
H	1.71576100	-3.14403400	-1.64040300
C	4.10320800	-3.19385100	0.76901400
H	4.35732600	-1.69204000	2.28338400
H	3.60986300	-4.51988300	-0.85134700
H	4.93486000	-3.79660500	1.11384000
C	1.16291700	1.71774600	-0.06247600
C	0.79759400	2.86731300	0.64269900
C	2.33619000	1.74424100	-0.82261900
C	1.57706100	4.01647600	0.58146900
H	-0.10957900	2.85996300	1.23667100
C	3.11493600	2.89351700	-0.88362700
H	2.63998300	0.85741900	-1.36788500
C	2.73884300	4.03408200	-0.18217500
H	1.27734600	4.89925800	1.13428400
H	4.02130200	2.89577800	-1.47783900
H	3.34894800	4.92842900	-0.22610600
C	-0.85316200	0.30844300	-1.10859300
H	-1.02784600	1.08479800	-1.85319400
C	0.29125300	0.50035100	-0.03961700
C	-1.79606300	0.20641400	0.08679500
C	-3.22472900	-0.09191300	0.12458200
C	-3.89996700	-0.39529800	-1.05975300
C	-3.93602700	-0.09172400	1.32967300
C	-5.25609600	-0.69991200	-1.04201900
H	-3.35275900	-0.39159100	-1.99667600
C	-5.28913400	-0.39190700	1.34668100
H	-3.41852600	0.14862600	2.25176100
C	-5.95317900	-0.69848400	0.16025100
H	-5.76900300	-0.93624800	-1.96665800
H	-5.83160100	-0.38819100	2.28458700
H	-7.01087200	-0.93282700	0.17529300
C	-0.82194500	0.37017400	0.99258600
H	-0.78739500	0.34135900	2.07583200

SCF Done: E(RM062X) = -925.129130739 A.U.

Zero-point correction= 0.324246 (Hartree/Particle)
Thermal correction to Energy= 0.393842
Thermal correction to Enthalpy= 0.395658
Thermal correction to Gibbs Free Energy= 0.191683

SCF Done: E(RB3LYP) = -925.614422382 A.U.

TS9

C	1.44522800	-0.22196000	-0.48029200
C	0.65860600	-0.30686700	-1.64330800
H	1.04718600	-0.66174000	-2.59466700
C	2.56005600	-1.06790100	-0.09663600
C	3.29610100	-0.75697200	1.05701100
C	2.94183600	-2.18761300	-0.85362300
C	4.36841600	-1.54740500	1.44892400
H	3.02807900	0.12631100	1.62790500
C	4.03003000	-2.95585800	-0.47427100
H	2.35933100	-2.46427300	-1.72464900
C	4.74506500	-2.64407200	0.68148700
H	4.92200700	-1.29677000	2.34611100
H	4.31342000	-3.81641100	-1.06900900
H	5.58919900	-3.25399400	0.97979000
C	0.45313000	1.99996300	0.14397500
C	-0.58396600	2.74109500	0.73860700
C	1.44043800	2.69058300	-0.58004500
C	-0.67741100	4.10671600	0.53684200
H	-1.31393100	2.22695500	1.35159200
C	1.34187200	4.05916300	-0.77944400
H	2.28273800	2.13831700	-0.97921600
C	0.27861500	4.77048200	-0.23193200
H	-1.48893500	4.66340600	0.99022500
H	2.10528900	4.57707100	-1.34763200
H	0.21019400	5.84223500	-0.37612000
C	-0.73790100	-0.18181100	-1.45946800
H	-1.37997100	-0.20012200	-2.33524900
C	0.61150000	0.57132500	0.40284100
C	-1.35909600	-0.32333800	-0.16058900
C	-2.72558500	-0.87059400	-0.02152400
C	-3.29142900	-1.70321100	-0.99402300
C	-3.47637000	-0.57623200	1.12093900
C	-4.57061200	-2.21698600	-0.82983200
H	-2.71220800	-1.97455200	-1.86906500
C	-4.75139300	-1.10126400	1.29196000

H	-3.05215400	0.08534400	1.86845600
C	-5.30530700	-1.91972700	0.31426200
H	-4.99078700	-2.86487400	-1.59015600
H	-5.31753700	-0.86102000	2.18427300
H	-6.30185700	-2.32528300	0.44185000
C	-0.49259000	-0.20049700	0.92309100
H	-0.49547200	-0.88271900	1.76585600

SCF Done: E(RM062X) = -925.080170547 A.U.

Zero-point correction= 0.322047 (Hartree/Particle)
Thermal correction to Energy= 0.390936
Thermal correction to Enthalpy= 0.392751
Thermal correction to Gibbs Free Energy= 0.193721

SCF Done: E(RB3LYP) = -925.580585446 A.U.

P2

C	0.73870200	-1.06294300	0.00112900
C	0.24765400	0.25527900	-0.00982300
C	1.14138400	1.44571900	-0.03736900
C	2.15665000	1.56815800	-0.98979100
C	0.95520600	2.47804900	0.88424600
C	2.96757500	2.69478000	-1.01420600
H	2.30734100	0.77408500	-1.71238400
C	1.77108200	3.60395100	0.86340200
H	0.17643800	2.38441500	1.63358100
C	2.78022500	3.71466200	-0.08558300
H	3.74828100	2.77820900	-1.76099100
H	1.61981200	4.39182400	1.59183500
H	3.41722400	4.59098300	-0.10343700
C	2.19075200	-1.38395700	0.05432700
C	2.73669900	-2.29864600	-0.84912100
C	3.02575000	-0.80827800	1.01595300
C	4.08760900	-2.62466200	-0.80056600
H	2.09695600	-2.74162000	-1.60488000
C	4.37309100	-1.13792600	1.06799100
H	2.61216700	-0.09946600	1.72456500
C	4.90963300	-2.04450800	0.15783600
H	4.49713200	-3.32999000	-1.51423700
H	5.00725200	-0.68635900	1.82160200
H	5.96262200	-2.29675500	0.19739700
C	-0.17899700	-2.11687400	-0.00806000

H	0.19676200	-3.13386800	0.01310600
C	-1.54646200	-1.89090800	-0.01599600
H	-2.23239600	-2.73000300	-0.04021800
C	-1.13228000	0.46631900	-0.01294500
H	-1.49921400	1.48739800	-0.01816400
C	-2.04574100	-0.58714000	-0.01462700
C	-3.50626000	-0.32732600	-0.02490500
C	-4.37447000	-1.10909400	0.74261200
C	-4.04419900	0.70164900	-0.80297000
C	-5.74268600	-0.86900800	0.73222200
H	-3.96861800	-1.89355300	1.37151300
C	-5.41231500	0.94207900	-0.81311400
H	-3.38678200	1.29983700	-1.42404400
C	-6.26672900	0.15757700	-0.04590900
H	-6.39957800	-1.47970500	1.34047700
H	-5.81298400	1.73785400	-1.42976600
H	-7.33364300	0.34498900	-0.05435000

SCF Done: E(RM062X) = -925.240360664 A.U.

Zero-point correction= 0.326744 (Hartree/Particle)
Thermal correction to Energy= 0.395544
Thermal correction to Enthalpy= 0.397359
Thermal correction to Gibbs Free Energy= 0.198351

SCF Done: E(RB3LYP) = -925.733576603 A.U.

TS1-2

C	3.88086500	0.02665900	-0.96150700
C	3.83930000	-1.34129600	-0.69925500
C	2.94554700	0.87676600	-0.39676700
H	4.64397100	0.42944800	-1.61663200
C	2.85281100	-1.85753500	0.13917000
H	4.57131300	-2.00269400	-1.14631200
C	1.94802200	0.36536400	0.45724500
H	2.96593600	1.93982200	-0.60203300
C	1.91898200	-1.01872100	0.72200700
H	2.81610700	-2.92137100	0.34049100
C	1.00007200	1.22358100	1.04194500
H	1.15076100	-1.41390000	1.37535900
C	-0.02220100	1.92559800	1.23076500
C	-1.26207700	1.80890500	-0.03463200
C	-1.36216100	2.87151300	-0.71254000

C	-1.94409100	0.50090300	-0.04216800
C	-2.73156700	0.17277700	-1.15396000
C	-1.85899900	-0.41172200	1.01109200
C	-3.40856400	-1.03516200	-1.20902900
H	-2.79717100	0.88190200	-1.97008600
C	-2.54470000	-1.62084600	0.95451300
H	-1.26133900	-0.17444100	1.88119400
C	-3.31836200	-1.93921800	-0.15377000
H	-4.00755000	-1.27485400	-2.07973700
H	-2.47290300	-2.31449000	1.78393300
H	-3.84775300	-2.88340600	-0.19755800
H	-0.97316400	3.84947100	-0.91606600
H	-0.38546600	2.59912600	1.98879300

SCF Done: E(UM062X) = -616.608446409 A.U.
<S**2> = 0.4126
Zero-point correction= 0.207669 (Hartree/Particle)
Thermal correction to Energy= 0.255857
Thermal correction to Enthalpy= 0.257672
Thermal correction to Gibbs Free Energy= 0.098355

SCF Done: E(UB3LYP) = -616.948492675 A.U.
<S**2> = 0.3235

TS1-3

C	2.67191500	-1.44413400	-1.16224800
C	3.87493700	-1.36822200	-0.47244400
C	1.62355800	-0.58639600	-0.84721800
H	2.54372700	-2.17434700	-1.95228100
C	4.02650000	-0.42876200	0.54446500
H	4.69113900	-2.03463300	-0.72409300
C	1.76731000	0.35634900	0.17299600
H	0.69237200	-0.65056100	-1.39540600
C	2.98254000	0.42334000	0.86746700
H	4.96220900	-0.36030400	1.08651700
C	0.68074000	1.26436400	0.57841700
H	3.09032700	1.15499200	1.65914200
C	0.44388600	2.00444500	1.57497300
C	-0.68076400	1.26439400	-0.57836200
C	-0.44390100	2.00458000	-1.57481800
C	-1.76731200	0.35633100	-0.17299900
C	-2.98257200	0.42338900	-0.86741200
C	-1.62351100	-0.58649700	0.84712300
C	-4.02652300	-0.42873100	-0.54442700

H	-3.09038500	1.15510300	-1.65902300
C	-2.67185800	-1.44425300	1.16213500
H	-0.69229800	-0.65070100	1.39526000
C	-3.87491500	-1.36827100	0.47239900
H	-4.96225700	-0.36022900	-1.08643100
H	-2.54363500	-2.17453200	1.95209700
H	-4.69111100	-2.03469500	0.72403700
H	0.19247800	2.73927400	-2.02651700
H	-0.19274500	2.73909000	2.02641600

SCF Done: E(UM062X) = -616.597664847 A.U.
<S**2> = 0.4746
Zero-point correction= 0.207215 (Hartree/Particle)
Thermal correction to Energy= 0.255625
Thermal correction to Enthalpy= 0.257440
Thermal correction to Gibbs Free Energy= 0.100142

SCF Done: E(UB3LYP) = -616.935634829 A.U.
<S**2> = 0.3678

TS1_con1

C	-0.02493900	2.34726100	0.37541400
C	-0.96616100	2.40910600	-0.66337500
C	-2.02564500	1.52865200	-0.70151100
C	-2.16024300	0.53912200	0.30010700
C	-1.21463700	0.49960500	1.34857400
C	-0.16876300	1.41309000	1.39051700
C	-3.06343400	-0.52473400	0.20007700
C	-2.92392600	-1.76252400	-0.06403700
H	0.80875500	3.03904000	0.38891500
H	-2.75122300	1.56201000	-1.50507700
H	-1.32467400	-0.25493900	2.11823700
H	0.55879900	1.36578700	2.19206000
C	3.49409700	0.13507700	-0.09270100
C	3.08685900	-0.80777300	0.85455000
C	1.84797700	-1.41083000	0.75685800
C	0.97327200	-1.07334100	-0.29953200
C	1.38471000	-0.10531200	-1.23732400
C	2.64019100	0.47785900	-1.13449800
C	-0.28340400	-1.68635400	-0.41534900
C	-1.38020400	-2.27808300	-0.58876100
H	4.47038600	0.59749000	-0.01336700
H	3.74977500	-1.07621600	1.66857500
H	1.52981800	-2.14673500	1.48536500

H	0.70648500	0.17121700	-2.03507600
H	2.94815600	1.21232800	-1.86955700
H	-0.85152000	3.14821700	-1.44789800
H	-1.56176100	-3.20342600	-1.11897800
H	-3.57750200	-2.61970300	-0.03724600

SCF Done: E(RM062X) = -616.618555116 A.U.

Zero-point correction= 0.209168 (Hartree/Particle)
Thermal correction to Energy= 0.256382
Thermal correction to Enthalpy= 0.258197
Thermal correction to Gibbs Free Energy= 0.105519

SCF Done: E(RB3LYP) = -616.961157306 A.U.

TS1_con2

C	-4.15950400	0.73504400	-0.86153800
C	-3.92579700	-0.63065900	-1.15482400
C	-3.01041200	-1.35181900	-0.43550700
C	-2.26739400	-0.72483600	0.59721700
C	-2.43444400	0.66498000	0.82756300
C	-3.44791200	1.36427900	0.12589200
C	-1.18023000	-1.29672400	1.24247000
C	0.03076300	-1.01015700	1.38666500
H	-4.92270200	1.27392400	-1.41049200
H	-2.83659900	-2.40083200	-0.64072100
H	-1.99271700	1.10508200	1.71172300
H	-3.65186300	2.39984200	0.37409600
C	4.70115300	-0.12263400	-0.47859900
C	3.82971600	-1.19686800	-0.62162500
C	2.47186200	-1.03446700	-0.37631800
C	1.96659500	0.21521700	-0.00978900
C	2.84650900	1.29206700	0.13014000
C	4.20568600	1.12032700	-0.09818600
C	0.52730800	0.41840100	0.20978900
C	-0.37559700	1.21750700	-0.11676900
H	5.76097300	-0.25375000	-0.66073700
H	4.20752900	-2.16700000	-0.92173700
H	1.78941900	-1.87029600	-0.47893600
H	2.45283000	2.25804600	0.42229100
H	4.87977900	1.96054800	0.01874000
H	-4.48769000	-1.10943000	-1.94791500
H	-0.78545200	2.06127000	-0.62550100

H	0.91667500	-1.21535400	1.95970800

SCF Done: E(RM062X) = -616.603923176 A.U.

Zero-point correction= 0.209371 (Hartree/Particle)
Thermal correction to Energy= 0.256690
Thermal correction to Enthalpy= 0.258505
Thermal correction to Gibbs Free Energy= 0.105800

SCF Done: E(RB3LYP) = -616.938737741 A.U.

TS-St

C	5.84613800	0.07236700	-0.40015900
C	5.11773600	1.25958500	-0.36635500
C	5.19282900	-1.14568400	-0.23323600
H	6.91711600	0.09646800	-0.56041100
C	3.74669400	1.23305900	-0.16790600
H	5.62261400	2.20922400	-0.49810400
C	3.82130300	-1.18310900	-0.03145800
H	5.75646300	-2.07077100	-0.26003100
C	3.07920700	0.01001100	0.01788800
H	3.17317000	2.15209000	-0.14848200
H	3.30704900	-2.12831000	0.09488200
C	1.65690100	-0.02248500	0.20243700
C	0.74842100	-0.20706700	1.16539100
C	-0.51220800	-0.11523100	0.46867000
C	-1.77673800	-0.12049700	0.47521600
C	-3.13901100	-0.04744200	0.14777000
C	-3.81035000	1.19422100	0.16059900
C	-3.87025500	-1.21099300	-0.17470500
C	-5.15812800	1.26333300	-0.14445800
H	-3.25119800	2.08709200	0.41156900
C	-5.21818600	-1.12677700	-0.47654800
H	-3.35766200	-2.16487500	-0.18180400
C	-5.86787100	0.10647700	-0.46346900
H	-5.66228900	2.22218900	-0.13502300
H	-5.76928200	-2.02581400	-0.72524300
H	-6.92323900	0.16548500	-0.70004900
H	0.90527500	-0.37388800	2.22924100
H	0.14308600	0.07248400	-0.60461000

SCF Done: E(UM062X) = -616.587903108 A.U.
<S**2> = 0.5692

Zero-point correction= 0.206232 (Hartree/Particle)
Thermal correction to Energy= 0.253712
Thermal correction to Enthalpy= 0.255528
Thermal correction to Gibbs Free Energy= 0.096800

SCF Done: E(UB3LYP) = -616.931280186 A.U.
<S**2> = 0.4401

TS4-2

C	-3.26300000	2.76161300	0.73630100
C	-2.60503300	3.02597100	-0.46394000
C	-2.81314900	1.73304200	1.55824200
H	-4.12286900	3.35376400	1.02632100
C	-1.51095400	2.26452300	-0.84495300
H	-2.95058000	3.82758000	-1.10637300
C	-1.71520700	0.96989000	1.18708900
H	-3.32755800	1.51561700	2.48682200
C	-1.03956100	1.23211500	-0.01670900
H	-1.00645800	2.45572400	-1.78489500
H	-1.37349000	0.15490300	1.81432100
C	0.03374900	0.38254100	-0.43634300
C	1.32328800	0.21708900	-0.22853000
C	2.14414100	-0.89345200	-0.75848600
C	3.44114500	-0.96877000	-0.59946800
C	4.69066600	-0.54620100	-0.14145200
C	5.17314500	-0.95744700	1.12551100
C	5.52645600	0.26445100	-0.94886000
C	6.42385800	-0.56068400	1.56068500
H	4.54330800	-1.58372500	1.74560500
C	6.77385500	0.65179500	-0.49635900
H	5.16786900	0.57812800	-1.92148300
C	7.23211200	0.24411400	0.75678600
H	6.77620500	-0.87862800	2.53479500
H	7.39853200	1.27833100	-1.12227100
H	8.21111600	0.55059200	1.10349200
H	1.85890200	0.94533400	0.38484100
H	1.61421400	-1.68762500	-1.28060000
C	-5.36316400	-0.30376200	-0.04434100
C	-4.22539400	-0.32342600	-0.83541700
C	-3.27095200	-1.33818900	-0.66668000
C	-3.48561800	-2.33337800	0.29929600
C	-4.62591700	-2.30172000	1.08697700
C	-5.56648800	-1.28807000	0.92003200
H	-6.08996100	0.48968000	-0.17199700

H	-4.04425500	0.45509500	-1.56678000
H	-2.74442900	-3.11273600	0.42724100
H	-4.78200200	-3.06885100	1.83610600
H	-6.45553200	-1.26679700	1.53892000
C	-2.07033400	-1.31502700	-1.42570000
C	-0.96175800	-1.09790300	-1.88505700
H	-0.14832200	-1.12107400	-2.57579700

SCF Done: E(UM062X) = -924.964743270 A.U.
<S**2> = 1.0715
Zero-point correction= 0.315802 (Hartree/Particle)
Thermal correction to Energy= 0.389267
Thermal correction to Enthalpy= 0.391082
Thermal correction to Gibbs Free Energy= 0.173473

SCF Done: E(UB3LYP) = -925.472212481 A.U.
<S**2> = 1.0450

TS4-3

C	-3.67104500	2.97903200	-0.80574100
C	-3.38249600	1.80168800	-1.49129400
C	-2.90536600	3.34174700	0.30017300
H	-4.48996500	3.61000900	-1.12955300
C	-2.33868400	0.98742000	-1.07832800
H	-3.97795200	1.51367500	-2.34979100
C	-1.85871700	2.53531900	0.72024700
H	-3.12694400	4.25718000	0.83598900
C	-1.55198200	1.34953600	0.02998800
H	-2.12312700	0.06047000	-1.59845200
H	-1.26382500	2.80706800	1.58455000
C	-0.50359800	0.49217400	0.50223400
C	0.79970300	0.36644000	0.35387600
C	1.58992800	1.23900200	-0.55567300
C	2.88040100	1.09540200	-0.71376600
C	4.09146600	0.43693000	-0.45642600
C	4.49644000	-0.66305200	-1.24898700
C	4.95652100	0.88003600	0.57132700
C	5.70277600	-1.29488800	-1.00679500
H	3.84277400	-1.00200600	-2.04339000
C	6.15878800	0.23582100	0.80121000
H	4.65818700	1.72831900	1.17535600
C	6.54057500	-0.85235500	0.01650700
H	5.99566600	-2.14099700	-1.61730700
H	6.80759900	0.58180000	1.59713700

H	7.48475800	-1.35012000	0.19984000
H	1.35080100	-0.39547200	0.89914700
H	1.03562800	2.01277000	-1.08375700
C	-4.47059600	-1.85777900	-0.00709300
C	-3.59911800	-1.31042300	0.92749000
C	-2.23813800	-1.61277800	0.87209100
C	-1.75724000	-2.46189300	-0.12772100
C	-2.63330900	-3.01066200	-1.05377500
C	-3.99155300	-2.70688300	-0.99797400
H	-5.52540500	-1.61450300	0.03731800
H	-3.96050500	-0.63482700	1.69334200
H	-0.69565500	-2.67321700	-0.17559000
H	-2.25586600	-3.67384800	-1.82293900
H	-4.67308100	-3.13080800	-1.72582000
C	-1.32117100	-1.00159600	1.81931900
C	-0.80195300	-0.86589300	2.92119500
H	-0.23288500	-0.56955100	3.77142200

SCF Done: E(UM062X) = -924.960632211 A.U.
<S**2> = 1.0318
Zero-point correction= 0.315481 (Hartree/Particle)
Thermal correction to Energy= 0.389115
Thermal correction to Enthalpy= 0.390930
Thermal correction to Gibbs Free Energy= 0.171267

SCF Done: E(UB3LYP) = -925.467885494 A.U.
<S**2> = 0.9810

TS4-4

C	-3.77492700	2.76917900	-1.24758700
C	-3.13759000	1.73154800	-1.92224800
C	-3.32831900	3.15038100	0.01605100
H	-4.61833800	3.27569800	-1.70119700
C	-2.06122100	1.07737100	-1.34159600
H	-3.48589700	1.42489700	-2.90139800
C	-2.25344400	2.50122100	0.60448000
H	-3.82375300	3.95667000	0.54444400
C	-1.59470400	1.46219500	-0.07350000
H	-1.57720100	0.24987500	-1.84844900
H	-1.91113500	2.78370600	1.59318900
C	-0.53769000	0.71902800	0.55316800
C	0.77097600	0.60254700	0.43919900
C	1.62007000	-0.35974500	1.17299100
C	2.89872800	-0.51070300	0.93372800

C	4.09569600	-0.23768100	0.26472600
C	5.00885200	0.72293600	0.76355300
C	4.44430400	-0.95068200	-0.90834900
C	6.20077900	0.96361600	0.10525900
H	4.75378300	1.26725800	1.66452200
C	5.64040800	-0.69659800	-1.55344700
H	3.75423800	-1.69214200	-1.29230000
C	6.52573700	0.25905800	-1.05410700
H	6.88627800	1.70672500	0.49543400
H	5.88905000	-1.24503400	-2.45437000
H	7.46192700	0.45179600	-1.56310800
H	1.29383500	1.24920600	-0.26851900
H	1.12437800	-0.96248600	1.93094600
C	-4.27421200	-1.82628100	-0.37707600
C	-3.60743100	-1.15028100	0.63799700
C	-2.25082000	-1.39021900	0.86005200
C	-1.56547100	-2.30137700	0.05332700
C	-2.23938700	-2.97893400	-0.95328500
C	-3.59409400	-2.74117900	-1.17229700
H	-5.32549000	-1.63025100	-0.55036000
H	-4.12305600	-0.42080500	1.25087900
H	-0.50542600	-2.46143800	0.21472800
H	-1.70545800	-3.68982100	-1.57242900
H	-4.11537700	-3.26555600	-1.96437900
C	-1.54786500	-0.64354300	1.89126600
C	-1.28276000	-0.35003300	3.05216800
H	-0.90604600	0.07075500	3.95552600

SCF Done: E(UM062X) = -924.958554917 A.U.
<S**2> = 1.0706
Zero-point correction= 0.315002 (Hartree/Particle)
Thermal correction to Energy= 0.388839
Thermal correction to Enthalpy= 0.390654
Thermal correction to Gibbs Free Energy= 0.170465

SCF Done: E(UB3LYP) = -925.465636809 A.U.
<S**2> = 1.0439

TS7-2

C	0.77782200	-0.16221600	-0.78075900
C	2.03447200	-0.99727200	-0.63511400
C	1.39944200	-2.07288200	-1.15686100
H	1.67053500	-3.10323200	-1.34040500
C	3.35959200	-0.77576000	-0.06719700

C	3.53200500	0.10024900	1.01092500
C	4.47007400	-1.46727400	-0.56452600
C	4.78743400	0.27716100	1.57828000
H	2.67130200	0.62347800	1.41235700
C	5.72278300	-1.28662900	0.00388900
H	4.34169400	-2.13334100	-1.41039900
C	5.88572100	-0.41240900	1.07535200
H	4.90782700	0.95368800	2.41594000
H	6.57703400	-1.82175000	-0.39349100
H	6.86553100	-0.26910300	1.51511800
C	0.39579300	1.20874600	-0.63135500
C	-0.97304400	1.54346800	-0.65934600
C	1.33629200	2.24217300	-0.46874400
C	-1.38064600	2.85729200	-0.50654200
H	-1.70834700	0.75658900	-0.78989200
C	0.91813100	3.55697800	-0.32707400
H	2.39391000	2.00731400	-0.48152200
C	-0.43830400	3.87210800	-0.33755400
H	-2.43860500	3.09396700	-0.52214900
H	1.65518600	4.34307100	-0.21156600
H	-0.75985700	4.89998700	-0.22235300
C	0.08393500	-1.28941500	-1.23851200
H	-0.71987000	-1.35403900	-1.95969300
C	-2.14769500	-1.68594300	0.51764700
C	-3.46835200	-1.18006500	0.47685900
C	-4.49630800	-1.89496300	-0.16322700
C	-3.77243900	0.05466200	1.08133900
C	-5.78365000	-1.38234200	-0.20206600
H	-4.26698400	-2.84835700	-0.62303800
C	-5.06474800	0.55168600	1.04218400
H	-2.97967500	0.60767800	1.57144700
C	-6.07523500	-0.16089700	0.39936500
H	-6.56665600	-1.93986800	-0.70225400
H	-5.28633200	1.50154400	1.51422100
H	-7.08360000	0.23308800	0.36827400
C	-0.96333800	-2.00057200	0.39739300
H	-0.11150600	-2.52600700	0.79326600

SCF Done: E(UM062X) = -925.005876077 A.U.
<S**2> = 0.5005
Zero-point correction= 0.316560 (Hartree/Particle)
Thermal correction to Energy= 0.388799
Thermal correction to Enthalpy= 0.390614
Thermal correction to Gibbs Free Energy= 0.178751

SCF Done: E(UB3LYP) = -925.506826665 A.U.
<S**2> = 0.6210

TS7-3

C	0.81766700	0.15490400	1.20290300
C	-0.62683100	0.06717300	1.43940300
C	-0.43833900	-0.99478000	2.31508100
H	-1.09984200	-1.62491400	2.89252500
C	-1.80425500	0.69398400	0.86014600
C	-1.77491700	1.15533800	-0.46202200
C	-3.00047300	0.77876700	1.58287400
C	-2.91444400	1.69599700	-1.04180300
H	-0.86129800	1.04964800	-1.03734600
C	-4.13620900	1.32276900	1.00038600
H	-3.02567300	0.42642500	2.60825200
C	-4.09634800	1.78591600	-0.31253100
H	-2.88225600	2.04063400	-2.06886200
H	-5.05506500	1.38963500	1.57091200
H	-4.98399500	2.21173600	-0.76477200
C	1.73774400	1.02741600	0.54587600
C	3.07201100	0.61001600	0.36302800
C	1.36743400	2.30631300	0.08670500
C	3.98994700	1.43315700	-0.26660900
H	3.36473500	-0.37689900	0.70736200
C	2.29509500	3.12423900	-0.53836300
H	0.35469800	2.65611700	0.24800100
C	3.60763500	2.69441500	-0.72287400
H	5.00984500	1.09370200	-0.40474000
H	1.99584800	4.10855700	-0.87886300
H	4.32784200	3.33778800	-1.21329400
C	1.01027700	-1.03773300	2.01602600
H	1.83561000	-1.26491100	2.67834200
C	2.07483300	-3.44864100	1.11925600
C	1.28156300	-2.61019300	0.66433500
C	0.43920900	-2.24450300	-0.46971100
C	0.99558900	-1.58364300	-1.56815600
C	-0.93102100	-2.51343600	-0.45261700
C	0.19260700	-1.21447100	-2.64018300
H	2.05636600	-1.36231400	-1.57319000
C	-1.73126200	-2.13581700	-1.52411300
H	-1.36153100	-3.01861600	0.40355900
C	-1.17208600	-1.48708800	-2.61952400
H	0.63537700	-0.70987600	-3.49078000

H	-2.79460000	-2.34177600	-1.49874900
H	-1.79864500	-1.19094500	-3.45261400
H	2.75003800	-3.90459100	1.80918400

SCF Done: E(UM062X) = -924.998504463 A.U.
<S**2> = 1.0454
Zero-point correction= 0.315700 (Hartree/Particle)
Thermal correction to Energy= 0.388208
Thermal correction to Enthalpy= 0.390023
Thermal correction to Gibbs Free Energy= 0.180763

SCF Done: E(UB3LYP) = -925.500943657 A.U.
<S**2> = 1.0436

TS7-4

C	-0.60468300	-0.42171700	2.08756600
C	-0.14877600	0.45490600	1.05203000
C	0.30512800	-1.40872700	1.73677700
H	-1.39004900	-0.35706500	2.82858400
H	0.55705400	-2.38629800	2.12067400
C	2.27165900	-0.41119100	0.33834000
C	2.86481600	0.85174000	0.26094800
C	3.07381600	-1.54291600	0.14314500
C	4.22328700	0.97789400	-0.01166500
H	2.26541600	1.73688800	0.43824700
C	4.42823400	-1.41521000	-0.12569300
H	2.61808900	-2.52640900	0.19402700
C	5.00863800	-0.15120000	-0.20876500
H	4.66894100	1.96437900	-0.06336300
H	5.03433900	-2.30161200	-0.27224700
H	6.06628600	-0.05011500	-0.42034700
C	-0.60238000	1.69714700	0.51443800
C	-1.59513400	2.44089200	1.18269700
C	-0.12315400	2.17807900	-0.72163400
C	-2.08125600	3.61789100	0.64133400
H	-1.97696000	2.07887800	2.13081600
C	-0.61844600	3.35690000	-1.25675100
H	0.61517000	1.59759500	-1.26380000
C	-1.59595100	4.08466200	-0.58056400
H	-2.84416500	4.17761900	1.16958500
H	-0.24589700	3.70977300	-2.21137000
H	-1.97969800	5.00549500	-1.00259300
C	0.84098400	-0.58233900	0.62620700
C	0.82062900	-1.38866100	-2.06173900

C	-0.01092000	-1.34697900	-1.13923600
C	-1.40023800	-1.62010500	-0.78374100
C	-1.74811400	-2.85090000	-0.22358900
C	-2.38296400	-0.64459600	-0.96238900
C	-3.06255700	-3.10505100	0.14622100
H	-0.98116600	-3.60449000	-0.08621200
C	-3.69538500	-0.90055600	-0.58329400
H	-2.11085400	0.31230600	-1.39173600
C	-4.03846500	-2.12851000	-0.02781300
H	-3.32483500	-4.06592900	0.57283200
H	-4.45042400	-0.13611100	-0.72409400
H	-5.06264000	-2.32561400	0.26590000
H	1.76878900	-1.27799100	-2.54188100

SCF Done: E(UM062X) = -924.995728152 A.U.
<S**2> = 1.0897
Zero-point correction= 0.315381 (Hartree/Particle)
Thermal correction to Energy= 0.388056
Thermal correction to Enthalpy= 0.389871
Thermal correction to Gibbs Free Energy= 0.179439

SCF Done: E(UB3LYP) = -925.496372969 A.U.
<S**2> = 1.0811

TS7-5

C	1.51084600	-0.64268900	-0.91176500
C	0.29261200	0.22514500	-1.08534000
C	-0.35143800	-0.76121300	-1.74486700
H	-1.27702900	-0.84106500	-2.29637600
C	-0.10309400	1.58306100	-0.71834900
C	0.83601000	2.61391500	-0.60737800
C	-1.45742200	1.87259600	-0.51030600
C	0.42963300	3.90266500	-0.28383600
H	1.88323600	2.40300600	-0.79353000
C	-1.85872300	3.16071100	-0.18558000
H	-2.18840400	1.07444700	-0.58751800
C	-0.91642300	4.17886900	-0.06677900
H	1.16559500	4.69398400	-0.20339900
H	-2.90903700	3.36875800	-0.01756900
H	-1.23003200	5.18301700	0.19245200
C	2.76201900	-0.55204500	-0.18721000
C	3.80984600	-1.44024900	-0.47777700
C	2.93815600	0.37416500	0.85087900
C	4.99474700	-1.39628500	0.23906600

H	3.68795300	-2.15420000	-1.28517900
C	4.12957800	0.41762700	1.56349000
H	2.12519900	1.04102800	1.11171900
C	5.16222000	-0.46298700	1.26075100
H	5.79580700	-2.08544800	-0.00102600
H	4.24874600	1.13749300	2.36466600
H	6.09091200	-0.42630700	1.81718400
C	0.87170000	-1.69076100	-1.53841600
H	1.23014500	-2.53991500	-2.10520000
C	-1.11612900	-2.29847600	0.11831100
C	-2.38678300	-1.72119000	0.38984400
C	-3.52011000	-2.06181500	-0.36699800
C	-2.51687700	-0.78079900	1.42546100
C	-4.74194600	-1.46272600	-0.10211900
H	-3.42371500	-2.79335400	-1.16041400
C	-3.74653400	-0.19475900	1.68636600
H	-1.64055500	-0.51102100	2.00260600
C	-4.86277100	-0.52694300	0.92291000
H	-5.60817600	-1.73023100	-0.69590700
H	-3.83216600	0.53215500	2.48550800
H	-5.82032900	-0.06337100	1.12617100
C	-0.00075600	-2.79797000	-0.03345900
H	0.75168900	-3.51606400	0.22440800

SCF Done: E(RM062X) = -925.012098338 A.U.

Zero-point correction= 0.318751 (Hartree/Particle)
Thermal correction to Energy= 0.390266
Thermal correction to Enthalpy= 0.392081
Thermal correction to Gibbs Free Energy= 0.181864

SCF Done: E(RB3LYP) = -925.510365733 A.U.

TS7-6

C	-0.81551500	2.70453800	1.34462800
C	-0.87970400	1.66799400	0.30294400
C	-2.00060900	0.97481100	-0.32124100
C	-3.24220500	1.61377200	-0.42064400
C	-1.88165200	-0.34340800	-0.78154100
C	-4.32864300	0.96451900	-0.99089700
H	-3.34514500	2.63048900	-0.05746300
C	-2.97216800	-0.99234900	-1.34352800
H	-0.94005700	-0.86926500	-0.66646200

C	-4.19676900	-0.34026000	-1.45641500
H	-5.28083100	1.47560300	-1.07077600
H	-2.86579700	-2.01570600	-1.68427400
H	-5.04596400	-0.84820600	-1.89764200
C	0.54864700	2.60289300	1.44622900
H	1.30845600	3.31510300	1.74220700
C	1.04063800	1.10084700	2.80706500
H	1.31682800	1.63303500	3.69386500
C	0.49105700	1.57949500	0.25770900
C	0.89346600	0.04289100	2.19181000
C	0.62848800	-1.21768800	1.58793000
C	1.52762800	-1.81358200	0.68767500
C	-0.58416100	-1.86995400	1.87378200
C	1.19999500	-3.01285500	0.07083700
H	2.46922700	-1.32454600	0.46935900
C	-0.89142000	-3.07508900	1.26266100
H	-1.27960000	-1.40665500	2.56307900
C	-0.00657600	-3.64823800	0.35153100
H	1.89653300	-3.45373900	-0.63271600
H	-1.83172500	-3.56390100	1.48848000
H	-0.25270700	-4.58656700	-0.13062000
H	-1.56676200	3.27106600	1.87781600
C	1.53827700	1.09481400	-0.60550900
C	1.27669600	0.41096600	-1.80380900
C	2.87684600	1.30094100	-0.23244300
C	2.31883100	-0.07767400	-2.57763400
H	0.25388300	0.27993900	-2.13295000
C	3.91491300	0.81251900	-1.01162000
H	3.09014200	1.82403800	0.69283100
C	3.64104300	0.11093700	-2.18333500
H	2.09844400	-0.60507100	-3.49829400
H	4.94119000	0.97509700	-0.70402400
H	4.45126700	-0.27575700	-2.78951900

SCF Done: E(RM062X) = -925.017835823 A.U.

Zero-point correction= 0.319007 (Hartree/Particle)
Thermal correction to Energy= 0.390093
Thermal correction to Enthalpy= 0.391908
Thermal correction to Gibbs Free Energy= 0.188632

SCF Done: E(RB3LYP) = -925.516228133 A.U.

TS7-7

C	-0.21509500	-1.06027500	-1.54648800
C	0.96506400	-0.74985800	-0.71654600
C	2.07518900	-1.55789300	-0.26082400
C	2.40745000	-2.73573200	-0.94549500
C	2.80947900	-1.22023200	0.88716100
C	3.45447200	-3.53571300	-0.51268000
H	1.84253500	-3.01081500	-1.82923100
C	3.85191500	-2.02595500	1.31991400
H	2.54393400	-0.32786400	1.44374000
C	4.18244300	-3.18432600	0.62038300
H	3.70372900	-4.43793400	-1.05857000
H	4.40641000	-1.75491500	2.21068800
H	4.99832400	-3.81087600	0.95955800
C	-0.76064800	0.15374700	-1.32614600
H	-1.59878300	0.71713100	-1.70985900
C	-1.78279700	0.02619400	0.86813100
C	0.48669600	0.52799400	-0.44902600
C	-0.66962600	0.30290300	1.31284100
H	-0.55372300	-1.94964100	-2.06172200
C	1.10345400	1.84144200	-0.25999800
C	2.49187300	2.00966800	-0.18767400
C	0.28556700	2.97691900	-0.19561900
C	3.04026700	3.27620100	-0.03780600
H	3.14109900	1.14719400	-0.28036600
C	0.83761600	4.24237300	-0.05303200
H	-0.79066700	2.85083200	-0.24860300
C	2.21754200	4.39673800	0.03293500
H	4.11686500	3.39115800	0.00878800
H	0.19032600	5.11034200	-0.00895100
H	2.64982200	5.38372000	0.14604900
C	-3.13741900	-0.29589800	0.55196500
C	-3.52429600	-1.63457400	0.39090000
C	-4.09537900	0.71526000	0.39063700
C	-4.83846500	-1.94869200	0.08204100
H	-2.77964100	-2.41248700	0.50994300
C	-5.40643400	0.39039700	0.07153300
H	-3.79935900	1.74925900	0.52248700
C	-5.78443700	-0.93957700	-0.08263000
H	-5.12733000	-2.98647700	-0.03451100
H	-6.13858400	1.17953200	-0.05276500
H	-6.80949700	-1.18907000	-0.32846800
H	0.03797900	0.52423700	2.08491500

SCF Done: E(RM062X) = -925.011009402 A.U.

Zero-point correction= 0.318480 (Hartree/Particle)
Thermal correction to Energy= 0.390168
Thermal correction to Enthalpy= 0.391983
Thermal correction to Gibbs Free Energy= 0.181470

SCF Done: E(RB3LYP) = -925.507939038 A.U.

TS7-8

C	1.56072300	-1.97986800	1.59681700
C	0.25743000	-1.53840900	2.04935200
C	1.64966900	-0.99201500	0.63469000
C	0.73902500	-1.82828600	-1.05921900
H	1.57320800	-2.25325200	-1.57832800
C	0.23149000	-0.48312200	1.18202700
C	-0.45042500	-1.52787900	-0.94831500
C	-1.83227100	-1.19024900	-0.98741800
C	-2.24973800	-0.02573700	-1.64830400
C	-2.78269400	-1.97215400	-0.31471300
C	-3.58553000	0.34804700	-1.62769500
H	-1.51330000	0.58558000	-2.15530600
C	-4.11794700	-1.59768600	-0.31270900
H	-2.45542100	-2.86410000	0.20682200
C	-4.52422600	-0.43513300	-0.96383900
H	-3.89289600	1.25826700	-2.12875500
H	-4.84585700	-2.21206400	0.20402100
H	-5.56715900	-0.14172500	-0.95167600
H	2.20453700	-2.80865900	1.85990200
H	-0.44203000	-1.90649400	2.78823400
C	2.82826300	-0.32497900	0.05485100
C	4.07765600	-0.47873400	0.66756900
C	2.74987600	0.44688200	-1.11257700
C	5.21190500	0.11889600	0.13229500
H	4.14580400	-1.05348600	1.58376200
C	3.88112600	1.05706600	-1.63666800
H	1.79465500	0.54721500	-1.61575200
C	5.11731600	0.89362900	-1.01800200
H	6.16947000	-0.01003800	0.62302600
H	3.80126500	1.65288400	-2.53831100
H	6.00004700	1.36646500	-1.43122300
C	-0.57932000	0.70526400	1.05342800
C	-0.12648900	1.84886700	0.38522700

C	-1.88237700	0.70537000	1.58110200
C	-0.95724100	2.95570400	0.24223000
H	0.88532900	1.87680000	0.00103000
C	-2.70454500	1.80799300	1.43249100
H	-2.25050900	-0.18189700	2.08405600
C	-2.24730300	2.94005100	0.75807900
H	-0.58926700	3.83710900	-0.27011300
H	-3.71125000	1.78409000	1.83296600
H	-2.89285800	3.80219600	0.64146000

SCF Done: E(RM062X) = -925.013651988 A.U.

Zero-point correction= 0.318486 (Hartree/Particle)
Thermal correction to Energy= 0.389813
Thermal correction to Enthalpy= 0.391628
Thermal correction to Gibbs Free Energy= 0.186834

SCF Done: E(RB3LYP) = -925.511199314 A.U.

TS8-2

C	0.33208000	-0.41700300	1.09554600
C	0.42435000	-1.33845100	2.16955400
H	-0.08827800	-1.41655000	3.12037600
C	-0.32283800	0.83462300	0.85631300
C	0.08006100	1.68239200	-0.19073200
C	-1.44554600	1.20037000	1.62178600
C	-0.60702500	2.86032400	-0.44503200
H	0.94287000	1.41297300	-0.79001700
C	-2.13212500	2.37314700	1.35272400
H	-1.78647100	0.53967600	2.41137100
C	-1.71601700	3.21192100	0.32065600
H	-0.27622100	3.50919800	-1.24779700
H	-3.00204100	2.63320200	1.94455600
H	-2.25310700	4.12945900	0.11342700
C	2.67381200	-0.57817500	-0.09591300
C	3.03174600	-0.38986500	-1.43041900
C	3.52014200	-0.08310100	0.90064000
C	4.21135600	0.27113400	-1.76342800
H	2.38047400	-0.74891700	-2.21906000
C	4.69409000	0.57831600	0.56963400
H	3.24514600	-0.21600600	1.94134800
C	5.04618000	0.75603900	-0.76574500
H	4.47363700	0.40741500	-2.80599700

H	5.33760700	0.95714400	1.35487200
H	5.96346700	1.27137000	-1.02382700
C	1.37985400	-2.10321500	1.55187700
H	1.90941300	-3.01394200	1.79548700
C	1.37812100	-1.24902000	0.29614300
C	-0.69091800	-1.58463700	-0.80873400
C	-2.02820100	-1.23272700	-0.81309800
C	-2.97031700	-1.92941700	-0.01096600
C	-2.46704100	-0.08798000	-1.52722700
C	-4.27792200	-1.49360200	0.06451800
H	-2.64139900	-2.79943200	0.54489200
C	-3.77770900	0.34020400	-1.42149800
H	-1.75506500	0.45269100	-2.13733500
C	-4.69239100	-0.35505900	-0.63223800
H	-4.98634600	-2.03837600	0.67770300
H	-4.09026000	1.22721400	-1.96006900
H	-5.71796200	-0.01545400	-0.55863100
C	0.57360200	-1.88732600	-0.83047200
H	1.04046600	-2.56501300	-1.54464900

SCF Done: E(UM062X) = -925.045033634 A.U.
<S**2> = 0.6926
Zero-point correction= 0.319411 (Hartree/Particle)
Thermal correction to Energy= 0.389647
Thermal correction to Enthalpy= 0.391462
Thermal correction to Gibbs Free Energy= 0.188746

SCF Done: E(UB3LYP) = -925.544885931 A.U.
<S**2> = 0.5643

M-Ph

C	4.82732400	0.00000000	0.00000000
C	4.13050000	-0.90055800	-0.79939600
C	2.74275100	-0.90357900	-0.80184200
C	2.03600700	0.00000000	0.00000000
C	2.74275100	0.90357900	0.80184200
C	4.13050000	0.90055800	0.79939500
H	5.91057200	0.00000000	-0.00000100
H	4.67020400	-1.60327600	-1.42270800
H	2.19179100	-1.60093200	-1.42068000
H	2.19179100	1.60093100	1.42068000
H	4.67020400	1.60327600	1.42270800
C	0.60289300	0.00000000	0.00000000
C	-0.60289300	0.00000000	0.00000100

C	-2.03600700	0.00000000	0.00000000
C	-2.74275100	-0.90357900	0.80184200
C	-2.74275100	0.90358000	-0.80184100
C	-4.13050000	-0.90055800	0.79939500
H	-2.19179100	-1.60093100	1.42068100
C	-4.13050000	0.90055800	-0.79939500
H	-2.19179100	1.60093200	-1.42068000
C	-4.82732400	0.00000000	-0.00000100
H	-4.67020400	-1.60327600	1.42270800
H	-4.67020400	1.60327600	-1.42270900
H	-5.91057200	0.00000000	-0.00000100

SCF Done: E(RM062X) = -539.353935316 A.U.

Zero-point correction= 0.182309 (Hartree/Particle)
Thermal correction to Energy= 0.222029
Thermal correction to Enthalpy= 0.223844
Thermal correction to Gibbs Free Energy= 0.085591

SCF Done: E(RB3LYP) = -539.639165338 A.U.

TS1-Ph

C	3.90508600	-3.21772600	1.42575200
C	4.24919600	-1.86725600	1.40423500
C	2.56176900	-3.58934600	1.41935300
H	4.67878900	-3.97533700	1.44788800
C	3.26692700	-0.89191100	1.38562400
H	5.29268400	-1.57492600	1.40607800
C	1.56775700	-2.62636900	1.38691800
H	2.29050200	-4.63851000	1.43477100
C	1.90513500	-1.25636800	1.36943600
H	3.52901500	0.15925300	1.37290300
H	0.52108600	-2.90700800	1.37400100
C	0.89501700	-0.28001300	1.34034400
C	-0.00543400	0.47897500	0.89091100
C	0.00568000	0.47911000	-0.89075200
C	-0.89456900	-0.28007200	-1.34025100
C	-1.90487000	-1.25623000	-1.36956800
C	-3.26659500	-0.89150000	-1.38537900
C	-1.56776300	-2.62628900	-1.38768200
C	-4.24905100	-1.86665300	-1.40425400
H	-3.52848200	0.15970800	-1.37216900
C	-2.56196200	-3.58906300	-1.42036000

H	-0.52114500	-2.90714000	-1.37504800
C	-3.90520700	-3.21718100	-1.42639800
H	-5.29248300	-1.57411700	-1.40581600
H	-2.29090100	-4.63827300	-1.43626100
H	-4.67906300	-3.97462900	-1.44875400
C	-1.03191000	1.37220000	1.45140800
C	-1.31359800	1.28724100	2.82107000
C	-1.71516900	2.31465800	0.67961500
C	-2.25749000	2.12047100	3.40025800
H	-0.78140000	0.55561200	3.41733000
C	-2.65741000	3.15261100	1.26663800
H	-1.50730600	2.39562200	-0.37992000
C	-2.93424000	3.05824100	2.62445600
H	-2.46764200	2.03768600	4.45999900
H	-3.17591400	3.88249600	0.65647500
H	-3.67198900	3.71011500	3.07672200
C	1.03194900	1.37263700	-1.45114500
C	1.31346800	1.28808000	-2.82087000
C	1.71517800	2.31498600	-0.67919600
C	2.25716800	2.12159500	-3.39996200
H	0.78130000	0.55653000	-3.41725100
C	2.65722800	3.15322400	-1.26612400
H	1.50744100	2.39564500	0.38038500
C	2.93389400	3.05925100	-2.62400100
H	2.46719200	2.03911700	-4.45975300
H	3.17572100	3.88300800	-0.65583100
H	3.67150100	3.71133900	-3.07618900

SCF Done: E(UM062X) = -1078.65736781 A.U.
<S**2> = 0.3059
Zero-point correction= 0.362618 (Hartree/Particle)
Thermal correction to Energy= 0.445245
Thermal correction to Enthalpy= 0.447060
Thermal correction to Gibbs Free Energy= 0.207925

SCF Done: E(UB3LYP) = -1079.24278685 A.U.
<S**2> = 0.1948

INT1-Ph

C	-3.84030300	-3.11591400	1.13371700
C	-2.58412400	-3.70616400	1.00270700
C	-3.94217600	-1.73942000	1.33583000
H	-4.73463100	-3.72481700	1.08158500
C	-1.43666900	-2.93546000	1.07515900

H	-2.50228700	-4.77457400	0.84199900
C	-2.80489800	-0.95433100	1.40544700
H	-4.91743200	-1.27762400	1.43777800
C	-1.52620400	-1.53926800	1.26670000
H	-0.45768100	-3.38787900	0.97003400
H	-2.87737300	0.11698300	1.55107600
C	-0.36497700	-0.75068100	1.34594000
C	0.56753700	-0.04267100	0.76533900
C	0.56742100	0.04277300	-0.76527200
C	-0.36516000	0.75081000	-1.34572400
C	-1.52643200	1.53930500	-1.26649400
C	-1.43700600	2.93553800	-1.07515800
C	-2.80509200	0.95423500	-1.40504400
C	-2.58452200	3.70614700	-1.00271000
H	-0.45804800	3.38805600	-0.97018300
C	-3.94243000	1.73923600	-1.33543600
H	-2.87748500	-0.11710400	-1.55052500
C	-3.84066100	3.11576700	-1.13352300
H	-2.50276700	4.77458700	-0.84215900
H	-4.91765500	1.27734000	-1.43723500
H	-4.73503900	3.72459800	-1.08139200
C	1.65524400	0.67559700	1.48251700
C	1.89400500	0.42915500	2.83926600
C	2.44523500	1.61783100	0.82138600
C	2.88890400	1.11663300	3.51729000
H	1.28860300	-0.30826900	3.35477700
C	3.44349500	2.30561400	1.50344000
H	2.27816600	1.81564500	-0.23101300
C	3.66852700	2.05949200	2.85154900
H	3.06093900	0.91469500	4.56799900
H	4.04681100	3.03460600	0.97573900
H	4.44799000	2.59403700	3.38130900
C	1.65499900	-0.67552900	-1.48261400
C	1.89354100	-0.42914100	-2.83941100
C	2.44508100	-1.61775000	-0.82157500
C	2.88832000	-1.11666100	-3.51757000
H	1.28806600	0.30827300	-3.35485000
C	3.44321800	-2.30557500	-1.50376500
H	2.27818200	-1.81551600	0.23086000
C	3.66803500	-2.05950700	-2.85192000
H	3.06018900	-0.91476500	-4.56831400
H	4.04660800	-3.03455600	-0.97613400
H	4.44740400	-2.59408300	-3.38178500

SCF Done: E(UM062X) = -1078.66559846 A.U.
<S**2> = 0.9994
Zero-point correction= 0.364878 (Hartree/Particle)
Thermal correction to Energy= 0.447647
Thermal correction to Enthalpy= 0.449462
Thermal correction to Gibbs Free Energy= 0.211528

SCF Done: E(UB3LYP) = -1079.24833505 A.U.
<S**2> = 0.9446

TS2-Ph

C	3.57287900	-2.70275500	0.52192400
C	2.79014400	-3.04758600	1.64758700
C	1.42000200	-2.99026900	1.58966200
C	0.77771900	-2.55138000	0.40327400
C	1.57385600	-2.17985700	-0.71630600
C	2.97341600	-2.30097000	-0.64988700
C	-0.57710200	-2.25170800	0.30688900
C	-1.18181500	-1.13744800	-0.03961700
H	4.65254000	-2.77528100	0.58101200
H	0.81103500	-3.25281800	2.44619200
H	1.08813000	-1.99282900	-1.66573400
H	3.57537000	-2.05090000	-1.51571700
C	4.63336100	2.10729900	-0.88628300
C	3.69228300	2.12460400	-1.91392300
C	2.46716100	1.49731000	-1.75303100
C	2.16062600	0.83460400	-0.54842900
C	3.12950800	0.80303500	0.47501600
C	4.34397300	1.44781000	0.30645000
C	0.94234800	0.13635200	-0.37474400
C	-0.31064000	0.14051100	-0.00938600
H	5.58824900	2.60189700	-1.01619800
H	3.91511300	2.63476300	-2.84356100
H	1.73240500	1.50844400	-2.55008500
H	2.90183600	0.26921100	1.39040100
H	5.07435700	1.43023000	1.10671600
H	3.27990400	-3.36208600	2.56152500
C	-0.94671200	1.35997800	0.58185400
C	-1.85931300	1.23030500	1.63096700
C	-0.62072400	2.63696900	0.12071400
C	-2.42786100	2.35696800	2.21102900
H	-2.12263900	0.24194900	1.99007800
C	-1.19477000	3.76183400	0.69926900
H	0.08419700	2.74553300	-0.69553800

C	-2.09968300	3.62600400	1.74662800
H	-3.13361600	2.24178500	3.02502600
H	-0.93533200	4.74664100	0.32919400
H	-2.54898400	4.50364900	2.19559300
C	-2.59525400	-1.02207200	-0.46871700
C	-3.01267700	-0.00578200	-1.33124800
C	-3.53211900	-1.96601600	-0.03593900
C	-4.33420800	0.06000600	-1.75542700
H	-2.29846000	0.73374000	-1.67500300
C	-4.85176400	-1.89691900	-0.45857500
H	-3.20793500	-2.74925400	0.63976100
C	-5.25885200	-0.88233800	-1.31990500
H	-4.64224400	0.85308800	-2.42632000
H	-5.56621900	-2.63362700	-0.11016700
H	-6.29039300	-0.82505900	-1.64625700

SCF Done: E(UM062X) = -1078.65593396 A.U.
<S**2> = 0.5882
Zero-point correction= 0.364262 (Hartree/Particle)
Thermal correction to Energy= 0.445293
Thermal correction to Enthalpy= 0.447108
Thermal correction to Gibbs Free Energy= 0.218370

SCF Done: E(UB3LYP) = -1079.24138820 A.U.
<S**2> = 0.4562

INT2-Ph

C	-3.29974100	-3.11104000	-0.25084100
C	-2.51453300	-3.73966100	-1.30511800
C	-1.18036000	-3.56901300	-1.37076100
C	-0.50353100	-2.71254500	-0.42737300
C	-1.29378400	-1.90275100	0.58543300
C	-2.74919600	-2.27307500	0.63396900
C	0.76126200	-2.29141300	-0.50233300
C	1.27012300	-1.10103100	-0.21014800
H	-4.35216900	-3.35889600	-0.17495300
H	-0.58170600	-4.04869100	-2.13596900
H	-0.88578600	-2.03449500	1.59873100
H	-3.34746200	-1.86117500	1.43853100
C	-4.25448800	2.33598700	0.81518800
C	-3.71743900	1.65894600	1.90528500
C	-2.66538700	0.76927100	1.72304300
C	-2.13075200	0.55366400	0.45035400
C	-2.68204200	1.22914100	-0.63933300

C	-3.73617500	2.11552200	-0.45645600
C	-1.00449300	-0.38960200	0.25152400
C	0.21293400	-0.01529400	-0.18750500
H	-5.07337500	3.03094600	0.95642800
H	-4.11598200	1.82546800	2.89919500
H	-2.23836000	0.25128100	2.57625700
H	-2.26773100	1.06214000	-1.62706800
H	-4.15294900	2.63632100	-1.31030700
H	-3.02196200	-4.36643900	-2.02864500
C	2.63755500	-0.87124700	0.28922600
C	2.94690300	0.19489900	1.14147000
C	3.65308200	-1.76889400	-0.06085500
C	4.23413700	0.34584000	1.63999900
H	2.17645000	0.90009600	1.42720200
C	4.93828600	-1.61463900	0.43876600
H	3.41612700	-2.58063300	-0.73901800
C	5.23434600	-0.55495600	1.29071900
H	4.45664900	1.17271100	2.30394200
H	5.71321100	-2.31730000	0.15595400
H	6.23937400	-0.42898400	1.67538100
C	0.60501600	1.36127400	-0.58848300
C	0.21468400	2.50366400	0.11870600
C	1.44094800	1.51494800	-1.69778600
C	0.63279600	3.76324200	-0.29015600
H	-0.40989100	2.40622100	0.99845400
C	1.85054400	2.77613600	-2.11176300
H	1.77158000	0.63191300	-2.23457700
C	1.44643300	3.90576000	-1.40953000
H	0.32548400	4.63698600	0.27250600
H	2.49407100	2.87404200	-2.97792400
H	1.77166900	4.88969200	-1.72557300

SCF Done: E(RM062X) = -1078.70071813 A.U.

Zero-point correction= 0.367785 (Hartree/Particle)
Thermal correction to Energy= 0.448477
Thermal correction to Enthalpy= 0.450292
Thermal correction to Gibbs Free Energy= 0.224686

SCF Done: E(RB3LYP) = -1079.27557089 A.U.

TS3-Ph

C	3.59941000	-3.22466600	0.09202500

C	2.68583300	-4.32861300	0.06440800
C	1.34923500	-4.11542000	0.03012100
C	0.76641400	-2.78572700	0.00412400
C	1.74554500	-1.64204800	-0.04614100
C	3.16080100	-1.94410000	0.05516600
C	-0.64655900	-2.60980300	0.03169000
C	-1.06126500	-1.28133600	-0.06866300
H	4.66218100	-3.42096800	0.16854200
H	0.62790200	-4.92253800	0.06183400
H	1.27829400	-2.22947800	-1.07244900
H	3.85538100	-1.11735200	0.12922000
C	3.88867500	3.01967700	0.15487900
C	3.90602700	2.17680400	-0.95113600
C	3.04054700	1.09056800	-1.01128200
C	2.14595600	0.83545200	0.03018900
C	2.14129400	1.68281000	1.13913400
C	3.00592000	2.76828300	1.19984800
C	1.20363000	-0.31765500	-0.04523200
C	-0.17476000	-0.14900500	-0.06824000
H	4.55910600	3.86937900	0.20109000
H	4.58852100	2.36830800	-1.77063600
H	3.04592400	0.43996400	-1.88048800
H	1.44304100	1.49415700	1.94653500
H	2.98736100	3.42101400	2.06434700
H	3.07560300	-5.33858200	0.09910500
C	-2.54032200	-1.05390200	-0.13059900
C	-3.12798900	-0.20032100	-1.06711600
C	-3.36900400	-1.75855700	0.74506500
C	-4.50747200	-0.03780300	-1.11184100
H	-2.50404900	0.33839200	-1.77105000
C	-4.74583200	-1.57972600	0.71657600
H	-2.90936600	-2.45917500	1.43191900
C	-5.32086800	-0.71662400	-0.21154300
H	-4.94587000	0.62335200	-1.85028900
H	-5.37338800	-2.12382500	1.41300400
H	-6.39579500	-0.58177000	-0.23906400
C	-0.71459100	1.24316800	-0.00199900
C	-0.42034100	2.18365400	-0.98853700
C	-1.51806600	1.61755700	1.07600500
C	-0.92658700	3.47497600	-0.90337500
H	0.20724400	1.89930800	-1.82622000
C	-2.01164400	2.91215100	1.16893500
H	-1.76248200	0.88286900	1.83561700
C	-1.72045600	3.84343100	0.17752900

H	-0.69724200	4.19506100	-1.67989700
H	-2.63164300	3.19119300	2.01256100
H	-2.11191300	4.85135500	0.24636900

SCF Done: E(RM062X) = -1078.66257231 A.U.

Zero-point correction= 0.363755 (Hartree/Particle)
Thermal correction to Energy= 0.443649
Thermal correction to Enthalpy= 0.445464
Thermal correction to Gibbs Free Energy= 0.222340

SCF Done: E(RB3LYP) = -1079.23357501 A.U.

P1-Ph

C	3.58027100	-3.25884500	0.09402800
C	2.67243300	-4.33974300	0.02681400
C	1.32749400	-4.09732700	-0.03267200
C	0.82933700	-2.76932800	-0.03587600
C	1.73835200	-1.67941600	0.00085800
C	3.12860200	-1.96565000	0.08278800
C	-0.55967000	-2.50737700	-0.06897900
C	-1.05478200	-1.22825300	-0.06175900
H	4.64347900	-3.45644700	0.16044500
H	0.61800500	-4.91680400	-0.07261600
H	-1.24820800	-3.34474700	-0.12341700
H	3.83397100	-1.14730500	0.14828500
C	3.90406800	2.99982700	0.12379900
C	3.89508900	2.15585100	-0.98163900
C	3.03592600	1.06324900	-1.01728200
C	2.17148300	0.80533700	0.04824100
C	2.19425400	1.65236400	1.15657000
C	3.05437200	2.74267800	1.19431200
C	1.22078400	-0.34436600	-0.00637400
C	-0.14556200	-0.12046900	-0.02719500
H	4.57023500	3.85386100	0.15047600
H	4.55483200	2.35024700	-1.81907600
H	3.02265700	0.40665200	-1.88131500
H	1.52117600	1.45836300	1.98407600
H	3.05719300	3.39485200	2.05958900
H	3.04497800	-5.35703100	0.03154200
C	-2.53081000	-1.03279000	-0.11543900
C	-3.12199100	-0.23124700	-1.09583800
C	-3.35255200	-1.67937300	0.80928600

C	-4.50059600	-0.07963700	-1.14576200
H	-2.49468500	0.27455800	-1.82053400
C	-4.73392200	-1.52245300	0.76335800
H	-2.89927600	-2.29382400	1.57973900
C	-5.31134900	-0.72132600	-0.21395100
H	-4.94395200	0.54297600	-1.91369300
H	-5.35702700	-2.02363800	1.49462700
H	-6.38689600	-0.59573600	-0.25006300
C	-0.68629700	1.27093800	0.02047900
C	-0.38298600	2.19734100	-0.97779200
C	-1.51205900	1.66159000	1.07577200
C	-0.89650400	3.48737600	-0.92309800
H	0.26067400	1.90164700	-1.79874400
C	-2.01878700	2.95362700	1.13614200
H	-1.75959300	0.94274500	1.84958000
C	-1.71397800	3.86973400	0.13524200
H	-0.65505500	4.19553400	-1.70690400
H	-2.65479700	3.24351300	1.96409000
H	-2.11142400	4.87671600	0.17970400

SCF Done: E(RM062X) = -1078.85194419 A.U.

Zero-point correction= 0.370436 (Hartree/Particle)
Thermal correction to Energy= 0.449984
Thermal correction to Enthalpy= 0.451799
Thermal correction to Gibbs Free Energy= 0.230343

SCF Done: E(RB3LYP) = -1079.42480109 A.U.

TS4-Ph

C	-1.34589000	4.07483900	-1.82629400
C	-0.88869800	3.06790100	-2.67441200
C	-1.53457500	3.80260100	-0.47399500
H	-1.56102900	5.06123900	-2.21931400
C	-0.61330600	1.80338500	-2.17512200
H	-0.74663700	3.26987300	-3.72952400
C	-1.26523700	2.53799400	0.03158300
H	-1.89337700	4.57955800	0.19117000
C	-0.78009200	1.52270000	-0.80766900
H	-0.24793300	1.02094100	-2.83126300
H	-1.42023800	2.32989800	1.08354200
C	0.60299700	-0.58694500	-0.43385900
C	1.88212700	-0.10189600	-1.10583900

C	2.51424300	0.92886200	-0.60154200
C	2.59456500	1.97800100	0.32852500
C	3.30293700	1.81927700	1.54165500
C	1.98815800	3.22694700	0.05763300
C	3.37180400	2.85853700	2.45345100
H	3.77650100	0.86703200	1.75014100
C	2.06638900	4.25481400	0.98068400
H	1.44640900	3.35900100	-0.87233900
C	2.75307300	4.07881900	2.18201100
H	3.91159400	2.72130400	3.38351500
H	1.58300200	5.20048300	0.76510500
H	2.80994900	4.88777000	2.89991600
C	0.63713000	-1.96917200	0.11205200
C	-0.46109200	-2.82023600	-0.03597900
C	1.75429400	-2.41746600	0.81819500
C	-0.44906200	-4.08797200	0.53099400
H	-1.32363100	-2.47053900	-0.59309800
C	1.76019100	-3.68133500	1.39552700
H	2.60936200	-1.75951400	0.92987800
C	0.65878600	-4.51904100	1.25524400
H	-1.30401900	-4.74259500	0.40592200
H	2.62554400	-4.01172200	1.95781100
H	0.66671200	-5.50694900	1.70041900
C	2.35309100	-0.85271400	-2.30109700
C	3.68409800	-0.76372300	-2.72178700
C	1.46573200	-1.63965700	-3.03847700
C	4.11239000	-1.43674500	-3.85599100
H	4.37805900	-0.16277300	-2.14473200
C	1.89678600	-2.31349200	-4.17620600
H	0.43261800	-1.72336100	-2.72020200
C	3.21951900	-2.21500600	-4.58888800
H	5.14735500	-1.35975900	-4.16776100
H	1.19560300	-2.91879800	-4.73827100
H	3.55598400	-2.74386800	-5.47252200
C	-0.44184700	0.21440100	-0.30343000
C	-1.74903500	-0.32065600	1.43435900
C	-2.88523200	-0.29662500	0.96722700
C	-0.77087600	-0.56436800	2.47630000
C	-4.05561900	-0.22807500	0.16920400
C	0.27346100	0.32573500	2.74646600
C	-0.86774700	-1.75249500	3.20850200
C	-4.53993500	1.00714300	-0.29249500
C	-4.73492000	-1.40596300	-0.18544300
C	1.19347200	0.03183200	3.74418100

H	0.38031300	1.23486400	2.16377500
C	0.06463800	-2.04659100	4.19313000
H	-1.66652200	-2.44650100	2.97803400
C	-5.67480800	1.05472000	-1.08738300
H	-4.00800200	1.91361700	-0.03126400
C	-5.86874800	-1.34554500	-0.98017400
H	-4.36016200	-2.35689100	0.17400700
H	1.99311500	0.73323700	3.94923600
H	-0.01147400	-2.97759600	4.74205000
C	-6.34302600	-0.11696200	-1.43310200
H	-6.03835500	2.01116200	-1.44325700
H	-6.38574900	-2.25902100	-1.24845400
H	-7.22922700	-0.07337200	-2.05446600
C	1.09642100	-1.15459800	4.46527500
H	1.82487700	-1.38412200	5.23386400

SCF Done: E(UM062X) = -1618.02365316 A.U.
<S**2> = 1.0342
Zero-point correction= 0.547786 (Hartree/Particle)
Thermal correction to Energy= 0.673029
Thermal correction to Enthalpy= 0.674844
Thermal correction to Gibbs Free Energy= 0.344581

SCF Done: E(UB3LYP) = -1618.89839863 A.U.
<S**2> = 0.9945

RAD3-Ph

C	1.02237300	0.12293100	-4.46577500
C	1.01447300	1.27133300	-3.67792200
C	0.85987900	-1.12227200	-3.86650000
H	1.16685600	0.19839500	-5.53705000
C	0.82897300	1.17804200	-2.30479400
H	1.16018700	2.24358400	-4.13382600
C	0.68167300	-1.21625100	-2.49168100
H	0.87123500	-2.02286200	-4.46960300
C	0.64260100	-0.06623500	-1.69432300
H	0.83307600	2.07633000	-1.69776400
H	0.55581000	-2.18968400	-2.02867300
C	-0.36999300	0.63972300	0.48675800
C	-1.27334800	1.67327300	-0.12878000
C	-2.26194900	1.24066900	-0.88274800
C	-2.87912900	0.11819300	-1.47573000
C	-3.89935100	-0.58804900	-0.80197100
C	-2.48524100	-0.31971400	-2.75885300

C	-4.46656300	-1.71438200	-1.37377000
H	-4.22271000	-0.24510500	0.17338400
C	-3.05887300	-1.45042300	-3.31566800
H	-1.71317300	0.22667600	-3.28910500
C	-4.04463100	-2.15648500	-2.62729700
H	-5.24094000	-2.25382100	-0.84069500
H	-2.73068400	-1.78767900	-4.29182500
H	-4.48755100	-3.04128200	-3.06799900
C	-0.48743500	0.50287000	1.96548200
C	0.64946400	0.51644900	2.77754200
C	-1.73967900	0.34297100	2.56039200
C	0.53838000	0.34304000	4.15081900
H	1.62184000	0.66033600	2.31915800
C	-1.85029300	0.15559600	3.93212600
H	-2.62560400	0.34595000	1.93557700
C	-0.71165600	0.15211000	4.73063400
H	1.42792600	0.35795100	4.76996600
H	-2.82687200	0.01224100	4.37928700
H	-0.79861800	0.00917500	5.80114800
C	-1.05274600	3.10581700	0.19735400
C	-2.06066300	4.05369900	-0.00698500
C	0.18339100	3.53153300	0.68824800
C	-1.83290600	5.39410000	0.26444500
H	-3.02534400	3.72377600	-0.37680100
C	0.41102000	4.87677500	0.95904400
H	0.97192500	2.80465100	0.85246000
C	-0.59465800	5.81130900	0.74817700
H	-2.62350800	6.11781500	0.10451800
H	1.37638900	5.19307000	1.33590300
H	-0.41873500	6.85873300	0.96230100
C	0.41177200	-0.19030000	-0.23414800
C	1.02859300	-1.39654000	0.43070300
C	2.33442100	-1.53730600	0.44482500
C	0.09180600	-2.39370200	1.02047800
C	3.59705100	-1.02685200	0.08038900
C	-1.15139200	-2.62064300	0.42256100
C	0.42913300	-3.10102500	2.17538200
C	4.08505500	-1.16175400	-1.23838200
C	4.41756800	-0.39931600	1.04331400
C	-2.03320300	-3.54729400	0.96453000
H	-1.43556000	-2.06685500	-0.46769800
C	-0.45659000	-4.02283100	2.71861600
H	1.38242500	-2.90256300	2.65268700
C	5.33516700	-0.67110700	-1.57294700

H	3.45821700	-1.63687200	-1.98324000
C	5.66446700	0.08851500	0.69288800
H	4.05612600	-0.31195200	2.06136300
H	-2.99087000	-3.71308700	0.48429900
H	-0.18891000	-4.55770400	3.62230200
C	6.13021800	-0.04475200	-0.61424300
H	5.69424200	-0.77192900	-2.59025500
H	6.28108200	0.57288100	1.44069900
H	7.10782800	0.33537200	-0.88422300
C	-1.68961900	-4.25000100	2.11462200
H	-2.38145500	-4.96581600	2.54282700

SCF Done: E(UM062X) = -1618.08181633 A.U.
<S**2> = 1.0645
Zero-point correction= 0.551548 (Hartree/Particle)
Thermal correction to Energy= 0.675953
Thermal correction to Enthalpy= 0.677769
Thermal correction to Gibbs Free Energy= 0.350263

SCF Done: E(UB3LYP) = -1618.95239042 A.U.
<S**2> = 1.0545

TS5-Ph

C	-3.19376800	-0.53439900	-2.28235600
C	-2.83164100	-1.89571900	-2.48943700
C	-1.54409900	-2.29635800	-2.27532400
C	-0.53185700	-1.39951500	-1.80051500
C	-0.94713000	-0.04296000	-1.49799500
C	-2.28033800	0.37293300	-1.82888800
C	0.79362100	-1.88701800	-1.61718000
C	1.68781300	-0.94923800	-1.09036700
H	-4.20902200	-0.21415800	-2.49314900
H	-1.21707100	-3.31144200	-2.47077600
H	-1.44306900	-0.87609700	-0.15134100
H	-2.56520500	1.40937100	-1.68818800
C	-1.16120400	4.86085700	0.02249000
C	-1.65332800	3.78474200	0.75404500
C	-1.26677700	2.49013300	0.42751900
C	-0.38166900	2.24796600	-0.62658000
C	0.10416000	3.33500200	-1.35261600
C	-0.28205600	4.63120200	-1.03022000
C	0.02956200	0.85136300	-0.95032700
C	1.32718700	0.40430100	-0.75535000
H	-1.45615600	5.87228500	0.27543700

H	-2.32872900	3.95666800	1.58483500
H	-1.63154700	1.64741200	1.00874300
H	0.80222500	3.15667300	-2.16270800
H	0.10961300	5.46522700	-1.60045500
H	-3.57533100	-2.59649200	-2.85184500
C	3.07868300	-1.44774700	-0.83841100
C	3.81285500	-1.14816000	0.31501700
C	3.64363700	-2.33440600	-1.76263400
C	5.06896500	-1.70634000	0.53048300
H	3.39470100	-0.48833300	1.06518000
C	4.90469100	-2.87752800	-1.55889000
H	3.05053400	-2.60442100	-2.62771300
C	5.62542300	-2.56688100	-0.40870800
H	5.61385900	-1.46309200	1.43602200
H	5.32392500	-3.55386900	-2.29544500
H	6.60760100	-2.99567700	-0.24513000
C	2.33627400	1.38128800	-0.24573600
C	2.18278200	1.98593500	1.00338500
C	3.45075400	1.70748400	-1.01958100
C	3.12516100	2.89247900	1.47222600
H	1.31957900	1.73279500	1.60947600
C	4.38874800	2.62227400	-0.55637300
H	3.58444600	1.22522400	-1.98205800
C	4.23083200	3.21552200	0.69206000
H	2.99497500	3.35014300	2.44628700
H	5.24932800	2.86650500	-1.16818500
H	4.96542900	3.92450100	1.05558700
C	-6.98085700	-0.42324700	0.35191600
C	-6.46736400	-1.71635200	0.25724800
C	-5.11937600	-1.94246000	0.47200600
C	-4.27805500	-0.86188400	0.78503400
C	-4.79990800	0.43839600	0.88774000
C	-6.15045800	0.65030500	0.66788100
H	-8.03622600	-0.25110600	0.17725300
H	-7.12126700	-2.54345700	0.01125700
H	-4.69494400	-2.93511200	0.38647100
H	-4.13346800	1.26258500	1.11283100
H	-6.55822300	1.65088700	0.73681500
C	-2.89943100	-1.08226900	0.98810200
C	-1.67060200	-1.22166900	1.05953600
C	-0.41843700	-1.48533700	1.76491900
C	0.39140400	-2.54870400	1.36478100
C	-0.03841100	-0.65132700	2.81860600
C	1.58242900	-2.78286500	2.03969500

H	0.12241100	-3.15295200	0.50708900
C	1.15493500	-0.89676400	3.48429400
H	-0.67238600	0.17927300	3.10643900
C	1.96234400	-1.96239700	3.09590600
H	2.23077700	-3.58499000	1.70940000
H	1.45696800	-0.25181800	4.30042900
H	2.90330500	-2.14036900	3.60303300

SCF Done: E(RM062X) = -1618.02862417 A.U.

Zero-point correction= 0.545092 (Hartree/Particle)
Thermal correction to Energy= 0.669014
Thermal correction to Enthalpy= 0.670829
Thermal correction to Gibbs Free Energy= 0.344562

SCF Done: E(UB3LYP) = -1618.90401402 A.U.
<S**2> = 0.4030

RAD1-Ph

C	-3.45771300	3.38830700	0.06419900
C	-2.51183300	4.43726400	0.01145800
C	-1.17462900	4.15164700	-0.03066700
C	-0.73440000	2.80429200	-0.03328900
C	-1.67921000	1.73676900	-0.00936400
C	-3.05723800	2.07774100	0.05690200
C	0.61030500	2.43058000	-0.04848800
C	1.11443100	1.17375500	-0.05482500
H	-4.51373500	3.62487200	0.11741500
H	-0.43095700	4.93907600	-0.05885900
H	-3.79464500	1.28711700	0.11349800
C	-4.00695300	-2.86186100	0.13633000
C	-3.96119600	-2.03149000	-0.97849100
C	-3.06391600	-0.97009800	-1.02087100
C	-2.19836300	-0.72995900	0.04786800
C	-2.25911500	-1.56210500	1.16599600
C	-3.15602100	-2.62201600	1.20985400
C	-1.20484000	0.38329500	-0.01066600
C	0.15217900	0.10093000	-0.02418800
H	-4.70230500	-3.69207700	0.16802100
H	-4.62169900	-2.21275100	-1.81825700
H	-3.02150400	-0.32516700	-1.89281900
H	-1.58541300	-1.38155000	1.99603300
H	-3.18658500	-3.26397500	2.08223600
H	-2.85004400	5.46642600	0.01427700

C	2.58911100	0.97450800	-0.11049400
C	3.18160200	0.07561800	-1.00149500
C	3.41020800	1.73993100	0.72114100
C	4.56258300	-0.05871200	-1.04930300
H	2.55863900	-0.51822300	-1.65973500
C	4.79235300	1.60126600	0.67508300
H	2.95327300	2.43898800	1.41288800
C	5.37258600	0.69913100	-0.20870000
H	5.00728000	-0.75838800	-1.74700700
H	5.41504100	2.19763300	1.33160500
H	6.44969400	0.58741900	-0.24465700
C	0.63921400	-1.30865400	0.02325800
C	0.29694100	-2.22237400	-0.97464400
C	1.45955200	-1.72715400	1.07181000
C	0.76774300	-3.52855200	-0.92548300
H	-0.34132600	-1.90354400	-1.79093000
C	1.92348000	-3.03561400	1.12600700
H	1.73890000	-1.01704700	1.84279600
C	1.58078400	-3.93909300	0.12588500
H	0.49671300	-4.22685300	-1.70837700
H	2.55689700	-3.34761500	1.94781500
H	1.94588600	-4.95845000	0.16511000

SCF Done: E(UM062X) = -1078.16580857 A.U.
<S**2> = 0.7663
Zero-point correction= 0.358360 (Hartree/Particle)
Thermal correction to Energy= 0.437347
Thermal correction to Enthalpy= 0.439162
Thermal correction to Gibbs Free Energy= 0.215878

SCF Done: E(UB3LYP) = -1078.73418626 A.U.
<S**2> = 0.7596

RAD2-Ph

H	0.92913400	-2.49546100	-0.00262700
C	-3.72628900	0.36220300	-1.20765000
C	-2.46024400	-0.18486200	-1.22209600
C	-1.78629500	-0.47550400	-0.00028400
C	-2.46062500	-0.18759000	1.22198800
C	-3.72664100	0.35951000	1.20830000
C	-4.37162700	0.63915600	0.00052500
H	-4.22369900	0.57800900	-2.14591600
H	-1.95817700	-0.40052300	-2.15696300
H	-1.95881900	-0.40544000	2.15650000

H	-4.22434100	0.57316600	2.14690200
H	-5.36623800	1.06667700	0.00088500
C	0.71445700	-1.42414400	-0.00143200
C	-0.52687800	-1.02652500	-0.00087200
C	1.90385100	-0.53897300	-0.00057300
C	1.78208200	0.85393800	0.00013500
C	3.17881900	-1.10535000	-0.00049800
C	2.91223400	1.65687900	0.00094600
H	0.79270200	1.29909700	0.00005900
C	4.31215400	-0.29962000	0.00029200
H	3.28101500	-2.18545700	-0.00106300
C	4.18227500	1.08334600	0.00101500
H	2.80497900	2.73519600	0.00152200
H	5.29609000	-0.75338200	0.00035200
H	5.06371800	1.71332700	0.00157200

SCF Done: E(UM062X) = -539.922858211 A.U.
<S**2> = 0.7878
Zero-point correction= 0.190985 (Hartree/Particle)
Thermal correction to Energy= 0.232174
Thermal correction to Enthalpy= 0.233989
Thermal correction to Gibbs Free Energy= 0.091207

SCF Done: E(UB3LYP) = -540.219134639 A.U.
<S**2> = 0.7846

TS6-Ph

C	-0.74226100	0.29490100	0.04634200
C	-1.22717400	-0.93932100	0.14304600
C	1.22727100	-0.93925300	-0.14297500
C	0.74229800	0.29494200	-0.04626200
C	2.41413600	-1.72438700	-0.10030100
C	2.79600300	-2.51730100	-1.19805200
C	3.20821800	-1.74801400	1.06265100
C	3.94234800	-3.29291700	-1.13756600
H	2.17767500	-2.51248400	-2.08795600
C	4.35341300	-2.52690800	1.11179900
H	2.91306900	-1.14113900	1.91048000
C	4.72485800	-3.30181200	0.01535700
H	4.22810500	-3.89662400	-1.99084400
H	4.96097200	-2.53130500	2.00914900
H	5.61884600	-3.91213500	0.05915700
C	-2.41404200	-1.72445300	0.10032900
C	-3.20813000	-1.74799000	-1.06261900

C	-2.79590400	-2.51744900	1.19802200
C	-4.35333100	-2.52687000	-1.11181900
H	-2.91297900	-1.14105500	-1.91040600
C	-3.94225600	-3.29305000	1.13748700
H	-2.17756700	-2.51271000	2.08792100
C	-4.72477500	-3.30185300	-0.01543100
H	-4.96089200	-2.53120200	-2.00916800
H	-4.22801400	-3.89681600	1.99072300
H	-5.61876700	-3.91216600	-0.05927000
C	1.61486900	1.49361800	0.04409800
C	1.31444100	2.53506200	0.92786100
C	2.77850800	1.57425000	-0.72598500
C	2.16531600	3.62776400	1.04019300
H	0.41329000	2.48520600	1.52862600
C	3.62694800	2.66747500	-0.61133200
H	3.01113900	0.77260300	-1.41789000
C	3.32261000	3.69831400	0.27156200
H	1.92292900	4.42695600	1.73058800
H	4.52504000	2.71563900	-1.21578700
H	3.98278800	4.55297200	0.35860700
C	-1.61490300	1.49352300	-0.04405300
C	-1.31458200	2.53491800	-0.92791000
C	-2.77850500	1.57414200	0.72608500
C	-2.16552900	3.62755900	-1.04028000
H	-0.41345600	2.48507100	-1.52871200
C	-3.62702000	2.66730600	0.61139100
H	-3.01105200	0.77253100	1.41806000
C	-3.32278900	3.69809600	-0.27159600
H	-1.92322400	4.42671700	-1.73074400
H	-4.52508500	2.71545800	1.21588600
H	-3.98302400	4.55270700	-0.35867400

SCF Done: E(UM062X) = -1078.65404318 A.U.
<S**2> = 0.8590
Zero-point correction= 0.365267 (Hartree/Particle)
Thermal correction to Energy= 0.446417
Thermal correction to Enthalpy= 0.448232
Thermal correction to Gibbs Free Energy= 0.213263

SCF Done: E(UB3LYP) = -1079.23745899 A.U.
<S**2> = 0.6402

INT3-Ph

C	-0.02300800	1.03158700	-0.00473900

C	1.01703100	0.17465600	0.00583900
C	0.02300800	-1.03158700	-0.00473900
C	-1.01703100	-0.17465600	0.00583900
C	0.19765400	-2.47492300	-0.01958600
C	1.28782200	-3.05982700	0.63870500
C	-0.71306200	-3.30563700	-0.68957600
C	1.45339100	-4.43960500	0.63825000
H	1.99439700	-2.42601900	1.16226000
C	-0.54160400	-4.68100200	-0.68803100
H	-1.54585200	-2.85602900	-1.21869200
C	0.54160400	-5.25375800	-0.02357400
H	2.29728800	-4.87938000	1.15647700
H	-1.24886600	-5.31078000	-1.21462600
H	0.67429000	-6.32894300	-0.02672800
C	-2.46685100	-0.27990700	0.02065600
C	-3.25190600	0.68784800	-0.62023900
C	-3.10589200	-1.34574700	0.67283300
C	-4.63779000	0.58325900	-0.62136600
H	-2.76716600	1.51323300	-1.12914600
C	-4.48825200	-1.44344400	0.66977900
H	-2.50446900	-2.08553800	1.18902400
C	-5.26007000	-0.48045200	0.02183100
H	-5.23162100	1.33490700	-1.12776200
H	-4.96961800	-2.26873800	1.18126200
H	-6.34058900	-0.55896800	0.02324100
C	-0.19765400	2.47492300	-0.01958600
C	-1.28782200	3.05982700	0.63870500
C	0.71306200	3.30563700	-0.68957600
C	-1.45339100	4.43960500	0.63825000
H	-1.99439700	2.42601900	1.16226000
C	0.54160400	4.68100200	-0.68803100
H	1.54585200	2.85602900	-1.21869200
C	-0.54160400	5.25375800	-0.02357400
H	-2.29728800	4.87938000	1.15647700
H	1.24886600	5.31078000	-1.21462600
H	-0.67429000	6.32894300	-0.02672800
C	2.46685100	0.27990700	0.02065600
C	3.25190600	-0.68784800	-0.62023900
C	3.10589200	1.34574700	0.67283300
C	4.63779000	-0.58325900	-0.62136600
H	2.76716600	-1.51323300	-1.12914600
C	4.48825200	1.44344400	0.66977900
H	2.50446900	2.08553800	1.18902400
C	5.26007000	0.48045200	0.02183100

H	5.23162100	-1.33490700	-1.12776200
H	4.96961800	2.26873800	1.18126200
H	6.34058900	0.55896800	0.02324100

SCF Done: E(RM062X) = -1078.73574715 A.U.

Zero-point correction= 0.368263 (Hartree/Particle)
Thermal correction to Energy= 0.449321
Thermal correction to Enthalpy= 0.451136
Thermal correction to Gibbs Free Energy= 0.223878

SCF Done: E(RB3LYP) = -1079.30814689 A.U.

TS7-Ph

C	-2.08896800	0.04733000	1.47830900
C	-0.85162200	0.09918600	1.39067200
C	0.38203000	-0.13319600	2.13257100
C	1.08962800	0.93394300	2.69128900
C	0.86550700	-1.43529500	2.29121300
C	2.24490100	0.69839300	3.42745800
H	0.72261000	1.94445600	2.55909700
C	2.02872000	-1.66381900	3.01621900
H	0.31900300	-2.25903400	1.84587700
C	2.71651900	-0.60044300	3.59251500
H	2.77619100	1.53230800	3.87089900
H	2.39782800	-2.67592300	3.13137600
H	3.61998500	-0.78356700	4.16218300
C	1.12972000	0.96563200	-0.55103500
C	1.63176900	-0.38731800	-0.79649600
C	-0.23131600	0.49447200	-0.60251600
C	0.34586300	-0.88801400	-0.91143800
C	-0.27845600	-2.18599700	-0.99849400
C	0.47581700	-3.37448500	-0.96156200
C	-1.67857200	-2.28887400	-1.07440700
C	-0.14811900	-4.60977700	-1.02113300
H	1.55252600	-3.31959300	-0.86081000
C	-2.29500300	-3.53067200	-1.14251000
H	-2.28036700	-1.38738200	-1.07642900
C	-1.53593000	-4.69671500	-1.12136900
H	0.44964500	-5.51316500	-0.98680400
H	-3.37602300	-3.58560000	-1.20996700
H	-2.01928200	-5.66468700	-1.17607500
C	-1.35686800	1.14980600	-1.30773700

C	-2.08892100	2.19987200	-0.75055300
C	-1.69062800	0.71864200	-2.59734300
C	-3.11515700	2.81057300	-1.46108700
H	-1.87362200	2.51761600	0.26156900
C	-2.71601400	1.32864100	-3.30849700
H	-1.13396200	-0.09990100	-3.04210400
C	-3.43293800	2.37782200	-2.74250700
H	-3.67513800	3.61918400	-1.00555600
H	-2.95599900	0.98241900	-4.30685700
H	-4.23674800	2.85043600	-3.29418900
C	-3.49417700	-0.00067400	1.39175900
C	-4.28116900	1.15551200	1.56310700
C	-4.14055200	-1.23086900	1.15502900
C	-5.66031600	1.08145900	1.47733600
H	-3.79203900	2.10154500	1.75998900
C	-5.52184300	-1.28992600	1.06880800
H	-3.53882700	-2.12567400	1.05310200
C	-6.28796000	-0.13733600	1.22459100
H	-6.25311200	1.97904800	1.60722100
H	-6.00631500	-2.24201900	0.88654900
H	-7.36779900	-0.18822000	1.15676700
C	1.75488400	2.25804300	-0.46981800
C	3.06093200	2.45386500	-0.95823900
C	1.08189500	3.36016300	0.08667100
C	3.66029000	3.70160500	-0.89121700
H	3.59000500	1.62372900	-1.41007200
C	1.68813100	4.60433500	0.15178500
H	0.08455200	3.22251200	0.48265600
C	2.98099400	4.78265700	-0.33467200
H	4.66299500	3.83387300	-1.28035000
H	1.15338800	5.43993200	0.58795200
H	3.45415600	5.75565500	-0.28095600
C	2.98636700	-0.94133300	-0.76158300
C	3.85137800	-0.53504100	0.26150500
C	3.44694500	-1.84765200	-1.72211600
C	5.13944500	-1.04611900	0.33637800
H	3.49272300	0.17195600	1.00226500
C	4.73993000	-2.35114500	-1.64820000
H	2.78861700	-2.14402800	-2.53149000
C	5.58738400	-1.95567100	-0.61729000
H	5.79410700	-0.73435600	1.14181000
H	5.08950100	-3.04927300	-2.39967700
H	6.59428000	-2.35170400	-0.56035700

SCF Done: E(UM062X) = -1618.07281077 A.U.
<S**2> = 0.8528
Zero-point correction= 0.548851 (Hartree/Particle)
Thermal correction to Energy= 0.672719
Thermal correction to Enthalpy= 0.674534
Thermal correction to Gibbs Free Energy= 0.352196

SCF Done: E(UB3LYP) = -1618.94378898 A.U.
<S**2> = 0.8664

INT4-Ph

C	-2.22000100	0.21701100	0.98180800
C	-0.93142000	0.28464000	0.81889500
C	-0.02770300	0.00808900	1.99208400
C	0.61918900	1.04326100	2.66684400
C	0.19217100	-1.31072400	2.39136400
C	1.47989600	0.76193400	3.72282200
H	0.45231500	2.06968000	2.36147700
C	1.05795500	-1.59113200	3.44301100
H	-0.31383400	-2.11386700	1.86560100
C	1.70485800	-0.55559200	4.10984100
H	1.97525400	1.57448400	4.24154900
H	1.22578000	-2.61930400	3.74094000
H	2.37732400	-0.77406300	4.93106000
C	1.19287700	0.95652000	-0.46539700
C	1.72962200	-0.32712300	-0.64327400
C	-0.24617200	0.41683000	-0.55727800
C	0.47598100	-0.91647400	-0.82362200
C	-0.06251100	-2.23621900	-0.98944700
C	0.74858500	-3.38452700	-0.89973500
C	-1.44347200	-2.40272000	-1.21125300
C	0.19375800	-4.64724200	-1.02884400
H	1.80964900	-3.27293800	-0.70988000
C	-1.98759500	-3.67203700	-1.33982000
H	-2.08019800	-1.52808300	-1.29141600
C	-1.17460200	-4.79919800	-1.24993500
H	0.82957200	-5.52166000	-0.95408800
H	-3.05146000	-3.78256400	-1.51644000
H	-1.60280600	-5.78910300	-1.35209600
C	-1.08723900	0.98116000	-1.68681500
C	-2.10328600	1.91654100	-1.48253100
C	-0.80420500	0.58834300	-2.99790200
C	-2.82143500	2.43497500	-2.55508900
H	-2.34473800	2.24521600	-0.47950500

C	-1.51870200	1.10559400	-4.06992800
H	-0.01742200	-0.13716400	-3.17512700
C	-2.53470000	2.03020000	-3.85227900
H	-3.60982700	3.15547500	-2.37174600
H	-1.28380600	0.78218300	-5.07709700
H	-3.09726300	2.43100900	-4.68693500
C	-3.57802700	0.11745200	1.17334300
C	-4.36928800	1.25605000	1.49803900
C	-4.23527100	-1.14036400	1.04214600
C	-5.73218100	1.13254500	1.67370800
H	-3.88138500	2.21629200	1.61600100
C	-5.59927400	-1.23698400	1.22363900
H	-3.63996400	-2.01412800	0.80331100
C	-6.36085200	-0.10785100	1.53805700
H	-6.31852700	2.00901200	1.92421200
H	-6.08269400	-2.20173100	1.12200700
H	-7.43081000	-0.19425600	1.67930600
C	1.70635000	2.28068200	-0.28196200
C	3.08709100	2.55272600	-0.35710200
C	0.82728000	3.34833900	-0.01916700
C	3.56014400	3.83950700	-0.16350300
H	3.77779100	1.74674700	-0.57386900
C	1.31030600	4.63273400	0.17325300
H	-0.23762600	3.15469700	0.03507100
C	2.67831000	4.88566600	0.10466700
H	4.62464300	4.03269600	-0.22472300
H	0.61852700	5.44217800	0.37448000
H	3.05524100	5.89026300	0.25326700
C	3.09503800	-0.86672100	-0.51394600
C	3.74926300	-0.73321300	0.71383300
C	3.73319700	-1.52038600	-1.56862600
C	5.02913300	-1.24745400	0.87989000
H	3.23938500	-0.23166900	1.53183700
C	5.01591600	-2.02985000	-1.39926500
H	3.22027700	-1.62587000	-2.51854100
C	5.66499500	-1.89376600	-0.17637700
H	5.52941500	-1.14559600	1.83568700
H	5.50945200	-2.53221100	-2.22287500
H	6.66386500	-2.29306200	-0.04634600

SCF Done: E(UM062X) = -1618.10714549 A.U.
<S**2> = 1.0720
Zero-point correction= 0.551229 (Hartree/Particle)
Thermal correction to Energy= 0.675298

Thermal correction to Enthalpy= 0.677113
Thermal correction to Gibbs Free Energy= 0.352355

SCF Done: E(UB3LYP) = -1618.97428006 A.U.
<S**2> = 1.0680

TS8-Ph

C	-0.61690400	-1.23029000	-1.25953900
C	0.59433900	-1.17652600	-0.77846900
C	1.81501500	-1.56074800	-1.55034500
C	2.79971400	-2.42130700	-1.05640500
C	1.99934300	-0.98627500	-2.81178500
C	3.94046200	-2.68919900	-1.80485300
H	2.68787800	-2.87902500	-0.08301200
C	3.14032100	-1.25367100	-3.55684400
H	1.24336400	-0.30853500	-3.19228100
C	4.11841800	-2.10401200	-3.05348100
H	4.69275400	-3.36063300	-1.40762900
H	3.26893000	-0.79068800	-4.52816500
H	5.01161600	-2.31186500	-3.63045200
C	0.98282500	1.03178100	0.37100700
C	-0.35607300	1.40562400	0.51870000
C	0.65266700	-0.44174500	0.57693100
C	-0.79507600	0.09890600	0.79166500
C	-2.06467700	-0.48186300	1.17411100
C	-3.26182900	0.12996100	0.75434800
C	-2.15095000	-1.68290500	1.89532100
C	-4.49032000	-0.43687600	1.05446300
H	-3.21836400	1.03620500	0.16205300
C	-3.38686400	-2.24133100	2.19509400
H	-1.24618200	-2.16221800	2.24445700
C	-4.56183400	-1.62514100	1.77787500
H	-5.39776900	0.04308600	0.70696200
H	-3.43006000	-3.16337200	2.76348200
H	-5.52343100	-2.06728100	2.00922900
C	1.30237400	-1.18428400	1.72234800
C	1.17497300	-2.57246200	1.82903900
C	1.97799300	-0.49784700	2.73210500
C	1.70705600	-3.25763500	2.91362300
H	0.64785000	-3.11527600	1.04969500
C	2.51206900	-1.18265500	3.81904500
H	2.08711300	0.57867400	2.66690400
C	2.38038500	-2.56237600	3.91391600
H	1.59732200	-4.33402000	2.97742600

H	3.03574800	-0.63353800	4.59266800
H	2.80055800	-3.09369700	4.75943900
C	-1.88731500	-1.36528900	-1.78526000
C	-2.67885900	-2.49789000	-1.46144100
C	-2.48328600	-0.32038600	-2.53990900
C	-3.99552900	-2.57086800	-1.87432400
H	-2.23807100	-3.29077500	-0.86999900
C	-3.79715600	-0.42079800	-2.95299300
H	-1.89441500	0.55979500	-2.77174900
C	-4.56449700	-1.54077300	-2.62322400
H	-4.58969000	-3.43653900	-1.60557000
H	-4.23778800	0.38387800	-3.53009600
H	-5.59649100	-1.60628500	-2.94481200
C	2.23274700	1.71093500	0.13818900
C	2.31133300	3.11766800	0.12722100
C	3.42009200	0.97765300	-0.03915300
C	3.52325000	3.75539200	-0.08146200
H	1.41709400	3.70390600	0.29832700
C	4.62728500	1.62419800	-0.25419500
H	3.38952200	-0.10412300	-0.01066800
C	4.68650700	3.01459000	-0.28150800
H	3.56327100	4.83831300	-0.08475500
H	5.52746800	1.03863900	-0.39905700
H	5.63125300	3.51761000	-0.44908500
C	-1.07794000	2.68516300	0.38838800
C	-0.97206200	3.43360500	-0.78631800
C	-1.89177000	3.15024300	1.42327600
C	-1.66628600	4.62969900	-0.92269500
H	-0.33646500	3.07067200	-1.58751900
C	-2.58154300	4.34868500	1.28701400
H	-1.98113700	2.56267100	2.33044800
C	-2.47079600	5.09013500	0.11479500
H	-1.57993800	5.20203200	-1.83872600
H	-3.20751800	4.70388200	2.09689100
H	-3.01002800	6.02399300	0.00998200

SCF Done: E(UM062X) = -1618.10412662 A.U.
<S**2> = 0.7003
Zero-point correction= 0.550903 (Hartree/Particle)
Thermal correction to Energy= 0.673561
Thermal correction to Enthalpy= 0.675376
Thermal correction to Gibbs Free Energy= 0.354885

SCF Done: E(UB3LYP) = -1618.97355066 A.U.

<S**2> = 0.5527

INT5-Ph

C	0.85185900	-1.18479100	-0.33815500
C	-0.48421500	-1.36565700	-0.35371700
C	-1.41629800	-2.28896500	-1.00782400
C	-1.08759900	-2.91238500	-2.21848500
C	-2.67902400	-2.52615000	-0.45006000
C	-1.98995800	-3.76236500	-2.84171700
H	-0.12575100	-2.70978700	-2.67549400
C	-3.57912200	-3.37988500	-1.07654700
H	-2.95112300	-2.04193200	0.48113200
C	-3.23716800	-4.00344100	-2.27083500
H	-1.72399600	-4.23227700	-3.78121700
H	-4.54994000	-3.55691300	-0.62867700
H	-3.93984800	-4.66813100	-2.75898700
C	0.79087900	0.11205400	0.46838100
C	0.48429400	1.36530900	-0.35493600
C	-0.79093300	-0.11167300	0.46835000
C	-0.85179300	1.18446600	-0.33936800
C	-2.01837600	1.87410600	-0.89383200
C	-2.03133800	3.26404300	-1.06477800
C	-3.16536800	1.14130500	-1.21514600
C	-3.15716700	3.89915400	-1.56964700
H	-1.15582300	3.84100800	-0.78744500
C	-4.28803900	1.77940600	-1.72745500
H	-3.16689500	0.06616200	-1.07091100
C	-4.28702400	3.15827800	-1.90799300
H	-3.15709100	4.97554900	-1.69455000
H	-5.16637600	1.19851000	-1.98285700
H	-5.16453800	3.65568900	-2.30334400
C	-1.49282500	-0.22353100	1.78516300
C	-1.30208900	-1.36619900	2.57050300
C	-2.26031500	0.82156500	2.29952700
C	-1.85833900	-1.45683200	3.83772900
H	-0.70175900	-2.18208500	2.18091000
C	-2.82660700	0.72538600	3.56837000
H	-2.41804500	1.71669000	1.70906300
C	-2.62633800	-0.41005000	4.34139400
H	-1.69099300	-2.34529700	4.43515100
H	-3.42371000	1.54489500	3.95082700
H	-3.06378800	-0.48245700	5.33004700
C	2.01836400	-1.87498700	-0.89209200
C	3.16536500	-1.14260000	-1.21433100

C	2.03110900	-3.26506800	-1.06183600
C	4.28784900	-1.78129900	-1.72628700
H	3.16700500	-0.06731400	-1.07116000
C	3.15675300	-3.90076900	-1.56639800
H	1.15556800	-3.84169200	-0.78386800
C	4.28663200	-3.16033500	-1.90561200
H	5.16621100	-1.20073800	-1.98237000
H	3.15646700	-4.97727100	-1.69039000
H	5.16401400	-3.65817400	-2.30071900
C	1.49256000	0.22513800	1.78519600
C	2.26058800	-0.81919600	2.30026700
C	1.30130900	1.36830200	2.56970400
C	2.82698700	-0.72175900	3.56898900
H	2.41870400	-1.71469900	1.71047800
C	1.85765700	1.46018100	3.83679300
H	0.70051600	2.18358200	2.17957200
C	2.62625900	0.41416800	4.34115700
H	3.42455400	-1.54066700	3.95200200
H	1.68989500	2.34901700	4.43354600
H	3.06381400	0.48753300	5.32969700
C	1.41649300	2.28806600	-1.00960700
C	1.08781300	2.91124100	-2.22039400
C	2.67943200	2.52502600	-0.45215900
C	1.99033400	3.76075300	-2.84403400
H	0.12585700	2.70879000	-2.67724400
C	3.57968600	3.37828100	-1.07904800
H	2.95157100	2.04102200	0.47913200
C	3.23771500	4.00161800	-2.27345300
H	1.72435800	4.23044700	-3.78364000
H	4.55064300	3.55512100	-0.63140600
H	3.94049600	4.66596500	-2.76192300

SCF Done: E(RM062X) = -1618.19179312 A.U.

Zero-point correction= 0.554942 (Hartree/Particle)
Thermal correction to Energy= 0.677153
Thermal correction to Enthalpy= 0.678968
Thermal correction to Gibbs Free Energy= 0.360225

SCF Done: E(RB3LYP) = -1619.04634017 A.U.

TS9-Ph

C	-1.13456400	0.92452300	-0.15982200

C	-0.00701300	1.59847900	0.41289400
C	0.81746800	2.60611500	-0.24859900
C	0.56357100	3.04436200	-1.55887600
C	1.93153900	3.12655500	0.42537500
C	1.40043000	3.96661100	-2.16608800
H	-0.28554600	2.64264800	-2.09986700
C	2.78332800	4.02979300	-0.19714500
H	2.11553500	2.81928300	1.44946400
C	2.51729200	4.45891300	-1.49191600
H	1.19187500	4.29455600	-3.17780100
H	3.64817500	4.40845400	0.33469500
H	3.17245700	5.17441300	-1.97430300
C	-0.88606800	-0.46669100	-0.23706400
C	0.54346800	-0.96732300	-0.29725800
C	0.56102900	0.60486300	1.26148300
C	1.44455100	-0.29162400	0.45881300
C	2.90935500	-0.32086100	0.49430100
C	3.55278800	0.04308600	1.68364000
C	3.69123500	-0.67514500	-0.61338600
C	4.93863300	0.03359800	1.77380300
H	2.95173300	0.32552200	2.54219800
C	5.07524400	-0.67707200	-0.52078800
H	3.21220600	-0.92866900	-1.55041200
C	5.70457900	-0.32898300	0.67164800
H	5.42040700	0.31055500	2.70396800
H	5.66795700	-0.94407000	-1.38787800
H	6.78603300	-0.33343000	0.73726100
C	-0.13459600	0.11636500	2.44598100
C	-1.03822100	0.96134800	3.11223700
C	0.12439400	-1.15222400	2.99589100
C	-1.71163800	0.52593600	4.24586400
H	-1.18807500	1.96597600	2.73511100
C	-0.54397200	-1.57699700	4.13128000
H	0.84039600	-1.80427300	2.50804800
C	-1.47168600	-0.74468700	4.75739000
H	-2.41043800	1.18842800	4.74301000
H	-0.34405300	-2.56239500	4.53528700
H	-1.98652100	-1.07894500	5.65007600
C	-2.31099100	1.59540400	-0.74854200
C	-3.01487900	1.04660400	-1.82842800
C	-2.71490600	2.83975500	-0.25305800
C	-4.09850900	1.71398400	-2.37991300
H	-2.70036800	0.09425700	-2.23963800
C	-3.79312900	3.51339200	-0.81374100

H	-2.16785200	3.27439200	0.57676600
C	-4.49276700	2.95049800	-1.87518300
H	-4.63217600	1.27282600	-3.21356800
H	-4.09013900	4.47778800	-0.41862600
H	-5.33674400	3.47208100	-2.31061000
C	-2.00370300	-1.43903400	-0.18774100
C	-3.00718700	-1.17692000	0.76064500
C	-2.11020200	-2.61307100	-0.95028100
C	-4.07373400	-2.04665300	0.93820300
H	-2.92999600	-0.28304800	1.37000000
C	-3.18644400	-3.47324800	-0.77748600
H	-1.37336500	-2.85160700	-1.70312400
C	-4.17037000	-3.19859700	0.16625200
H	-4.82908800	-1.82352800	1.68235200
H	-3.25453000	-4.36548000	-1.38882500
H	-5.00425200	-3.87779500	0.29822800
C	0.90317100	-2.04553300	-1.25166400
C	1.42424200	-3.26353700	-0.81945300
C	0.73117900	-1.82163500	-2.62068200
C	1.75830500	-4.24964000	-1.74117500
H	1.55925100	-3.43339300	0.24284000
C	1.06770300	-2.80544300	-3.54155400
H	0.33139200	-0.86790200	-2.95168600
C	1.57908200	-4.02410700	-3.10198300
H	2.15589100	-5.19683800	-1.39620300
H	0.93340400	-2.62268500	-4.60123000
H	1.83838600	-4.79408900	-3.81876500

SCF Done: E(RM062X) = -1618.13624634 A.U.

Zero-point correction= 0.552247 (Hartree/Particle)
Thermal correction to Energy= 0.673725
Thermal correction to Enthalpy= 0.675540
Thermal correction to Gibbs Free Energy= 0.358862

SCF Done: E(RB3LYP) = -1619.00537982 A.U.

P2-Ph

C	0.00000000	1.40494000	0.00000000
C	-1.21671400	0.70247000	0.00000000
C	-1.21671400	-0.70247000	0.00000000
C	0.00000000	-1.40494000	0.00000000
C	1.21671400	-0.70247000	0.00000000

C	1.21671400	0.70247000	0.00000000
C	0.00000000	2.89993700	0.00000000
C	0.57941800	3.60858900	1.05281700
C	-0.57941800	3.60858900	-1.05281700
C	0.57619800	4.99778100	1.05562600
H	1.04124600	3.06271800	1.86825800
C	-0.57619800	4.99778100	-1.05562600
H	-1.04124600	3.06271800	-1.86825800
C	0.00000000	5.69661000	0.00000000
H	1.02810100	5.53471200	1.88119300
H	-1.02810100	5.53471200	-1.88119300
H	0.00000000	6.78007900	0.00000000
C	-2.51141900	1.44996900	0.00000000
C	-3.41483900	1.30250400	-1.05281700
C	-2.83542100	2.30608500	1.05281700
C	-4.61630400	1.99988800	-1.05562600
H	-3.17301500	0.62961400	-1.86825800
C	-4.04010600	2.99789300	1.05562600
H	-2.13176900	2.43310400	1.86825800
C	-4.93340900	2.84830500	0.00000000
H	-5.30725200	1.87699400	-1.88119300
H	-4.27915100	3.65771800	1.88119300
H	-5.87172100	3.39004000	0.00000000
C	-2.51141900	-1.44996900	0.00000000
C	-2.83542100	-2.30608500	-1.05281700
C	-3.41483900	-1.30250400	1.05281700
C	-4.04010600	-2.99789300	-1.05562600
H	-2.13176900	-2.43310400	-1.86825800
C	-4.61630400	-1.99988800	1.05562600
H	-3.17301500	-0.62961400	1.86825800
C	-4.93340900	-2.84830500	0.00000000
H	-4.27915100	-3.65771800	-1.88119300
H	-5.30725200	-1.87699400	1.88119300
H	-5.87172100	-3.39003900	0.00000000
C	0.00000000	-2.89993700	0.00000000
C	0.57941800	-3.60858900	-1.05281700
C	-0.57941800	-3.60858900	1.05281700
C	0.57619800	-4.99778100	-1.05562600
H	1.04124600	-3.06271800	-1.86825800
C	-0.57619800	-4.99778100	1.05562600
H	-1.04124600	-3.06271800	1.86825800
C	0.00000000	-5.69661000	0.00000000
H	1.02810100	-5.53471200	-1.88119300
H	-1.02810100	-5.53471200	1.88119300

H	0.00000000	-6.78007900	0.00000000
C	2.51141900	-1.44996900	0.00000000
C	3.41483900	-1.30250400	-1.05281700
C	2.83542100	-2.30608500	1.05281700
C	4.61630400	-1.99988800	-1.05562600
H	3.17301500	-0.62961400	-1.86825800
C	4.04010600	-2.99789300	1.05562600
H	2.13176900	-2.43310400	1.86825800
C	4.93340900	-2.84830500	0.00000000
H	5.30725200	-1.87699400	-1.88119300
H	4.27915100	-3.65771800	1.88119300
H	5.87172100	-3.39004000	0.00000000
C	2.51141900	1.44996800	0.00000000
C	3.41483900	1.30250400	1.05281700
C	2.83542100	2.30608500	-1.05281700
C	4.61630400	1.99988800	1.05562600
H	3.17301500	0.62961400	1.86825800
C	4.04010600	2.99789300	-1.05562600
H	2.13176900	2.43310400	-1.86825800
C	4.93340900	2.84830500	0.00000000
H	5.30725200	1.87699400	1.88119300
H	4.27915100	3.65771800	-1.88119300
H	5.87172100	3.39003900	0.00000000

SCF Done: E(RM062X) = -1618.27449305 A.U.

Zero-point correction= 0.556398 (Hartree/Particle)
Thermal correction to Energy= 0.678034
Thermal correction to Enthalpy= 0.679849
Thermal correction to Gibbs Free Energy= 0.368405

SCF Done: E(RB3LYP) = -1619.13457663 A.U.

TS1-Ph-con

C	3.79168100	-2.33350100	0.98182000
C	2.95687000	-2.56364800	2.08992700
C	1.58849700	-2.58646800	1.94248000
C	1.00956600	-2.33867600	0.67378300
C	1.86070600	-2.11774700	-0.43503800
C	3.24373200	-2.13439700	-0.27408300
C	-0.35502600	-2.13788800	0.46171900
C	-1.05372800	-1.17658700	-0.02282500
H	4.86746800	-2.33006600	1.11217700

H	0.93742700	-2.76005300	2.79053200
H	1.41948800	-1.98266000	-1.41396100
H	3.88844400	-1.96064000	-1.12780700
C	4.57760300	2.08690800	-1.42371100
C	3.52436900	2.09142400	-2.33724000
C	2.28577700	1.58605400	-1.98244500
C	2.08318000	1.04118400	-0.69668600
C	3.16172300	1.02396700	0.21542900
C	4.38557400	1.55950900	-0.14788800
C	0.83360700	0.53267600	-0.31336500
C	-0.33632900	0.33527000	0.13036700
H	5.54176900	2.49204800	-1.70520000
H	3.67032500	2.50137000	-3.32966500
H	1.46143500	1.59425500	-2.68534600
H	3.01016700	0.58772300	1.19562700
H	5.20243600	1.55470300	0.56408700
H	3.39630500	-2.72321500	3.06769500
C	-1.22134500	1.29081600	0.85285700
C	-2.13364900	0.85405000	1.81316900
C	-1.11779800	2.65765000	0.58079500
C	-2.92373400	1.77244500	2.49455600
H	-2.22094700	-0.20453500	2.02655100
C	-1.91482100	3.57013000	1.25717700
H	-0.40855700	2.99528200	-0.16698800
C	-2.82084700	3.13048500	2.21779900
H	-3.62615100	1.42144300	3.24118100
H	-1.82839200	4.62694700	1.03404100
H	-3.44381800	3.84274200	2.74517400
C	-2.36978100	-1.13202200	-0.68915700
C	-2.72670400	-0.08829600	-1.54499700
C	-3.27492000	-2.17980700	-0.48454500
C	-3.95928100	-0.09432700	-2.18619400
H	-2.03545700	0.72836800	-1.71449600
C	-4.50691600	-2.17835300	-1.12154800
H	-2.99299300	-2.98747200	0.18041700
C	-4.85489100	-1.13555700	-1.97577200
H	-4.22023000	0.72138800	-2.84974600
H	-5.19953400	-2.99404000	-0.95056900
H	-5.81787800	-1.13535900	-2.47200400

SCF Done: E(RM062X) = -1078.65021494 A.U.

Zero-point correction= 0.364412 (Hartree/Particle)
Thermal correction to Energy= 0.445788

Thermal correction to Enthalpy= 0.447603
Thermal correction to Gibbs Free Energy= 0.217565

SCF Done: E(RB3LYP) = -1079.23690214 A.U.

TS4-Ph-2

C	2.30207500	-4.73917100	1.41584600
C	1.71765600	-3.92969500	2.38635100
C	2.42456000	-4.26713300	0.11287100
H	2.66310300	-5.72704600	1.67501800
C	1.25742500	-2.66469400	2.05722300
H	1.61943500	-4.28709400	3.40459900
C	1.96868000	-3.00052300	-0.22488200
H	2.88450000	-4.88837800	-0.64667900
C	1.36297800	-2.17881200	0.73959500
H	0.79427600	-2.03598100	2.80899400
H	2.08921600	-2.63232600	-1.23483700
C	-0.26621800	-0.22905300	0.76184600
C	-0.47485500	1.24773100	0.62183500
C	-1.68102900	1.74212800	0.45710700
C	-3.02416900	2.02585100	0.31303100
C	-3.60163100	2.23722200	-0.97095800
C	-3.87388100	2.14392900	1.44876600
C	-4.94723200	2.52025000	-1.09978100
H	-2.96835500	2.18880100	-1.84871700
C	-5.21499200	2.43073600	1.29646300
H	-3.44810600	1.99811900	2.43343900
C	-5.76658800	2.61585500	0.02646900
H	-5.36679600	2.67568500	-2.08714700
H	-5.84523400	2.50915100	2.17461100
H	-6.82046600	2.83819000	-0.08353700
C	-1.44507100	-1.04018900	1.19466900
C	-1.85839800	-2.13107500	0.42713700
C	-2.15126300	-0.72485200	2.35783800
C	-2.95594200	-2.88955900	0.81468800
H	-1.31889500	-2.37454600	-0.48287200
C	-3.24525500	-1.48752800	2.74821300
H	-1.83134400	0.12052900	2.95857700
C	-3.65217600	-2.57112600	1.97571500
H	-3.26966000	-3.72800600	0.20376100
H	-3.78209900	-1.23556200	3.65547400
H	-4.50960700	-3.16164600	2.27632700
C	0.69269300	2.17836400	0.69874100

C	0.74590300	3.30250800	-0.12888600
C	1.71863100	1.97032700	1.62213000
C	1.79536200	4.20634400	-0.02778600
H	-0.04511600	3.45886400	-0.85474500
C	2.77027300	2.87350800	1.72055600
H	1.69487600	1.09331700	2.25906400
C	2.81092700	3.99423100	0.89922800
H	1.82424500	5.07265700	-0.67861500
H	3.56466500	2.69623200	2.43592800
H	3.63793600	4.69079600	0.97126100
C	0.87744800	-0.84392900	0.46419300
C	1.97261300	-0.02253100	-1.26148300
C	1.12978700	-0.34225300	-2.10235400
C	-0.07493100	-0.87296900	-2.63762600
C	-0.11452900	-2.15599100	-3.20589000
C	-1.27076700	-0.15325200	-2.48745800
C	-1.32876200	-2.70962500	-3.58515500
H	0.80720500	-2.71045500	-3.33293600
C	-2.47993400	-0.71707200	-2.86259200
H	-1.22714100	0.83057500	-2.03915900
C	-2.51303300	-1.99799400	-3.40761100
H	-1.35357100	-3.70423800	-4.01397500
H	-3.39999200	-0.16537600	-2.70745700
H	-3.45920700	-2.44160600	-3.69305000
C	3.23811400	0.54325100	-0.83629200
C	4.01334100	-0.05094300	0.16463300
C	3.70404700	1.69790300	-1.47108900
C	5.23779500	0.50023100	0.51370800
H	3.65397200	-0.94200600	0.66340100
C	4.92787100	2.24664900	-1.11188000
H	3.09151400	2.16127800	-2.23473800
C	5.69853100	1.65043900	-0.12053700
H	5.83443900	0.02915000	1.28586500
H	5.27583500	3.14679500	-1.60495800
H	6.65405500	2.07918600	0.15754200

SCF Done: E(UM062X) = -1618.01803691 A.U.
<S**2> = 1.0805
Zero-point correction= 0.547612 (Hartree/Particle)
Thermal correction to Energy= 0.672493
Thermal correction to Enthalpy= 0.674308
Thermal correction to Gibbs Free Energy= 0.348428

SCF Done: E(UB3LYP) = -1618.89322544 A.U.

<S**2> = 1.0538

TS7-Ph-2

C	-0.69400800	0.67031600	-1.41965700
C	0.54287700	0.75428900	-1.42901700
C	1.87928600	0.68194200	-1.94830600
C	2.27107800	-0.51420500	-2.57087900
C	2.81656200	1.71543500	-1.81070600
C	3.56998500	-0.67806800	-3.02684600
H	1.54508200	-1.31250800	-2.67102900
C	4.11801600	1.53725000	-2.26330900
H	2.52709400	2.64778900	-1.34318400
C	4.50247600	0.34343100	-2.86648600
H	3.85848100	-1.60960700	-3.49905800
H	4.83576200	2.34040800	-2.14463600
H	5.51920400	0.21285100	-3.21696100
C	-0.85794300	0.31650900	0.77894200
C	-0.54862300	-1.03139600	0.88296900
C	0.69558300	0.59545100	0.80115400
C	0.88673500	-0.77378200	0.92286000
C	2.04972800	-1.65669300	1.00236500
C	1.93556000	-2.90125900	1.63794800
C	3.28938900	-1.29401500	0.45653300
C	3.02584400	-3.75683000	1.72134000
H	0.98659800	-3.19021000	2.07487900
C	4.37423500	-2.15558600	0.53688200
H	3.40046100	-0.33904900	-0.04443100
C	4.24820600	-3.38996500	1.16788500
H	2.91973100	-4.71273600	2.22057500
H	5.31984300	-1.86072900	0.09693600
H	5.09699900	-4.06072900	1.22807300
C	1.46497700	1.80058200	1.09110800
C	0.96953000	3.05749200	0.70674100
C	2.71415500	1.74090400	1.72131900
C	1.70635400	4.21030600	0.93198900
H	0.01074300	3.11398600	0.20367100
C	3.45486800	2.89684300	1.93396200
H	3.09635700	0.78450800	2.05645100
C	2.95876800	4.13444400	1.53777700
H	1.30871800	5.17030100	0.62426700
H	4.42070800	2.82962400	2.42074300
H	3.53814600	5.03419400	1.70648300
C	-2.02530600	0.62937600	-1.95312000
C	-2.60265900	-0.60668500	-2.27800200

C	-2.78237700	1.79680400	-2.09465900
C	-3.90937400	-0.66526100	-2.73834200
H	-2.02393200	-1.51349400	-2.14297400
C	-4.09065000	1.72893000	-2.55576900
H	-2.34144000	2.74938600	-1.82537000
C	-4.65958200	0.50126100	-2.87606200
H	-4.34716200	-1.62543100	-2.98461900
H	-4.66987000	2.63920800	-2.65527500
H	-5.68180100	0.45117700	-3.23126700
C	-2.01064200	1.10589800	1.21866100
C	-3.31982200	0.75695200	0.84736200
C	-1.83220600	2.20421800	2.07105900
C	-4.40357200	1.49232900	1.30186900
H	-3.48488500	-0.08968000	0.19182700
C	-2.92407400	2.93687200	2.52392800
H	-0.83756900	2.46696500	2.40614100
C	-4.21243000	2.59036400	2.13717400
H	-5.40324500	1.21039000	0.99246300
H	-2.76224600	3.77742200	3.18853400
H	-5.06178700	3.16524300	2.48654200
C	-1.34077600	-2.26181400	0.80083100
C	-0.89438300	-3.31182300	-0.01147500
C	-2.54920300	-2.40597300	1.49042100
C	-1.65008200	-4.46918100	-0.14724800
H	0.04760300	-3.20654700	-0.53980900
C	-3.30093400	-3.56584200	1.35468000
H	-2.88973700	-1.60449200	2.13557600
C	-2.85721500	-4.59794300	0.53307500
H	-1.29707000	-5.27141000	-0.78443600
H	-4.23468900	-3.66669100	1.89518100
H	-3.44619500	-5.50138800	0.42901300

SCF Done: E(RM062X) = -1618.08018439 A.U.

Zero-point correction= 0.550872 (Hartree/Particle)
Thermal correction to Energy= 0.673976
Thermal correction to Enthalpy= 0.675791
Thermal correction to Gibbs Free Energy= 0.356401

SCF Done: E(RB3LYP) = -1618.94633990 A.U.

compound 3

C	3.20800700	-0.34948800	-0.00001800

C	4.37268200	-0.64385900	0.00000200
H	5.40278200	-0.90857000	0.00006300
C	1.82235800	0.01734600	-0.00001000
C	0.84047200	-0.94697000	-0.00000800
C	1.46017700	1.39460200	-0.00000600
C	-0.52913500	-0.58951200	-0.00000200
H	1.11647500	-1.99552800	-0.00001200
C	0.14539100	1.76159800	0.00000000
H	2.24665100	2.13879700	-0.00000700
C	-1.55713800	-1.56796700	0.00000000
C	-0.88575800	0.78580100	0.00000300
H	-0.12899900	2.81097600	0.00000400
C	-2.87391200	-1.19615400	0.00000600
H	-1.27887200	-2.61634800	-0.00000300
C	-2.25842100	1.13976500	0.00000900
C	-3.22884300	0.17391800	0.00001100
H	-3.65214500	-1.94978600	0.00000800
H	-2.52586800	2.19105500	0.00001200
H	-4.27529700	0.45492100	0.00001600

SCF Done: E(RM062X) = -461.950327155 A.U.

Zero-point correction= 0.148701 (Hartree/Particle)
Thermal correction to Energy= 0.181941
Thermal correction to Enthalpy= 0.183756
Thermal correction to Gibbs Free Energy= 0.065088

SCF Done: E(RB3LYP) = -462.192150471 A.U.

Transition state for the dimerization of compound 3

C	1.47804100	-0.36038800	-0.87834600
C	0.24724800	-0.18098100	-0.72617200
C	-0.29505800	0.15784500	0.96625000
C	-1.52815900	0.34578100	1.09898200
H	-0.63355400	-0.15481900	-1.34518800
H	0.58124500	0.14613600	1.59113800
C	2.84478600	-0.48423800	-0.58175100
C	3.66189200	0.63615100	-0.48998500
C	3.41996300	-1.78291900	-0.38465300
C	5.03905000	0.51294300	-0.20592600
H	3.23452900	1.62089900	-0.64287700
C	4.74706600	-1.91754000	-0.11226400
H	2.77481100	-2.64949400	-0.45957800

C	5.88679600	1.64795700	-0.10575100
C	5.59911400	-0.78116700	-0.01663900
H	5.17676000	-2.90254600	0.03595000
C	7.22072900	1.50204300	0.16560100
H	5.45656400	2.63322700	-0.24951600
C	6.98073700	-0.89945800	0.26010100
C	7.77561600	0.21431800	0.34979300
H	7.85872000	2.37468000	0.23809500
H	7.40194100	-1.88916400	0.40111800
H	8.83293200	0.11215700	0.56218800
C	-2.87002500	0.47282100	0.70110900
C	-3.72726900	-0.62056900	0.70452000
C	-3.37039800	1.74750200	0.27583300
C	-5.06995700	-0.49577300	0.28801900
H	-3.35843300	-1.58570300	1.03297500
C	-4.66210300	1.88220800	-0.13398200
H	-2.69636600	2.59510500	0.28321800
C	-5.95771000	-1.60435900	0.28250700
C	-5.55177300	0.77162900	-0.14339200
H	-5.03202900	2.84716000	-0.46363700
C	-7.25439500	-1.45906400	-0.13150100
H	-5.58837800	-2.56877500	0.61383700
C	-6.89603200	0.88939400	-0.56664700
C	-7.73016200	-0.19876800	-0.56251500
H	-7.92290300	-2.31158000	-0.13104500
H	-7.25600200	1.85813500	-0.89610000
H	-8.75781700	-0.09762000	-0.88971300

SCF Done: E(UM062X) = -923.854302195 A.U.
<S**2> = 0.3065
Zero-point correction= 0.297666 (Hartree/Particle)
Thermal correction to Energy= 0.366389
Thermal correction to Enthalpy= 0.368204
Thermal correction to Gibbs Free Energy= 0.162607

SCF Done: E(UB3LYP) = -924.352104927 A.U.
<S**2> = 0.1903

compound 4

C	2.34696100	-0.95944600	-0.00010000
C	3.17510200	-1.82990900	-0.00004500
H	3.91295600	-2.59579200	0.00036300
C	1.35781700	0.07733000	-0.00004600
C	-0.03414400	-0.25881100	-0.00001700

C	1.74949100	1.39828600	-0.00002700
C	-0.48997300	-1.60069800	-0.00003500
C	-0.98862600	0.79279100	0.00003000
C	0.79295900	2.43401900	0.00002000
H	2.80656900	1.63360600	-0.00004900
C	-1.83042800	-1.88069300	-0.00000700
H	0.24178800	-2.39955000	-0.00007000
C	-2.37011000	0.46855700	0.00005700
C	-0.54372900	2.13924900	0.00004800
H	1.12678900	3.46441900	0.00003400
C	-2.78273900	-0.83563700	0.00003900
H	-2.16757900	-2.91034300	-0.00002100
H	-3.09224300	1.27777400	0.00009300
H	-1.28377500	2.93213600	0.00008400
H	-3.83998000	-1.07248700	0.00006100

SCF Done: E(RM062X) = -461.950802245 A.U.

Zero-point correction= 0.148682 (Hartree/Particle)
Thermal correction to Energy= 0.181937
Thermal correction to Enthalpy= 0.183752
Thermal correction to Gibbs Free Energy= 0.065105

SCF Done: E(RB3LYP) = -462.192677805 A.U.

Transition state for the dimerization of compound 4

C	-1.53568300	-0.54974300	-0.92876500
C	-0.32613100	-0.23103400	-0.85466400
C	0.32632100	-0.08157500	0.83908900
C	1.50649400	0.33092300	0.92105100
H	0.48757400	-0.00740400	-1.52258600
H	-0.46390300	-0.38958000	1.50185500
C	-2.82456400	-0.90696200	-0.50764600
C	-3.83127900	0.10230200	-0.28400000
C	-3.14466700	-2.24723400	-0.30346300
C	-3.57021900	1.47874600	-0.47496800
C	-5.12185200	-0.30203700	0.14712000
C	-4.42672300	-2.62599700	0.12343100
H	-2.38414800	-2.99779000	-0.48013100
C	-4.54706800	2.41364800	-0.24684800
H	-2.58380000	1.78147400	-0.80621200
C	-6.11100100	0.68876800	0.37436300
C	-5.39664600	-1.68030700	0.34462400

H	-4.64469700	-3.67579300	0.27829900
C	-5.83204200	2.01545900	0.18280500
H	-4.33462800	3.46520000	-0.39781700
H	-7.09480500	0.37271800	0.70385700
H	-6.38796400	-1.97252400	0.67252900
H	-6.59559100	2.76390000	0.35819500
C	2.76486200	0.80516900	0.52455600
C	3.85031600	-0.11169600	0.27239500
C	2.97867000	2.17361700	0.37470100
C	3.69904600	-1.51105100	0.40905000
C	5.10698600	0.41023000	-0.13145500
C	4.22949900	2.66931400	-0.02357300
H	2.15965300	2.85384700	0.57261000
C	4.74861900	-2.35596000	0.15392300
H	2.73852400	-1.90295900	0.72268100
C	6.17269500	-0.48936600	-0.38893000
C	5.27287400	1.81267300	-0.27241300
H	4.36491700	3.73841000	-0.13501900
C	5.99963400	-1.84039600	-0.25057900
H	4.61976300	-3.42612000	0.26352800
H	7.12977100	-0.08427500	-0.69941900
H	6.23967700	2.19429300	-0.58119600
H	6.82080500	-2.51835300	-0.44999700

SCF Done: E(UM062X) = -923.857037520 A.U.
<S**2> = 0.3047
Zero-point correction= 0.297295 (Hartree/Particle)
Thermal correction to Energy= 0.366115
Thermal correction to Enthalpy= 0.367930
Thermal correction to Gibbs Free Energy= 0.159777

SCF Done: E(UB3LYP) = -924.355087127 A.U.
<S**2> = 0.1910

compound 5

C	0.00004800	2.43947900	-0.00003800
C	0.00035600	3.64176900	0.00004900
H	0.00054800	4.70541100	0.00007900
C	0.00000600	1.00861300	-0.00001900
C	-1.22609100	0.31209100	-0.00001000
C	1.22606500	0.31202500	-0.00001000
C	-2.48640800	0.98404100	-0.00001700
C	-1.21645200	-1.11999500	0.00000700
C	1.21635300	-1.12005900	0.00000600

C	2.48641600	0.98391200	-0.00001800
C	-3.65193400	0.27977200	-0.00000900
H	-2.49444700	2.06688100	-0.00002900
C	-2.46265200	-1.82049400	0.00001500
C	-0.00006700	-1.80003200	0.00001400
C	2.46251800	-1.82062100	0.00001400
H	2.49450900	2.06675100	-0.00003100
C	3.65190700	0.27958400	-0.00001100
C	-3.64312300	-1.14516600	0.00000700
H	-4.59957800	0.80485200	-0.00001500
H	-2.44243900	-2.90473000	0.00002700
H	-0.00009600	-2.88570900	0.00002600
C	3.64302300	-1.14535300	0.00000600
H	2.44225000	-2.90485700	0.00002600
H	4.59957700	0.80461700	-0.00001700
H	-4.58214300	-1.68519400	0.00001300
H	4.58201600	-1.68542900	0.00001200

SCF Done: E(RM062X) = -615.560399781 A.U.

Zero-point correction= 0.193173 (Hartree/Particle)
Thermal correction to Energy= 0.236909
Thermal correction to Enthalpy= 0.238724
Thermal correction to Gibbs Free Energy= 0.097811

SCF Done: E(RB3LYP) = -615.881482474 A.U.

Transition state for the dimerization of compound 5

C	-1.62006200	-0.25839100	-0.87109600
C	-0.37772200	-0.38399800	-0.85652200
C	0.37772200	-0.38400000	0.85652200
C	1.62006200	-0.25839200	0.87109600
H	0.44897100	-0.49994800	-1.53376200
H	-0.44897100	-0.49995300	1.53376100
C	-2.94868100	-0.10916500	-0.47926500
C	-3.51703500	1.19486100	-0.36062400
C	-3.74578100	-1.26166700	-0.20579800
C	-2.76205800	2.37125600	-0.61880900
C	-4.88451600	1.33032900	0.03028200
C	-5.10896500	-1.09389000	0.18779500
C	-3.22360700	-2.58013700	-0.30692400
C	-3.32791600	3.60814300	-0.49635300
H	-1.72637000	2.26744800	-0.91992200

C	-5.44076400	2.64019900	0.14773500
C	-5.64875600	0.19061700	0.29438500
C	-5.89234600	-2.25403300	0.47001000
H	-2.19235300	-2.70728800	-0.61381000
C	-4.00275800	-3.66663400	-0.02887300
C	-4.68742500	3.74626400	-0.10680400
H	-2.73903300	4.49436000	-0.70016700
H	-6.47928300	2.73265300	0.44613500
H	-6.68597600	0.30599900	0.59252400
C	-5.35736500	-3.50260600	0.36754400
H	-6.92518200	-2.11584800	0.77036500
H	-3.58824400	-4.66408800	-0.11229300
H	-5.12018300	4.73515300	-0.01409900
H	-5.96062600	-4.37534700	0.58687300
C	2.94868100	-0.10916500	0.47926500
C	3.51703400	1.19486100	0.36062400
C	3.74578200	-1.26166700	0.20579800
C	2.76205600	2.37125600	0.61880700
C	4.88451600	1.33033000	-0.03028100
C	5.10896600	-1.09388900	-0.18779400
C	3.22360700	-2.58013700	0.30692200
C	3.32791400	3.60814300	0.49635100
H	1.72636800	2.26744700	0.91991800
C	5.44076300	2.64019900	-0.14773300
C	5.64875600	0.19061800	-0.29438200
C	5.89234700	-2.25403200	-0.47000900
H	2.19235300	-2.70728900	0.61380700
C	4.00275900	-3.66663400	0.02887100
C	4.68742400	3.74626500	0.10680400
H	2.73903100	4.49436000	0.70016400
H	6.47928300	2.73265400	-0.44613200
H	6.68597700	0.30600000	-0.59252000
C	5.35736600	-3.50260500	-0.36754500
H	6.92518300	-2.11584600	-0.77036300
H	3.58824400	-4.66408800	0.11229000
H	5.12018100	4.73515400	0.01410000
H	5.96062800	-4.37534600	-0.58687300

SCF Done: E(UM062X) = -1231.08226481 A.U.
<S**2> = 0.2876
Zero-point correction= 0.385206 (Hartree/Particle)
Thermal correction to Energy= 0.475324
Thermal correction to Enthalpy= 0.477139
Thermal correction to Gibbs Free Energy= 0.228149

SCF Done: E(UB3LYP) = -1231.73871692 A.U.
<S**2> = 0.1606

compound 6

C	-0.00000300	2.05430500	-0.00000300
C	1.20463500	1.36476700	0.00002300
C	1.21026800	-0.03444700	0.00002500
C	0.00000200	-0.72981800	0.00000200
C	-1.21026600	-0.03445200	-0.00002400
C	-1.20463700	1.36476300	-0.00002600
H	-0.00000400	3.13724400	-0.00000400
H	2.14738000	1.89715800	0.00004100
H	0.00000500	-1.81217300	0.00000300
H	-2.14738500	1.89715000	-0.00004600
C	2.45127800	-0.75276300	0.00005000
C	3.49154000	-1.35221200	0.00007000
H	4.41198000	-1.88518800	0.00007700
C	-2.45127400	-0.75277000	-0.00004700
C	-3.49154200	-1.35220900	-0.00006700
H	-4.41198700	-1.88517600	-0.00008700

SCF Done: E(RM062X) = -384.471634298 A.U.

Zero-point correction= 0.113172 (Hartree/Particle)
Thermal correction to Energy= 0.142082
Thermal correction to Enthalpy= 0.143897
Thermal correction to Gibbs Free Energy= 0.032794

SCF Done: E(RB3LYP) = -384.667705127 A.U.

Transition state for the dimerization of compound 6

C	-4.35612000	1.59774200	-0.23797900
C	-3.09224000	1.96977100	-0.68302400
C	-4.64719400	0.24459000	-0.01674900
H	-5.12359500	2.34049500	-0.06183100
C	-2.11266900	1.01699900	-0.90585300
H	-2.87113000	3.01638800	-0.85418900
C	-3.67261700	-0.72250900	-0.24764800
C	-2.38937200	-0.34936100	-0.68752100
H	-1.12555300	1.30349900	-1.24716200
C	-1.39822300	-1.31794800	-0.91748800
C	-0.39315400	-2.05557800	-0.78707900

C	0.39314500	-2.05557600	0.78704200
C	1.39821300	-1.31794500	0.91745200
C	2.38936400	-0.34935900	0.68749600
C	2.11265500	1.01700200	0.90581400
C	3.67261900	-0.72250800	0.24765200
C	3.09222900	1.96977400	0.68299900
H	1.12553100	1.30350300	1.24709900
C	4.64720000	0.24459100	0.01676800
C	4.35611900	1.59774300	0.23798500
H	2.87111500	3.01639200	0.85415300
H	5.12359900	2.34049600	0.06185000
H	0.15298800	-2.74657500	-1.40924300
H	-0.15299800	-2.74657200	1.40920600
H	3.90155900	-1.76814700	0.08648900
H	-3.90155300	-1.76814700	-0.08647400
C	-5.94909900	-0.14579300	0.44190300
C	-7.03965000	-0.46918600	0.82624600
H	-8.00520000	-0.75807500	1.16599600
C	5.94911600	-0.14579300	-0.44185100
C	7.03967700	-0.46918700	-0.82616700
H	8.00523500	-0.75807800	-1.16589000

SCF Done: E(UM062X) = -768.896094846 A.U.
<S**2> = 0.3292
Zero-point correction= 0.225318 (Hartree/Particle)
Thermal correction to Energy= 0.285803
Thermal correction to Enthalpy= 0.287618
Thermal correction to Gibbs Free Energy= 0.096312

SCF Done: E(UB3LYP) = -769.302310197 A.U.
<S**2> = 0.2244

compound 7

C	0.69221100	1.20810200	0.00000100
C	-0.69218200	1.20811900	0.00000100
C	-1.39863700	0.00003400	0.00000000
C	-0.69221100	-1.20806800	-0.00000100
C	0.69218200	-1.20808400	-0.00000100
C	1.39863700	0.00000100	0.00000000
H	1.24090300	2.14145900	0.00000200
H	-1.24085200	2.14148900	0.00000200
H	-1.24090300	-2.14142400	-0.00000200
H	1.24085200	-2.14145400	-0.00000200
C	-2.83113600	0.00005200	0.00000100

C	-4.03206900	0.00002600	-0.00000300
H	-5.09562600	-0.00067600	-0.00004100
C	2.83113600	-0.00001600	-0.00000100
C	4.03206900	-0.00003600	0.00000300
H	5.09562600	-0.00018400	0.00004900

SCF Done: E(RM062X) = -384.472298283 A.U.

Zero-point correction= 0.113259 (Hartree/Particle)
Thermal correction to Energy= 0.142163
Thermal correction to Enthalpy= 0.143978
Thermal correction to Gibbs Free Energy= 0.032872

SCF Done: E(RB3LYP) = -384.668523909 A.U.

Transition state for the dimerization of compound 7

C	-1.46121300	4.18436500	0.93611500
C	-0.58825500	3.16285300	1.33988900
C	-1.73040200	4.35301600	-0.43061900
C	-0.00421800	2.32877600	0.40879500
H	-0.38130400	3.03386900	2.39504400
C	-1.14403500	3.52903700	-1.36890700
C	-0.27409100	2.49202800	-0.96811000
H	0.66511400	1.53670100	0.72131400
C	0.31743600	1.64300600	-1.91153900
C	0.58825500	0.66201000	-2.64115800
C	-0.58825500	-0.66201000	-2.64115800
C	-0.31743600	-1.64300600	-1.91153900
C	0.27409100	-2.49202800	-0.96811000
C	0.00421800	-2.32877600	0.40879500
C	1.14403500	-3.52903700	-1.36890700
C	0.58825500	-3.16285300	1.33988900
H	-0.66511400	-1.53670100	0.72131400
C	1.73040200	-4.35301600	-0.43061900
C	1.46121300	-4.18436500	0.93611500
H	0.38130400	-3.03386900	2.39504400
H	1.37776700	0.37511200	-3.31624600
H	-1.37776700	-0.37511200	-3.31624600
H	1.34609400	-3.66772000	-2.42360500
H	-1.34609400	3.66772000	-2.42360500
H	2.40187000	-5.14381700	-0.74119500
H	-2.40187000	5.14381700	-0.74119500
C	-2.06661100	5.04382600	1.90444100

C	-2.57637500	5.76614900	2.71865900
H	-3.02617100	6.40602400	3.43928600
C	2.06661100	-5.04382600	1.90444100
C	2.57637500	-5.76614900	2.71865900
H	3.02617100	-6.40602400	3.43928600

SCF Done: E(UM062X) = -768.899798457 A.U.
<S**2> = 0.2897
Zero-point correction= 0.225113 (Hartree/Particle)
Thermal correction to Energy= 0.285583
Thermal correction to Enthalpy= 0.287398
Thermal correction to Gibbs Free Energy= 0.096958

SCF Done: E(UB3LYP) = -769.306787373 A.U.
<S**2> = 0.1656

compound 8

C	-2.34840000	-0.69603400	-0.00003100
C	-1.14766300	-1.38957200	0.00000500
C	0.07084000	-0.70462800	0.00001800
C	0.07083600	0.70463200	-0.00000500
C	-1.14767000	1.38957000	-0.00004300
C	-2.34840300	0.69602700	-0.00005600
H	-3.28414300	-1.24128300	-0.00004100
H	-1.13448500	-2.47212900	0.00002400
H	-1.13449700	2.47212700	-0.00006200
H	-3.28414900	1.24127100	-0.00008500
C	1.29957200	-1.43825400	0.00005500
C	2.32316600	-2.06556600	0.00007700
H	3.23360400	-2.61531200	-0.00000600
C	1.29956500	1.43826300	0.00000900
C	2.32316100	2.06557300	0.00001300
H	3.23364200	2.61525100	-0.00007700

SCF Done: E(RM062X) = -384.470914846 A.U.

Zero-point correction= 0.113113 (Hartree/Particle)
Thermal correction to Energy= 0.142053
Thermal correction to Enthalpy= 0.143868
Thermal correction to Gibbs Free Energy= 0.032855

SCF Done: E(RB3LYP) = -384.667164394 A.U.

Transition state for the dimerization of compound 8

C	-4.69443100	-1.89908300	-0.06342100
C	-3.51523900	-2.40528700	0.48712200
C	-4.80703400	-0.54151300	-0.32713500
H	-5.52072400	-2.56209500	-0.28695400
C	-2.45921400	-1.56128500	0.77204100
H	-3.42377200	-3.46537300	0.69058300
C	-3.75645900	0.33242000	-0.04401700
H	-5.71478300	-0.13712900	-0.75765900
C	-2.55322600	-0.17668500	0.51577200
H	-1.54001900	-1.94533000	1.19688800
C	-1.48237800	0.67016500	0.82288700
C	-0.41814800	1.32748300	0.77850000
C	0.41814700	1.32737000	-0.77878900
C	1.48238100	0.67005500	-0.82307700
C	2.55325700	-0.17671400	-0.51583100
C	2.45939500	-1.56132500	-0.77208600
C	3.75639500	0.33250600	0.04406000
C	3.51547400	-2.40522700	-0.48707100
H	1.54027200	-1.94546400	-1.19700600
C	4.80703000	-0.54132400	0.32726300
C	4.69457800	-1.89890700	0.06355200
H	3.42411600	-3.46532400	-0.69052200
H	5.71470900	-0.13684700	0.75784900
H	5.52092000	-2.56183500	0.28715400
H	0.16062100	1.95131000	1.43942000
H	-0.16053500	1.95125700	-1.43972800
C	-3.88662900	1.72656200	-0.32982800
C	-4.00035900	2.89760200	-0.57376900
H	-4.10255700	3.93485700	-0.78494700
C	3.88640100	1.72665600	0.32990800
C	4.00000100	2.89770100	0.57388900
H	4.10208800	3.93496000	0.78510300

SCF Done: E(UM062X) = -768.898217679 A.U.
<S**2> = 0.2996
Zero-point correction= 0.225298 (Hartree/Particle)
Thermal correction to Energy= 0.285777
Thermal correction to Enthalpy= 0.287592
Thermal correction to Gibbs Free Energy= 0.096410

SCF Done: E(UB3LYP) = -769.304918724 A.U.
<S**2> = 0.1689

3. Full Citation of Reference 27

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