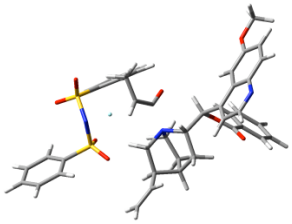
Structure: TS-A

```
****************************************
 Gaussian 09:  IA32W-G09RevA.02    8-May-2009
               27-Jan-2011
****************************************
 %mem=10000MB
 %nprocshared=4
 Will use up to    4 processors via shared memory.
 %nosave
 ----------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput
 ----------------------------------------------------------------
---------------------
 - Thermochemistry -
 ---------------------
Zero-point correction=                          0.778412 (Hartree/Particle)
 Thermal correction to Energy=                  0.829888
 Thermal correction to Enthalpy=                0.830832
 Thermal correction to Gibbs Free Energy=       0.685917
 Sum of electronic and zero-point Energies=          -3286.884913
 Sum of electronic and thermal Energies=             -3286.833437
 Sum of electronic and thermal Enthalpies=           -3286.832493
 Sum of electronic and thermal Free Energies=        -3286.977408
```



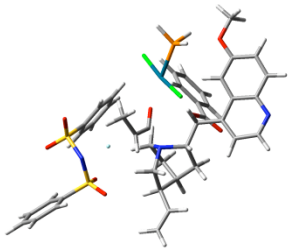
C	-0.00554700	0.01938400	-1.44760600	C	3.82064900	3.83174400	0.78768300
C	0.71262100	-0.22704000	-2.60275400	C	1.93045500	3.04044400	-0.53987400
N	-0.17261400	-1.25513200	-0.43524400	C	1.06826600	3.79415600	0.25604800
C	-1.56490200	-1.89489900	-0.60637400	C	2.94743900	4.59424500	1.56193100
C	0.04651400	-0.73811000	0.97528200	H	4.88652200	3.82282200	0.98129500
C	0.84002900	-2.35747300	-0.68920900	H	1.53707400	2.44023900	-1.34772500
H	1.10360200	-0.47087200	1.01480700	H	0.00270100	3.75872900	0.05240900
H	-0.54643300	0.16712700	1.06852100	H	3.33954900	5.20027000	2.37373900
H	0.54784300	-2.84118400	-1.62422400	H	0.89916300	5.16440600	1.91118400
H	1.80635600	-1.87676600	-0.81846700	C	6.15315100	-0.78233300	0.45679200
H	-1.55016300	-2.20485600	-1.65439900	C	8.75606000	-1.69626400	0.25298300
H	1.08785800	-1.21284700	-2.82972200	C	6.38693600	-2.04877400	-0.08522400
N	4.20404500	0.43910700	-0.98527500	C	7.19414100	0.03684600	0.89744500
F	2.61407800	0.16661400	-1.40429000	C	8.50320500	-0.43253700	0.79202500
C	-0.31943900	-1.82510500	2.00669100	C	7.70118800	-2.50260800	-0.18394300
H	-1.25796700	-1.57778400	2.51088000	H	5.55377100	-2.66211600	-0.40994700
H	0.46114800	-1.87074200	2.77340200	H	6.97819600	1.01787000	1.30281900
C	-1.64508400	-3.13648300	0.33138300	H	9.32545000	0.19159400	1.12930400
H	-1.67314300	-4.04914600	-0.27435500	H	7.90126100	-3.48570800	-0.60019800
H	-2.57772200	-3.11050000	0.89635700	H	9.77863200	-2.05452400	0.17232900
C	0.86851100	-3.37888200	0.47725600	O	5.80323900	2.39913100	-0.82594200
H	1.71725000	-3.12830200	1.12272100	O	4.40047800	0.81895100	1.65278000
C	-0.43653900	-3.17835700	1.28607400	O	-0.55899100	1.03961700	-1.02675400
H	-0.56492400	-3.99041900	2.00884300	C	0.82634500	0.82086600	-3.67126600
S	4.46558300	-0.20830700	0.60984200	H	1.86987400	1.13076800	-3.80949800
O	3.58711800	-1.38321900	0.69072000	H	0.46486500	0.43880900	-4.63607700
S	4.43390500	2.13747100	-1.28403100	H	0.23673100	1.70549000	-3.41499600
O	4.05546700	2.30818600	-2.68300300	C	1.07135500	-4.78037100	-0.03481600
C	3.29766900	3.06586500	-0.25672100	H	0.29403100	-5.17914600	-0.68955600
C	1.57492100	4.57252800	1.29922400	C	2.12594500	-5.54380800	0.25535800

H	2.22529300	-6.55337500	-0.13411000	O	-5.72383500	3.21341400	-0.94859400
H	2.93037700	-5.18508600	0.89404300	C	-6.69649300	4.20233700	-1.24831600
C	-2.73426100	-0.88614000	-0.51439500	H	-6.33204500	5.12445000	-0.79202200
H	-2.38499900	0.03526800	-0.98024000	H	-6.80154900	4.35320800	-2.33066200
C	-3.99649100	-1.30576200	-1.25833300	H	-7.67613900	3.95166300	-0.82062000
C	-4.99736600	-0.31147500	-1.53160400	C	-4.13522900	-0.15219700	2.88734500
C	-4.20200000	-2.57148200	-1.76073000	C	-5.01450500	-0.65440300	3.85844600
C	-4.91207600	1.03363100	-1.10307500	C	-3.50702200	1.08615400	3.08928400
C	-6.14053300	-0.72082000	-2.29794100	C	-5.26167700	0.07245000	5.01990600
C	-5.36923900	-2.86401800	-2.50820200	H	-5.49331000	-1.61167700	3.68123100
H	-3.49406000	-3.37326700	-1.58409700	C	-3.75760200	1.80960100	4.25434700
C	-5.91035700	1.94457600	-1.41085700	H	-2.83355300	1.47736200	2.33534500
H	-4.07135400	1.38731900	-0.51825900	C	-4.63270800	1.30495900	5.21947100
C	-7.14456600	0.23467800	-2.59150400	H	-5.94355400	-0.31940000	5.76935000
H	-5.51633400	-3.87276000	-2.89285700	H	-3.27126200	2.76874600	4.40821500
C	-7.04316400	1.53905000	-2.16300300	H	-4.82558900	1.87232800	6.12610200
H	-7.99792300	-0.10163700	-3.17168700	C	-3.91348400	-0.97925900	1.66661000
H	-7.82798300	2.24635700	-2.40548500	O	-2.97820100	-0.42488500	0.85023000
N	-6.31211000	-1.98794500	-2.77462700	O	-4.48177600	-2.03001500	1.44593100

Structure: TS-B

```
*****************************************
 Gaussian 09:  IA32W-G09RevA.02  8-May-2009
               21-Jan-2011
 *****************************************
 %nosave
 %mem=10000MB
 %nprocshared=4
 Will use up to    4 processors via shared memory.
 ----------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput
 ----------------------------------------------------------------
-------------------
 - Thermochemistry -
 -------------------

Zero-point correction=                           0.811550 (Hartree/Particle)
 Thermal correction to Energy=                    0.871522
 Thermal correction to Enthalpy=                  0.872466
 Thermal correction to Gibbs Free Energy=         0.708845
 Sum of electronic and zero-point Energies=          -4677.236551
 Sum of electronic and thermal Energies=             -4677.176579
 Sum of electronic and thermal Enthalpies=           -4677.175635
 Sum of electronic and thermal Free Energies=        -4677.339256
```



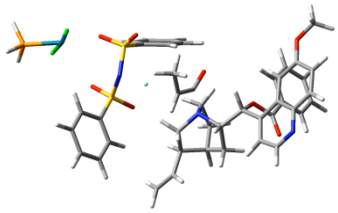
C	-0.34528500	0.15119700	-1.34972100	H	-0.15151100	0.20237700	1.19543500
C	-1.15667700	0.02296700	-2.46542900	H	-1.14081300	2.85993400	-1.90548200
N	-0.44019200	1.45347400	-0.48965200	H	-2.40582300	1.81335000	-1.22465500
C	0.87193700	2.30201200	-0.49629000	H	0.96135200	2.58112900	-1.54956500
C	-0.83536200	0.99943000	0.92415300	H	-1.63158100	0.89348800	-2.89135600
C	-1.52776400	2.40573300	-0.99017600	N	-4.55435500	-0.70398500	-0.91633600
H	-1.83394100	0.57939900	0.80311400	F	-2.88114500	-0.35848000	-1.32326500

C	-0.80903000	2.18483300	1.90378000
H	0.04637700	2.10926800	2.58178200
H	-1.71700100	2.15469600	2.51487000
C	0.61672500	3.56434300	0.38740500
H	0.64822600	4.45693100	-0.24582100
H	1.42406700	3.65955100	1.11538600
C	-1.88399800	3.47535400	0.07277000
H	-2.80240900	3.15095800	0.57272400
C	-0.73897100	3.49467700	1.10753600
H	-0.84126700	4.35539400	1.77619700
S	-5.07421500	0.71069500	-0.08169500
O	-4.67597500	1.81816500	-0.96158000
S	-4.52233900	-2.25830200	-0.15175400
O	-4.04020200	-3.15209200	-1.19891600
C	-3.32932500	-2.26251800	1.18286900
C	-1.50829000	-2.38159000	3.26513200
C	-3.76938300	-2.01614200	2.48660000
C	-1.99834600	-2.57981200	0.90405000
C	-1.08553200	-2.63805000	1.95848600
C	-2.84639200	-2.07465500	3.52932900
H	-4.81236000	-1.79263500	2.67265800
H	-1.68254400	-2.78766800	-0.11077200
H	-0.05232200	-2.88901800	1.74213900
H	-3.17425000	-1.88653200	4.54783800
H	-0.79192200	-2.42572700	4.08139200
C	-6.85411300	0.55820800	-0.15949700
C	-9.61101400	0.39192700	-0.28550300
C	-7.49062500	0.77461700	-1.38475000
C	-7.56719100	0.26158300	1.00210000
C	-8.95768300	0.18345300	0.93142400
C	-8.88017600	0.68705700	-1.44022300
H	-6.90695600	1.00976400	-2.26794000
H	-7.03829900	0.10009600	1.93396100
H	-9.52946100	-0.04442400	1.82618400
H	-9.39229200	0.85021000	-2.38395000
H	-10.69424400	0.32419300	-0.33525400
O	-5.86174600	-2.40685600	0.43178200
O	-4.64615200	0.73619700	1.32663300
O	0.41310300	-0.71161300	-0.82829300
Pd	1.99534900	-1.84627600	-1.75748000
P	3.77521700	-3.00249500	-2.48091500
H	4.85778900	-2.99458300	-1.58347500
H	4.37340700	-2.58037800	-3.68219700
H	3.59130100	-4.37757800	-2.71138700
Cl	2.30701400	-0.23836600	-3.47008400
Cl	1.90857100	-3.51332400	-0.05982800
C	-1.15580100	-1.21817000	-3.30185300
H	-2.16280800	-1.39282900	-3.69193800
H	-0.46229600	-1.11543500	-4.14579000
H	-0.85751700	-2.09462900	-2.72112000
C	-2.16203500	4.80318900	-0.58395100
H	-1.30283200	5.33828400	-0.99281200
C	-3.37902200	5.33426300	-0.70812600
H	-3.53482500	6.29297300	-1.19554700
H	-4.26346800	4.81986200	-0.34003800
C	2.17478000	1.52495700	-0.19991700
H	2.17477300	0.65527000	-0.85328500
C	3.46069900	2.28184800	-0.53198600
C	4.71652600	1.57879200	-0.48761900
C	3.48591400	3.58594100	-0.97432700
C	4.85530900	0.21562200	-0.13024200
C	5.89691300	2.31461600	-0.84347300
C	4.71160400	4.20799800	-1.31809100
H	2.58357900	4.17687500	-1.05946300
C	6.09930100	-0.39519200	-0.11802400
H	3.99656200	-0.38543200	0.14255900
C	7.15478400	1.66460400	-0.79572300
H	4.70448600	5.24409700	-1.65512600
C	7.26737100	0.33976400	-0.44058200
H	8.02749600	2.25207100	-1.06214100
H	8.24313900	-0.13191800	-0.42148400
N	5.88217300	3.61831800	-1.24731500
O	6.11379500	-1.72716400	0.20245200
C	7.36361000	-2.35184500	0.46359900
H	7.12555700	-3.36214600	0.80095800
H	7.98798500	-2.41054100	-0.43789900
H	7.91651600	-1.82709400	1.25263000
C	2.84177600	0.50852100	3.33667700
C	3.23735200	1.00128300	4.58951100
C	2.59053000	-0.86308200	3.17010200
C	3.37480500	0.13306900	5.66918800
H	3.43344700	2.06340700	4.69366100
C	2.73589700	-1.72768100	4.25497800
H	2.29532700	-1.25223100	2.20148400
C	3.12409000	-1.23249200	5.50266900
H	3.67914800	0.51776700	6.63856500
H	2.55285000	-2.79004000	4.12066400
H	3.23533700	-1.91061100	6.34477300
C	2.71627700	1.48655400	2.21988600
O	3.03034500	2.65839300	2.29429300
O	2.17700900	0.90562600	1.11526500

Structure: TS-C

```
 ******************************************
 Gaussian 09:  IA32W-G09RevA.02  8-May-2009
               21-Jan-2011
 ******************************************
 %nosave
 %mem=10000MB
 %nprocshared=4
 Will use up to    4 processors via shared memory.
 ----------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput
 ----------------------------------------------------------------
---------------------
 - Thermochemistry -
 ---------------------
```

Zero-point correction= 0.809936 (Hartree/Particle)
Thermal correction to Energy= 0.870672
Thermal correction to Enthalpy= 0.871616
Thermal correction to Gibbs Free Energy= 0.704317
Sum of electronic and zero-point Energies= -4677.223914
Sum of electronic and thermal Energies= -4677.163179
Sum of electronic and thermal Enthalpies= -4677.162235
Sum of electronic and thermal Free Energies= -4677.329534

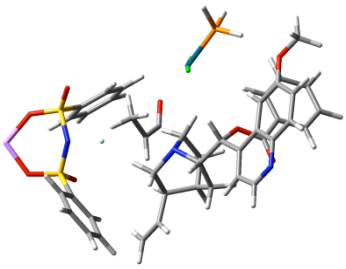


C	-1.34510900	0.46261800	1.03252100	H	5.08480200	2.15200400	1.12000500
C	-0.69063800	1.30742500	1.90296400	H	5.54447800	4.52860800	1.65851200
N	-1.76370200	1.15373900	-0.42342100	H	2.53716900	5.77155600	-1.16733500
C	-3.17530500	1.75188900	-0.33615600	H	4.27500100	6.33880300	0.52035100
C	-1.66542300	0.07084300	-1.47730200	O	4.44952100	-1.72933000	1.07822500
C	-0.83446300	2.27660200	-0.83264100	O	4.50456500	0.30503700	-1.19254300
H	-0.60012000	-0.15610700	-1.55502100	O	-1.70255300	-0.71325900	1.11022700
H	-2.16949700	-0.80339400	-1.07697300	Pd	6.55281900	-1.17440000	0.56486100
H	-1.04245400	3.12020000	-0.17117100	P	8.68254900	-0.86037400	0.04291900
H	0.17922300	1.92875600	-0.65001700	H	9.52019600	-1.98072200	0.18100400
H	-3.06444700	2.50258300	0.45003500	H	9.38024600	0.12119600	0.76931000
H	-0.53660000	2.34822500	1.65702300	H	8.93753700	-0.48302000	-1.28712700
N	2.90767800	0.31794400	0.80980000	Cl	6.71465000	0.45888700	2.26297200
F	1.32376300	0.68875400	1.05609800	Cl	6.66100600	-2.83377900	-1.13828200
C	-2.25962300	0.56497300	-2.81172800	C	-0.38296200	0.85993600	3.30362300
H	-3.22352200	0.08575200	-3.00619300	H	0.60385700	1.21817300	3.61358000
H	-1.58850200	0.28937100	-3.63235800	H	-1.12102400	1.24355700	4.02395500
C	-3.50085400	2.43324500	-1.69917800	H	-0.38107000	-0.23033600	3.37046500
H	-3.55679400	3.51873600	-1.56036000	C	-0.94061000	4.16774300	-2.50843000
H	-4.48394200	2.11414400	-2.04765800	H	-1.59966000	4.78971200	-1.89987600
C	-1.05528200	2.67815200	-2.31666900	C	-0.10965600	4.75914900	-3.36980600
H	-0.27703100	2.19980300	-2.92333900	H	-0.08218700	5.83914800	-3.48654500
C	-2.42403300	2.09133500	-2.74606400	H	0.56689300	4.18410900	-3.99908400
H	-2.71638300	2.49215000	-3.72165400	C	-4.22486400	0.76075000	0.21977100
S	3.25382400	0.94602000	-0.77259800	H	-3.71537700	0.15749100	0.97168200
O	2.07892600	0.88409900	-1.65290500	C	-5.41399600	1.41395600	0.91339900
S	3.01676200	-1.37910100	1.17552400	C	-6.24258000	0.60666800	1.76543200
O	2.33838500	-1.51939800	2.45353200	C	-5.70187600	2.75822600	0.83062000
C	2.15746900	-2.31870500	-0.07577300	C	-6.05590300	-0.78091200	1.96540500
C	0.82282500	-3.82423000	-1.96464700	C	-7.31401300	1.26614600	2.45779900
C	2.88614100	-2.86293500	-1.13719600	C	-6.78554000	3.30375900	1.56180400
C	0.78025800	-2.50745600	0.06857500	H	-5.12661000	3.42365100	0.19663800
C	0.11726800	-3.27048800	-0.89263200	C	-6.88922600	-1.49822800	2.80958500
C	2.19953800	-3.62087200	-2.08624800	H	-5.26395500	-1.32329600	1.46277900
H	3.95871200	-2.71664300	-1.21098100	C	-8.14796300	0.50314300	3.31215000
H	0.23479600	-2.07339600	0.89864800	H	-7.00099800	4.36863500	1.48018800
H	-0.95175900	-3.43390900	-0.79240500	C	-7.95059600	-0.84743200	3.49068800
H	2.74864800	-4.05865800	-2.91448100	H	-8.94944500	1.02655200	3.82358100
H	0.29854500	-4.42256800	-2.70528300	H	-8.60562000	-1.40304000	4.15179900
C	3.54651100	2.65136900	-0.32267700	N	-7.57128400	2.60144500	2.34731500
C	4.07058900	5.29901500	0.27969400	O	-6.61899700	-2.82839300	2.92593500
C	2.82539300	3.65044100	-0.97743000	C	-7.42023200	-3.61893700	3.79104100
C	4.53382100	2.94491700	0.62208900	H	-7.01357900	-4.62984700	3.72940600
C	4.78640300	4.28328100	0.92065900	H	-7.36127500	-3.26958200	4.82999500
C	3.09423200	4.98428100	-0.66773100	H	-8.47060500	-3.63260300	3.47172500
H	2.07313700	3.39071000	-1.71242300	C	-5.99426800	-1.45520500	-2.23643200

C	-7.02035800	-1.45487900	-3.19343100	H	-8.14307200	-2.62486700	-4.60661500
C	-5.30303600	-2.64346400	-1.95558100	H	-5.10317500	-4.73676000	-2.40907000
C	-7.34843400	-2.62897900	-3.86591400	H	-6.91312600	-4.72742500	-4.11034300
H	-7.54674500	-0.52720200	-3.39190900	O	-4.60132700	-0.27050300	-0.74464700
C	-5.63647200	-3.81666800	-2.63080400	C	-5.68968000	-0.16520300	-1.55463800
H	-4.51749900	-2.64438200	-1.20855000	O	-6.31991300	0.85894700	-1.72589800
C	-6.65615100	-3.81087800	-3.58604200				

Structure: TS-D

```
*****************************************
 Gaussian 09:  IA32W-G09RevA.02  8-May-2009
               21-Jan-2011
*****************************************
 %nosave
 %mem=10000MB
 %nprocshared=4
 Will use up to    4 processors via shared memory.
 ----------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput
 ----------------------------------------------------------------------------
 - Thermochemistry -
 -------------------
Zero-point correction=                          0.813283 (Hartree/Particle)
 Thermal correction to Energy=                  0.874512
 Thermal correction to Enthalpy=                0.875456
 Thermal correction to Gibbs Free Energy=       0.710329
 Sum of electronic and zero-point Energies=          -4684.653697
 Sum of electronic and thermal Energies=             -4684.592468
 Sum of electronic and thermal Enthalpies=           -4684.591524
 Sum of electronic and thermal Free Energies=        -4684.756651
```



C	-0.63741100	0.00387900	-0.48788100	H	0.24111700	3.61740300	2.08765900
C	-1.24706200	0.76911300	-1.45195600	H	1.68956200	2.73248400	2.51289800
N	-0.41243700	0.72057700	0.92906500	C	-1.64121900	1.78532300	2.89102700
C	0.60844400	1.87633900	0.82806100	H	-2.12511000	1.03210400	3.52447500
C	0.01512900	-0.31617400	1.96063700	C	-0.13908900	1.82813000	3.26486800
C	-1.72806100	1.31991600	1.41242600	H	-0.00947900	2.30165100	4.24251800
H	-0.82881700	-1.00102200	2.04787800	S	-5.85612000	0.52829900	-0.08574700
H	0.84658700	-0.87846000	1.55064300	O	-5.45424600	0.37153500	1.30830500
H	-1.95722800	2.15665100	0.75169900	S	-4.89808100	-2.18426300	-1.11819100
H	-2.49344500	0.56018600	1.26209300	O	-4.13863200	-2.57028700	-2.28970500
H	0.16788600	2.51950600	0.06585100	C	-4.11904400	-2.75095200	0.36619000
H	-1.47757100	1.80621700	-1.23666300	C	-2.89237100	-3.76729700	2.61492200
N	-4.93108700	-0.42344100	-1.20277900	C	-4.89172400	-2.96440400	1.51543500
F	-3.40394800	0.01012700	-0.93918400	C	-2.74841600	-3.02649400	0.31642600
C	0.35950800	0.37593600	3.29557300	C	-2.13721600	-3.54165400	1.46098400
H	1.43786700	0.34496100	3.46902500	C	-4.26162200	-3.47832100	2.64493000
H	-0.11342000	-0.17068000	4.11848800	H	-5.95441100	-2.75373100	1.52290000
C	0.65222100	2.60846600	2.20029800	H	-2.17002000	-2.84698500	-0.58170200

H	-1.07340800	-3.76035900	1.43297500	C	2.76990000	2.55096600	-0.41471200
H	-4.84155400	-3.66359500	3.54368000	C	3.94580300	2.22227300	-1.17297900
H	-2.41209200	-4.17911500	3.49793500	C	2.37884800	3.87166600	-0.38447900
C	-5.51064700	2.16323400	-0.67629800	C	4.46482200	0.91394500	-1.30884700
C	-5.07698700	4.75154600	-1.52506800	C	4.62611000	3.30328000	-1.82928100
C	-5.02573300	3.09725100	0.24246300	C	3.12614200	4.85694600	-1.07611700
C	-5.78665600	2.48955600	-2.00908500	H	1.51265900	4.19964400	0.17951500
C	-5.55891900	3.79788300	-2.42828000	C	5.60436900	0.67380300	-2.05826500
C	-4.81311900	4.40417800	-0.19811800	H	3.98360500	0.07070200	-0.83109400
H	-4.82236900	2.81228600	1.26911000	C	5.79122700	3.02224300	-2.58475200
H	-6.15752300	1.74196800	-2.70151000	H	2.80345300	5.89663800	-1.03618600
H	-5.76013400	4.07367100	-3.45854700	C	6.27956100	1.74093400	-2.70259900
H	-4.44579300	5.14991500	0.50001200	H	6.28463400	3.85821600	-3.06950500
H	-4.90871700	5.77083100	-1.85959300	H	7.17198500	1.55989300	-3.28983100
O	-6.35119000	-2.52832500	-1.03963500	N	4.20840600	4.60039100	-1.77404600
O	-7.26896200	0.18364800	-0.44711100	O	6.01778800	-0.62966300	-2.12730200
O	-0.27624400	-1.19998900	-0.50554900	C	7.21811900	-0.92874100	-2.83336400
Pd	1.53883300	-2.23135500	-1.15877000	H	7.36742200	-2.00456800	-2.72599300
P	3.39035400	-3.26867400	-1.88864900	H	7.13190200	-0.68036400	-3.89824300
H	4.50474000	-2.42598500	-2.05084200	H	8.07795900	-0.40255600	-2.40187100
H	3.28002600	-3.88225200	-3.14814500	C	4.50170100	0.09779600	2.66528900
H	3.88673200	-4.31298600	-1.08769600	C	5.53334200	0.52851900	3.51574300
Cl	1.78114700	-0.98663200	-3.15369800	C	4.26672700	-1.27560100	2.48978300
Cl	1.53061100	-3.54002200	0.82431400	C	6.32544300	-0.40402500	4.17881300
C	-1.42813800	0.31340400	-2.86954500	H	5.69870900	1.59354700	3.63933600
H	-2.40576200	0.63210700	-3.24554200	C	5.05983200	-2.20352500	3.16371600
H	-0.65694300	0.74420200	-3.51787000	H	3.46989200	-1.62175700	1.84135200
H	-1.35349600	-0.77190600	-2.95162800	C	6.08861700	-1.77123200	4.00448500
C	-2.36646300	3.09007500	3.09776200	H	7.12537500	-0.06782200	4.83202700
H	-1.98195400	3.95166600	2.54916400	H	4.86935400	-3.26474400	3.03204800
C	-3.41219000	3.25349500	3.91187500	H	6.70525000	-2.49852700	4.52559700
H	-3.88040000	4.22380000	4.05294700	Li	-7.84086000	-1.45812600	-1.06474100
H	-3.82760900	2.42647900	4.48385400	O	2.73024400	0.61601500	1.17748500
C	1.96845100	1.42701700	0.24089800	C	3.69185000	1.14916800	1.99744200
H	1.75718600	0.70603900	-0.55612300	O	3.83481200	2.34194200	2.17091700

Structure: BQ

```
 ****************************************
 Gaussian 09:  IA32W-G09RevA.02  8-May-2009
               21-Jan-2011
 ****************************************
 %nosave
 %mem=10000MB
 %nprocshared=4
 Will use up to    4 processors via shared memory.
 ----------------------------------------------------------------
 # opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput
 ----------------------------------------------------------------

 -------------------
 - Thermochemistry -
 -------------------
Zero-point correction=                          0.502429 (Hartree/Particle)
 Thermal correction to Energy=                  0.528881
 Thermal correction to Enthalpy=                0.529825
 Thermal correction to Gibbs Free Energy=       0.443068
 Sum of electronic and zero-point Energies=          -1380.340698
 Sum of electronic and thermal Energies=             -1380.314247
 Sum of electronic and thermal Enthalpies=           -1380.313303
 Sum of electronic and thermal Free Energies=        -1380.400060
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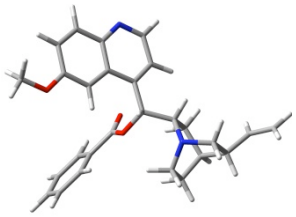

N	-2.60352300	-0.33510600	1.64834800	C	2.42308200	-2.78567200	-0.94525500
C	-2.00607400	-0.76313900	0.35788600	C	0.55327400	-3.29926200	-2.15807900
C	-2.61874700	1.13433800	1.79918500	H	-1.27206900	-2.23917500	-1.72041500
C	-3.99074500	-0.82081300	1.68988000	C	3.78315600	-1.35994200	1.07014200
H	-3.11525400	1.34852100	2.75245400	H	1.96634100	-0.33355800	1.43352100
H	-1.59124300	1.49067600	1.88458600	C	3.79476300	-3.02396300	-0.68148700
H	-3.98056100	-1.90984000	1.57533400	H	0.08950300	-3.88933700	-2.94807800
H	-4.39417600	-0.60010200	2.68455200	C	4.46970300	-2.33429300	0.30076700
H	-2.16529600	-1.84729000	0.33828900	H	4.29455800	-3.77532200	-1.28464500
C	-3.35956100	1.82452800	0.61397200	H	5.51888900	-2.54116900	0.47808400
H	-2.66967700	2.44941800	0.03385600	N	1.82911700	-3.52148200	-1.92942500
H	-4.15926800	2.48227200	0.97723200	O	4.36859000	-0.62887900	2.06361000
C	-2.77036200	-0.11858200	-0.84300300	C	5.73886100	-0.84833000	2.35685300
H	-3.14517800	-0.90126500	-1.51357100	H	5.98089100	-0.16557700	3.17356400
H	-2.11821500	0.51310300	-1.44904800	H	5.92462500	-1.88007500	2.68356700
C	-4.88592400	-0.16415900	0.56850400	H	6.38105900	-0.62096000	1.49570200
H	-5.60715500	0.50493100	1.05857400	C	0.94053900	2.67339100	-0.71836900
C	-3.94312700	0.71879500	-0.28608000	C	1.25288400	3.39740900	-1.87816900
H	-4.50355200	1.16342600	-1.11746700	C	1.20860800	3.22939400	0.54102100
C	-5.67593100	-1.16427700	-0.25094400	C	1.82407400	4.66364300	-1.78053500
H	-5.48017800	-1.17876800	-1.32440500	H	1.04111000	2.94791400	-2.84258400
C	-6.58645200	-2.01026700	0.23646600	C	1.78115700	4.49736300	0.63441000
H	-7.12281200	-2.70311500	-0.40640800	H	0.97343000	2.66725200	1.43754000
H	-6.83791300	-2.04272200	1.29534400	C	2.08838700	5.21568200	-0.52380400
C	-0.46688200	-0.62530700	0.40842900	H	2.06412600	5.22046900	-2.68206100
H	-0.21787900	-0.84132800	1.45193400	H	1.98933100	4.92441100	1.61155000
C	0.33527800	-1.59406500	-0.45011500	H	2.53445600	6.20382300	-0.44728900
C	1.72861200	-1.79934600	-0.16691400	C	0.32946700	1.32197600	-0.89588400
C	-0.22930700	-2.35584800	-1.44844000	O	0.13731100	0.80713600	-1.97915900
C	2.44267000	-1.10075300	0.83507500	O	0.00341600	0.75905500	0.29364200