Mechanism and Origins of Selectivity in the Enantioselective *oxa*-Pictet-Spengler Reaction: A Cooperative Catalytic Complex from a Hydrogen Bond Donor and Chiral Phosphoric Acid

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Supporting Information

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General Information

All reactions were carried out under an argon atmosphere in oven-dried glassware with magnetic stirring. Reagents were purified prior to use following the guidelines of Perrin and Armarego unless otherwise stated.[1] Purification of select reaction products was carried out by flash chromatography using a Biotage Isolera instrument (230–400 mesh silica). Analytical thin layer chromatography was performed on EM Reagent 0.25 mm silica gel 60-F plates. Visualization was accomplished with UV light and ceric ammonium nitrate stain, anisaldehyde stain, or potassium permanganate stain followed by heating. Infrared spectra were recorded on a Bruker Tensor 37 FTIR spectrometer and a Thermo Scientific Nicolet iS5 FTIR spectrometer. ^{1}H-NMR spectra were recorded on a Bruker Avance 500 MHz with direct cryoprobe (500 MHz) spectrometer and an Agilent DD2 500 MHz spectrometer and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 7.26 ppm, CD_3OD at 3.31 ppm, toluene-d_8 at 2.08 ppm). Data are reported as (ap = apparent, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad; coupling constant(s) in Hz; integration). Proton-decoupled ^{13}C-NMR spectra were recorded on a Bruker Avance 500 MHz with direct cryoprobe (126 MHz) spectrometer and are reported in ppm using solvent as an internal standard ($CDCl_3$ at 77.0 ppm, CD_3OD at 49.0 ppm, toluene-d_8 at 20.43 ppm). ^{31}P-NMR spectra were recorded on an Agilent DD2 500 MHz spectrometer and are reported in ppm.

Substrates and catalysts were prepared in accordance with our prior report.[2] Toluene was dried by passing through activated alumina and stored under dry argon prior to use. Deuterated solvents were purchased from Cambridge Isotope Laboratories (toluene-d_8, methanol-d_4, chloroform-d) and Sigma-Aldrich (toluene-d_8); chloroform-d was stored over potassium carbonate, methanol-d_4 and toluene-d_8 were used as received.

DOSY Analysis

^{1}H-DOSY spectra were recorded on a Bruker Avance III 600 MHz spectrometer with gradient suppression from 5-100% over 16 steps in toluene-d_8 at –40° C and were processed with MestReNova Bayesian DOSY transforms (resolution factor = 1.00, repetitions = 1; 128 points in diffusion dimension). Diffusion constants were obtained from the maxima of the 1D projection of the DOSY data.

The viscosity of toluene was utilized as a stand-in for that of toluene-d_8; data for the deuterated species is not available at –40 °C.[3] Due to large relative changes in viscosity in the low-temperature regime, the viscosity of toluene at –40 °C was modeled using the high-precision reference curve[4] below as defined by Santos *et al.*:

$for\ viscosity\ \eta\ and\ temperature\ T,\ let$

$$\eta^* = \eta(T)/\eta(298.15) \text{ and } T^* = T/298.15$$

$\eta(298.15\ K) = 554.2\ \mu Pa \cdot s$

$$\ln(\eta^*) = -5.2203 + \frac{8.964}{T^*} - \frac{5.834}{(T^*)^2} + \frac{2.089}{(T^*)^3}$$

$for\ T = -40\ °C = 233.15\ K$

$\eta(233.15\ K) = 1617.2\ \mu Pa \cdot s$

Stokes radii were determined in the spherical case as the following:

$$r = \frac{k_B T}{6\pi\eta D}$$

$$k_B = 1.380649x10^{-23}\frac{m^2 \cdot kg}{s^2 \cdot K}$$

Ternary Complex (CPA + urea + unreactive substrate analogue)

$for\ D = 1.907x10^{-10}\ m^2/s$

$$r = \frac{k_B T}{6\pi\eta D} = 5.537x10^{-10}\ m \sim 5.5\ \text{Å}$$

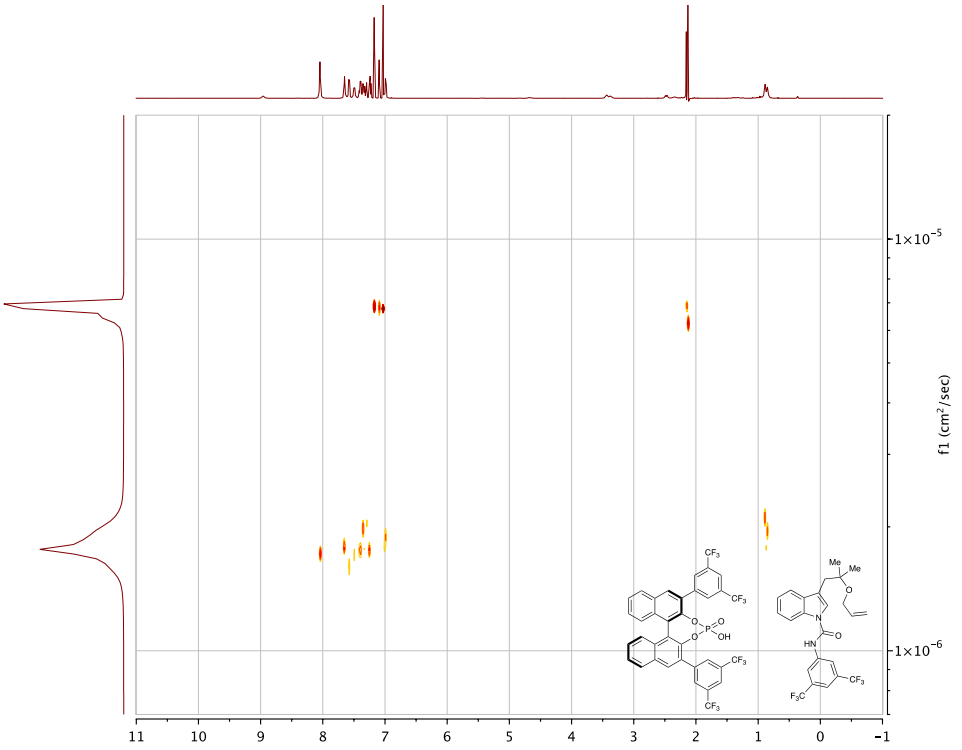
Binary Complex (CPA + unreactive substrate analogue)

$for\ D = 1.761x10^{-10}\ m^2/s$

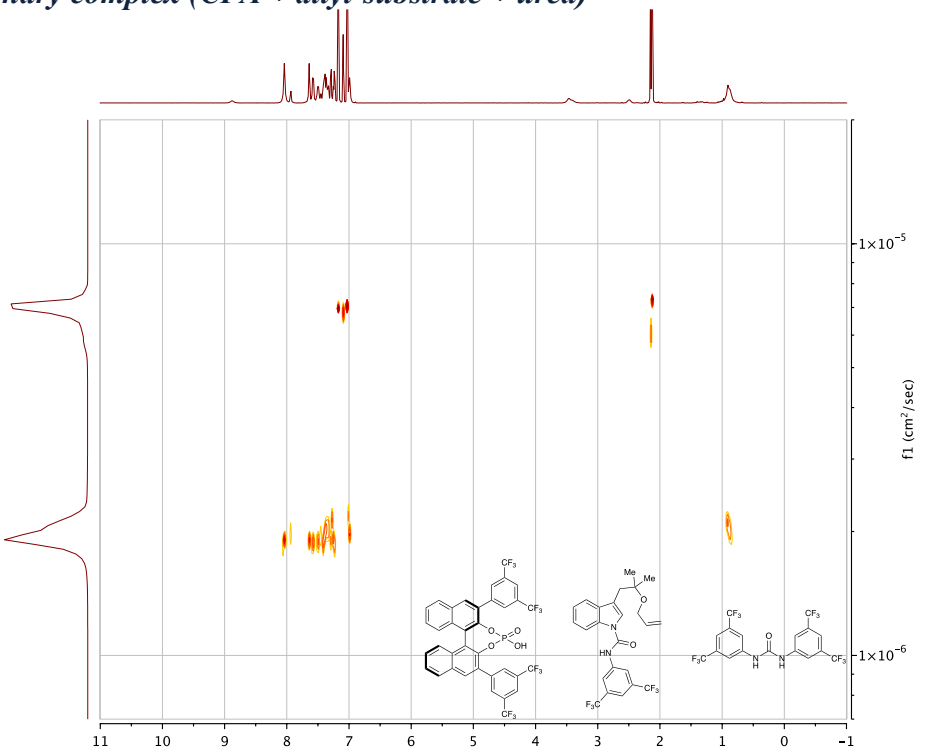
$$r = \frac{k_B T}{6\pi\eta D} = 5.996x10^{-10}\ m \sim 6\ \text{Å}$$

Selected DOSY Spectra

Binary complex (CPA + allyl-substrate, toluene-d8, –40 °C)

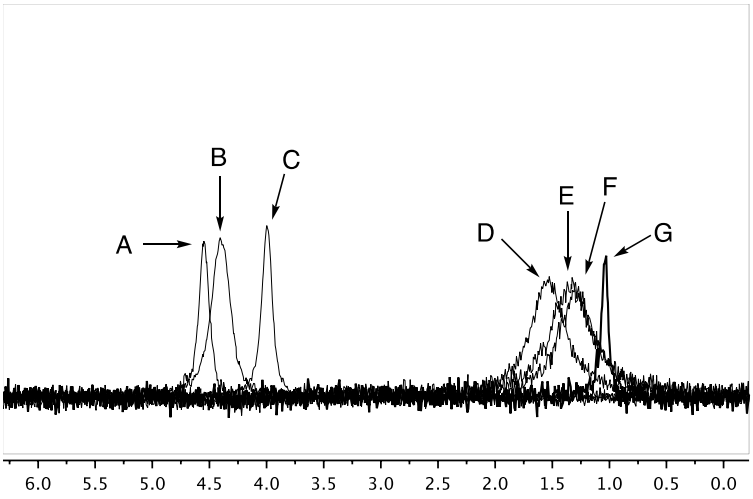


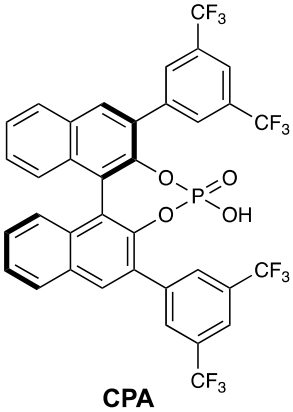
Ternary complex (CPA + allyl-substrate + urea)



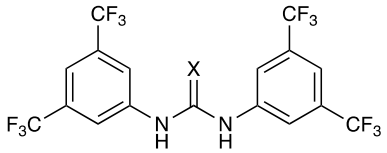
^{31}P-NMR CPA/HBD Spectra

tol-d_8, –40 °C

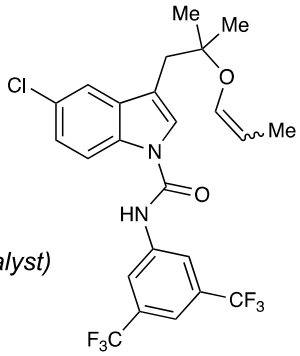




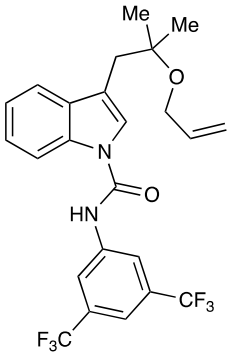
CPA



urea: X = O *(optimal co-catalyst)*
thiourea: X = S



S1

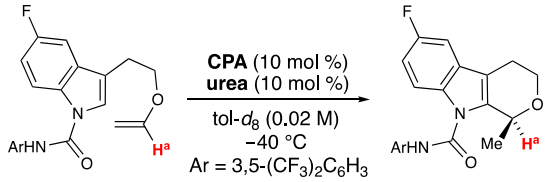


S2

A:	free CPA:	4.58 ppm
B:	CPA + urea:	4.40 ppm
C:	CPA + thiourea:	4.00 ppm
D:	CPA + thiourea + **S2**:	1.54 ppm
E:	CPA + urea + **S2**:	1.35 ppm
F:	CPA + **S2**:	1.29 ppm
G:	CPA + urea + **S1** (post rxn):	1.04 ppm

Kinetics Data Analysis

NMR spectrographic kinetic studies were undertaken on substrate **S3** (20 mM). Due to changing homogeneity of the reaction as identified in earlier studies,[2] analysis of the resulting data was conducted by the method of initial rates. Previous experiments demonstrated that the cyclization of **S3** to **1o** proceeds with a rate amenable to monitoring on the NMR timescale by ^{1}H NMR spectroscopy.[2] All experiments were conducted in quadruplicate.



S3 **1o**

Proton **H^a** was monitored by ^{1}H NMR; generation of the cyclization product **1o** was characterized by the appearance of a broadened apparent quartet at 5.4 ppm. Experiments were conducted on an Agilent DD2 500 MHz spectrometer regulated at −40 °C every six seconds and consisted of two 45° pulse scans. FID data was processed in MestReNova with phase correction and Whittaker baseline corrections. Integration of the product peak was normalized against the integration of 0.333 equivalents of 2-methoxynaphthalene as an inert internal standard. Normalized integration data were processed by subjecting the data to a polynomial fit; the linear potion of the fitted curve was extracted, and the slope of the line determined. The slope is equated to the initial rate in [product]/time (mM/s).

To determine the order of a given component of the reaction milieu, the concentration of the component of interest was varied while holding all other components constant in concentration. Under Initial Rate conditions, the concentrations of components are considered constant over the brief linear domain, and permits the following derivation:

$for\ rate\ law\ of\ the\ form\ r = k[A]^n[B]^m$

$vary\ [A]\ holding\ B = B^0\ constant$

$for\ concentrations\ [A_1] \neq [A_2]$:

$r_1 = k[A_1]^n[B^0]^m$

$r_2 = k[A_2]^n[B^0]^m$

$$\rightarrow \frac{r_1}{r_2} = \frac{k[A_1]^n[B^0]^m}{k[A_2]^n[B^0]^m} = \frac{[A_1]^n}{[A_2]^n} = \left(\frac{[A_1]}{[A_2]}\right)^n$$

$$\rightarrow \ln\left(\frac{r_1}{r_2}\right) = \ln\left(\frac{[A_1\}}{[A_2]}\right)^n = n \cdot \ln\left(\frac{[A_1]}{[A_2]}\right)$$

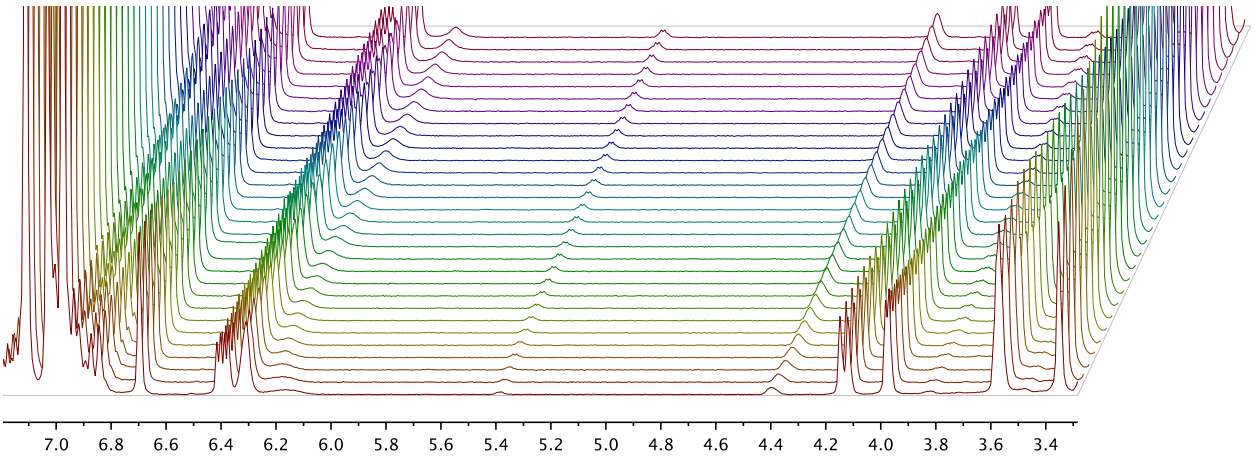
$$\rightarrow n = \frac{\ln\left(\frac{r_1}{r_2}\right)}{\ln\left(\frac{[A_1]}{[A_2]}\right)} \equiv reaction\ order\ with\ respect\ to\ reagent\ A$$

Four experiments were designed to probe the three components of the reaction:

1) 0.020 mmol **S3** with 0.05 equivalents **CPA** and 0.1 equivalents **urea**
2) 0.020 mmol **S3** with 0.025 equivalents **CPA** and 0.1 equivalents **urea**
3) 0.020 mmol **S3** with 0.05 equivalents **CPA** and 0.05 equivalents **urea**
4) 0.040 mmol **S3** with 0.025 equivalents **CPA** and 0.05 equivalents **urea**

Experiment 1 functions as the baseline control; all other experiments are compared to experiment 1. Experiment 2 probes the reaction order of **CPA**. Experiment 3 probes the reaction order of the **urea**. Experiment 4 probes the reaction order of the substrate **S3**. Reaction volume is constant (1 mL of toluene-d_8) producing constant concentrations of the un-probed reagents.

Representative NMR Data: Trial of 0.020 mmol **S3** with 0.025 equiv **CPA A** and 0.1 equiv **urea**

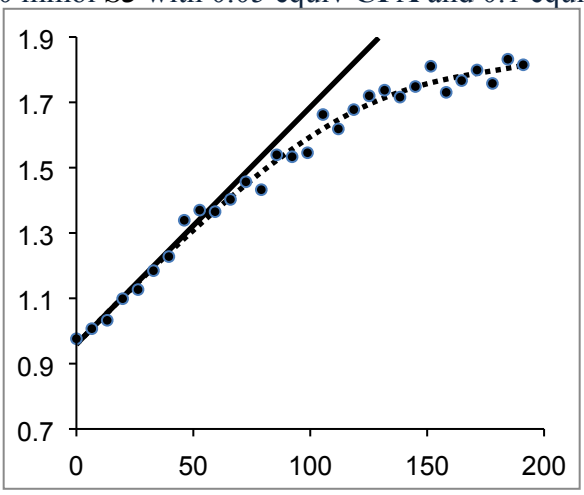


Representative Integration Curves:

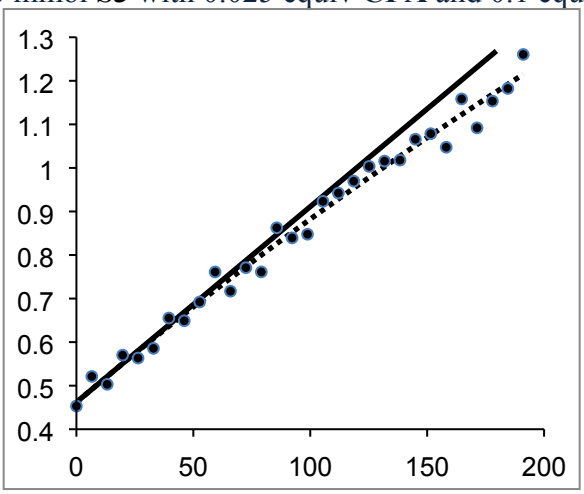
Dotted lines are polynomial fits, solid lines are extracted linear fits of linear domains

Vertical axes are [product **1o**] (mM); horizontal axes are time (s).

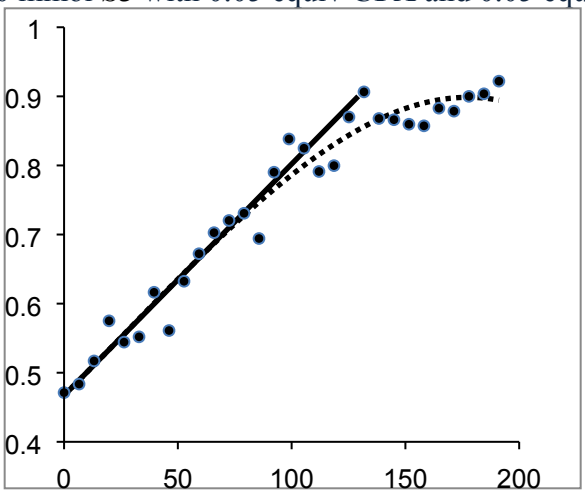
1) 0.020 mmol **S3** with 0.05 equiv **CPA** and 0.1 equiv **urea**



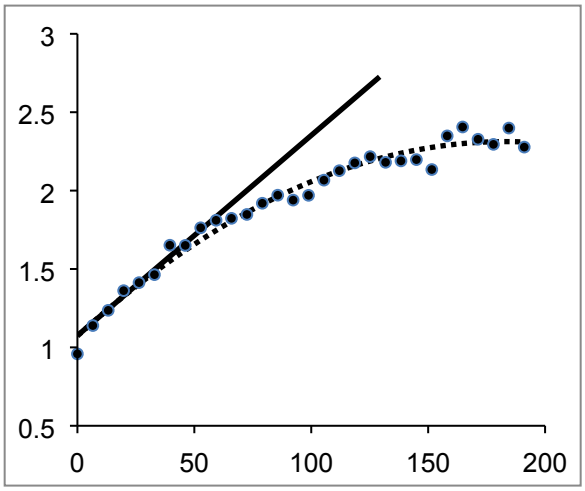
2) 0.020 mmol **S3** with 0.025 equiv **CPA** and 0.1 equiv **urea**



3) 0.020 mmol **S3** with 0.05 equiv **CPA** and 0.05 equiv **urea**



4) 0.040 mmol **S3** with 0.025 equiv **CPA** and 0.05 equiv **urea**



Raw Slope Data:

Experiment 1

Trial	**Slope**
1	0.0077169
2	0.0072575
3	0.0070965
4	0.0057761
Avr:	0.0069618

Experiment 3

Trial	**Slope**
1	0.0029104
2	0.0032138
3	0.0040785
4	0.0033492
Avr:	0.0033880

Experiment 2

Trial	**Slope**
1	0.0039595
2	0.0060217
3	0.0044901
4	0.0050888
Avr:	0.0048900

Experiment 4

Trial	**Slope**
1	0.017940
2	0.0094425
3	0.012770
4	0.013972
Avr:	0.013531

Data Analysis:

*Determination of Reaction Order of **CPA** with respect to **S3** and **urea**:*

$$\frac{\ln\left(\frac{r_{exp1}}{r_{exp2}}\right)}{\ln\left(\frac{[CPA_{exp1}]}{[CPA_{exp2}]}\right)} = \frac{\ln\left(\frac{0.0069618}{0.0048900}\right)}{\ln(2)} = 0.50963 \approx 0.5$$

*Determination of Reaction Order of **urea** with respect to **CPA A** and **S3**:*

$$\frac{\ln\left(\frac{r_{exp1}}{r_{exp3}}\right)}{\ln\left(\frac{[urea_{exp1}]}{[urea_{exp3}]}\right)} = \frac{\ln\left(\frac{0.0069618}{0.0033880}\right)}{\ln(2)} = 1.0390 \approx 1$$

*Determination of Reaction Order of **S3** with respect to **urea** and **CPA A**:*

$$\frac{\ln\left(\frac{r_{exp1}}{r_{exp4}}\right)}{\ln\left(\frac{[1o_{exp1}]}{[1o_{exp4}]}\right)} = \frac{\ln\left(\frac{0.0069618}{0.013531}\right)}{\ln(0.5)} = 0.95874 \approx 1$$

Complete Authorship of Gaussian 09

Gaussian 09, Revision **D.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

General Computational Procedure

Manual, exhaustive conformation searches were performed to locate all relevant structures. All conformers were optimized using the Gaussian 09 computational package (see above reference) using PBE[5]-D3BJ[6]/6-31G(d)[7] with implicit solvent modelled using SMD[8] (Solvation Model based on Density) for toluene. Minima were confirmed with vibrational frequency computations, with ground state structures having zero imaginary vibrational frequencies and transition states having one imaginary vibrational frequency.

All results discussed in the manuscript are at the following level of theory. Single point electronic energies were obtained at the PBE/def2-TZVPP[9, 10] level of theory with ORCA 4.0.1.[11] Solvation

corrections were computed using PBE-D3BJ/6-311++G(2df,p)[12, 13] in toluene using SMD. Final free energies were calculated by adding the ORCA single point energies, solvation free energies, and the thermal correction to Gibbs free energy obtained from the vibration frequency calculations. All three-dimensional images were generated with CYLview.[14]

Assembly Model Systems

The transition state model proposed in our initial report[2] leading to the major product could not be located computationally. To rationalize this outcome, we computed model systems to identify critical interactions for the assembly of the substrate, catalyst, and co-catalyst. We used the spirocycle (see **Figure 3**) to avoid the reactive oxocarbenium uncontrollably collapsing to either the spirocycle or the phosphate-ketal (analogous to **Major-TS**, **II**, and **I** in **Figure 7**, respectively). We identified four important observations, all summarized in **Figure S1**: (1) π-π interactions are worth ~3-4 kcal/mol, (2) urea-substrate interactions are weak (ΔG = 24.9 kcal/mol), (3) urea-phosphate interactions are moderate (ΔG = –2.1 kcal/mol), and (4) substrate-phosphate interactions are strong (ΔG = –69.3 kcal/mol).

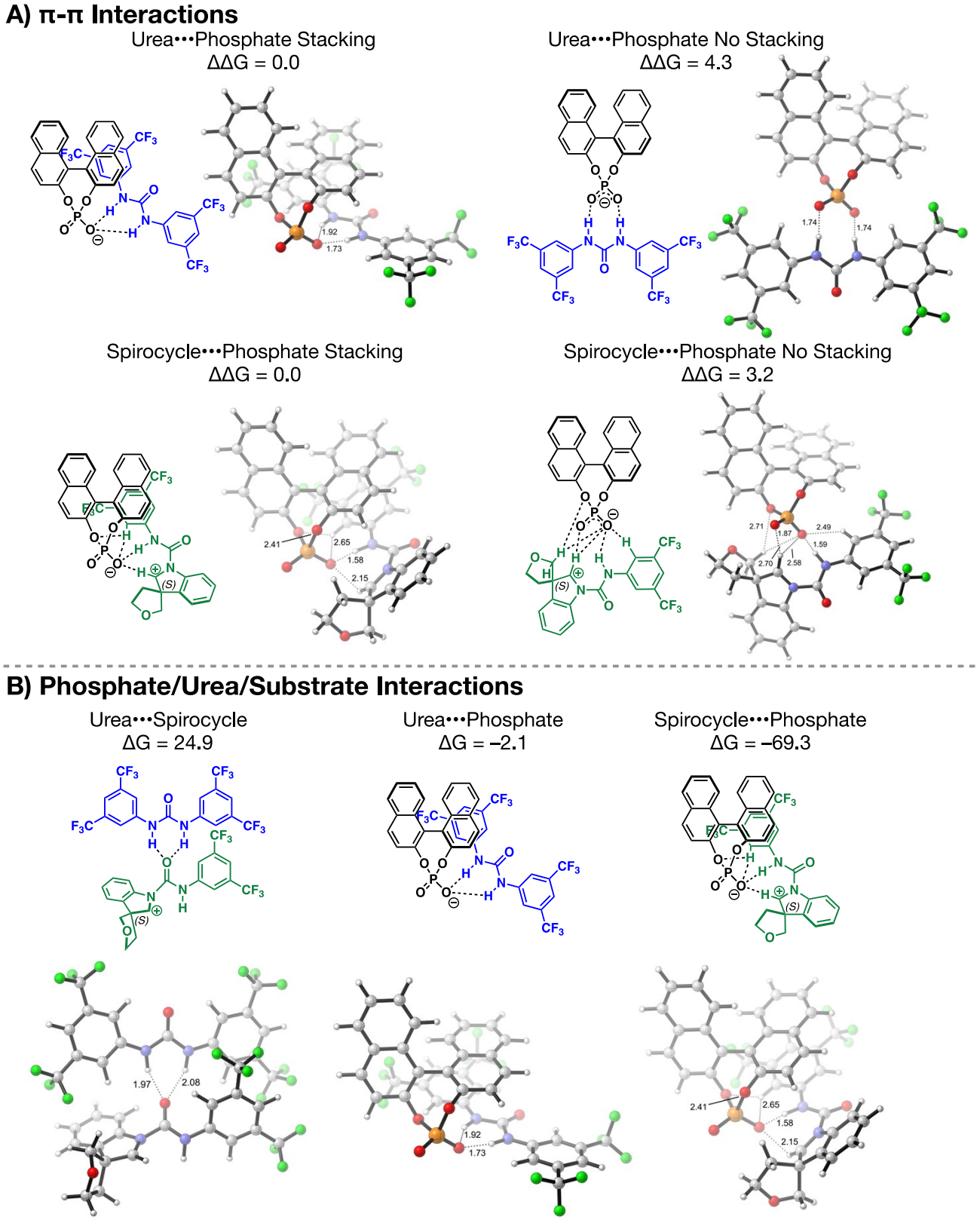


Figure S1. Model systems for the assembly of the catalyst, co-catalyst, and substrate. Energies reported in kcal/mol at PBE-D3BJ/6-31G(d)/SMD(Toluene). Distances are in Ångströms.

Rationalizing Transition State Motifs

The computed reaction coordinate diagram involving the CPA mediated process shown in Figure S2 reveals a low-energy phosphate-acetal analogous to that observed by List and co-workers.[15] We hypothesized that the spirocyclization transition state conformations are closely related to the phosphate-acetal conformations, as the size and bulkiness of the CPA and the short life-time of the oxo-carbenium ion preceding the transition state would not allow for drastic structural reorganization.

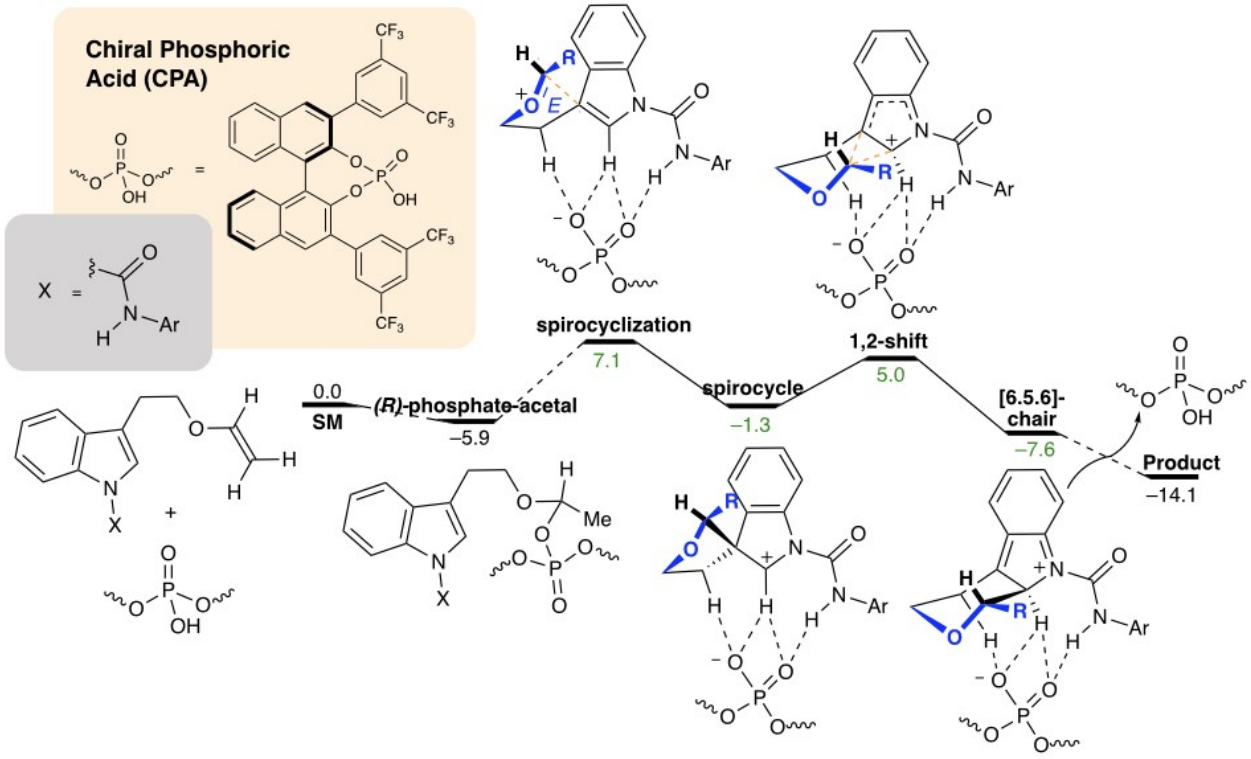


Figure S2. Reaction coordinate diagram of CPA-mediated process. Energies reported in kcal/mol at PBE-D3BJ/6-311++G(2df,p)//PBE-D3BJ/3-21G(d) with PBE-D3BJ/6-31+G(d,p)/SMD(Toluene) solvation corrections.

We performed a manual conformational search of both the *(R)*- and *(S)*-phosphate-acetal intermediates and optimized the structures using quantum mechanics. Three observations appear important: (1) The acetal favors stacking arrangements between the CPA aryl substituent and the top π-face of the substrate (Figure S3, top). (2) This is favored by 0.9 kcal/mol compared to the conformation in which the CPA aryl is in close proximity to the bottom face of the substrate (Figure S3, middle). (3) We also explored the torsions around the substrate carboxamide and

discovered that the *syn*-orientation between the carbonyl and the indole benzene group is favored over the *anti*-orientation (Figure S3, top vs. bottom) by 8.1 kcal/mol.

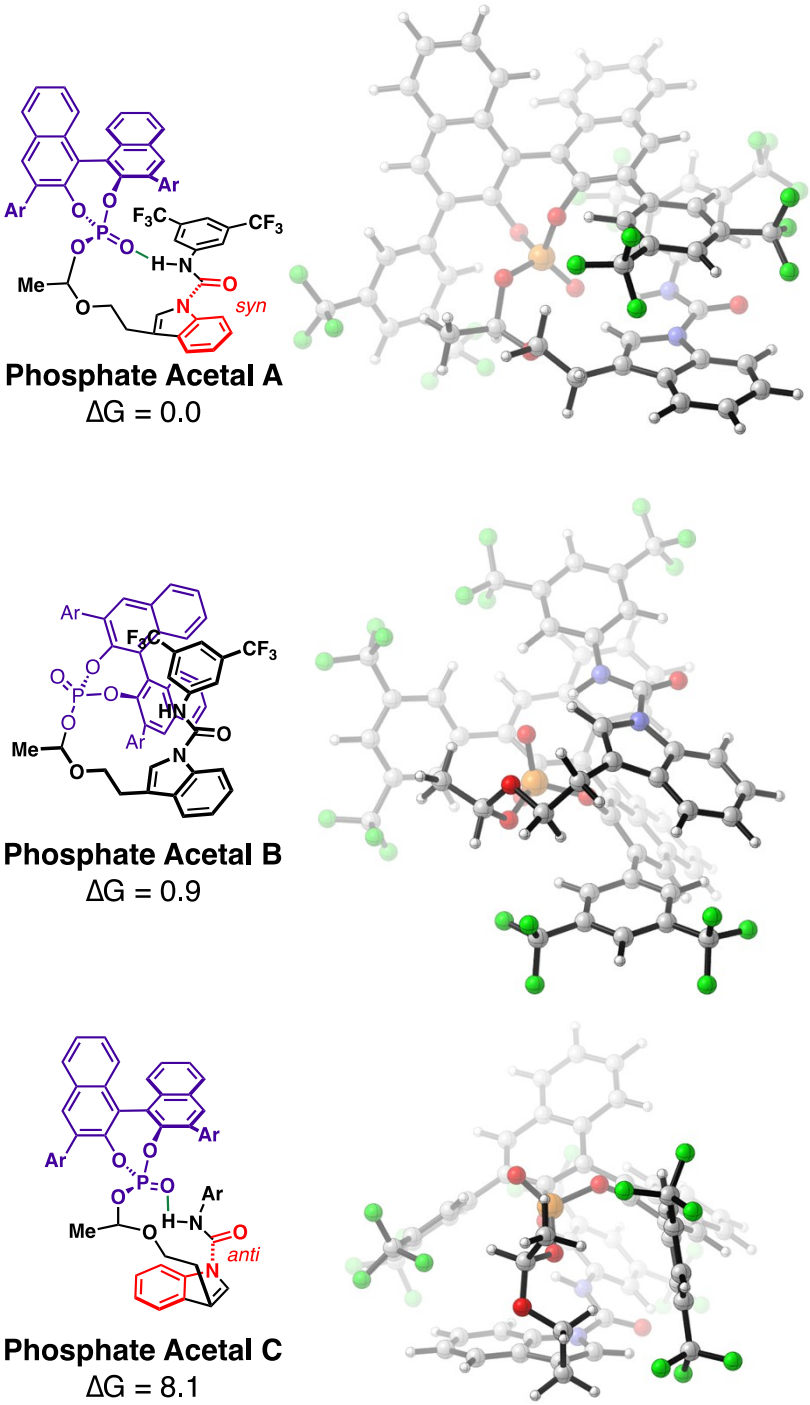


Figure S3. Three representative phosphate acetal conformations. Energies reported in kcal/mol at PBE/def2-TZVPP//PBE-D3BJ/6-31G(d)/SMD(toluene) with PBE-D3BJ/6-311++G(2df,p)/SMD(toluene) solvation corrections.

In order to deduce the binding motif of the urea to the CPA-mediated spirocyclization transition state, we coordinated the urea to the two exposed oxygens of the system: (1) the substrate carbonyl oxygen or (2) one of the CPA phosphate oxygens. Spirocyclization transition states involving the urea coordination to the substrate carbonyl oxygen was 5.6 kcal/mol disfavored compared to the transition state where the urea coordinates to the exposed CPA phosphate oxygen (Figure S4).

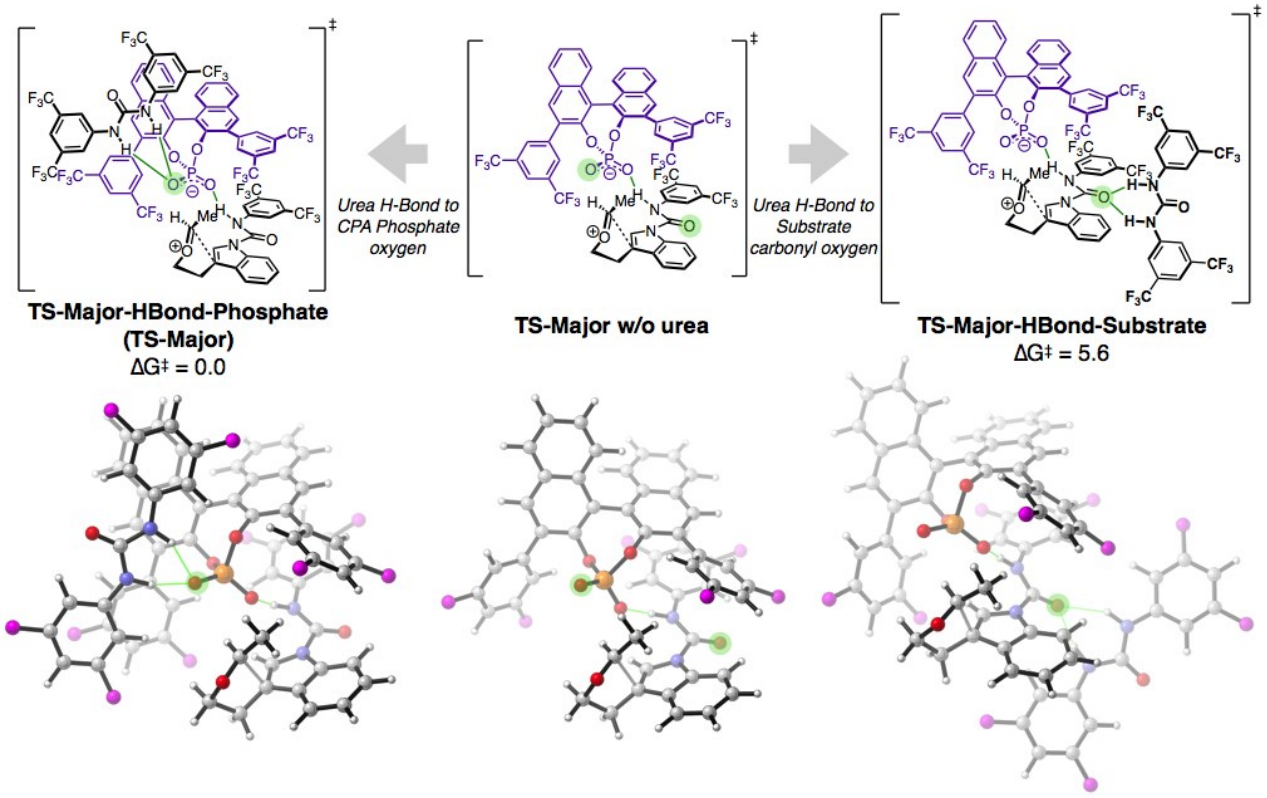


Figure S4. The two binding motifs of urea to the spirocyclization transition state. Energies reported in kcal/mol at PBE/def2-TZVPP//PBE-D3BJ/6-31G(d)/SMD(toluene) with PBE-D3BJ/6-311++G(2df,p)/SMD(toluene) solvation corrections.

Origins of Stereoselectivity Model System

The origins of stereoselectivity involve the differential interactions between the substrate aryl group and the CPA naphthyl & aryl groups found in the major and minor transition states. To probe these interactions, we computed model systems involving these groups in the exact geometry as found in the transition states. The model complex from the **Major-TS** was favored by 4.6 kcal/mol over that from the **Minor-TS**.

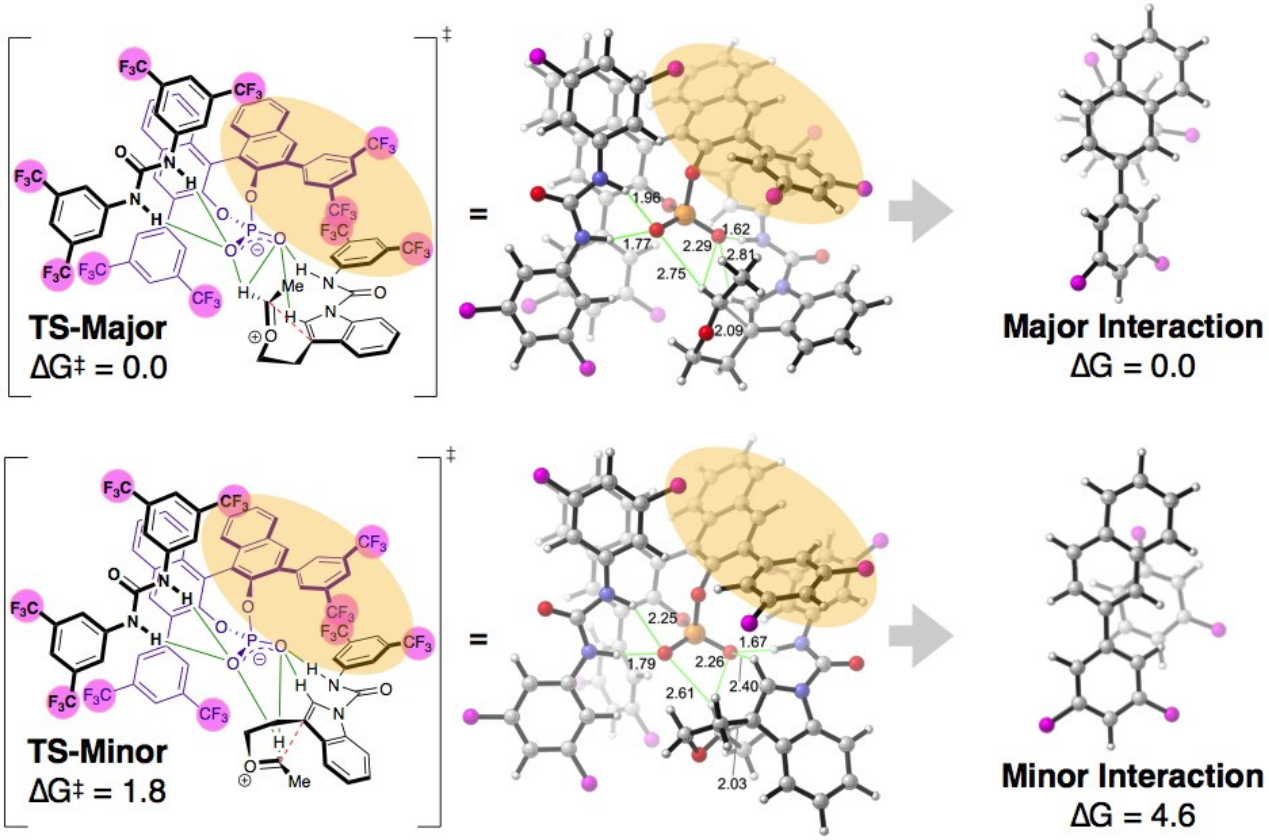


Figure S5. Two model complexes of substrate aryl group and the CPA naphthyl & aryl groups as found in the **Major-TS** and **Minor-TS**. The geometries of all atoms are as found in the transition states, except for the capping hydrogen atoms, which were quantum mechanically optimized. Energies reported in kcal/mol at PBE/def2-TZVPP//PBE-D3BJ/6-31G(d)/SMD(toluene) with PBE-D3BJ/6-311++G(2df,p)/SMD(toluene) solvation corrections. Distances are in Ångströms.

Computed Geometries, Energies, and Thermal & Dispersion & Solvation Corrections

Major-TS

```
---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
===========================================================================
 #pbepbe/6-31G(d)/auto EmpiricalDispersion=GD3BJ
 scf=(maxcycle=300,direct,tight) density=current
 opt=(maxcycle=250,modredundant) iop(1/8=18) Temperature=233.15
 SCRF=(SMD,SOLVENT=Toluene)
 Modredundant Input:  B       7      11 F
 Modredundant Input:
--link 1--
#pbepbe/6-31G(d)/auto EmpiricalDispersion=GD3BJ
 scf=(direct,tight,maxcycle=300,xqc)
 opt=(nofreeze,maxcycle=250,ts,calcfc,noeigentest) iop(1/8=18) freq=noraman
 Temperature=233.15 geom=check guess=read SCRF=(SMD,SOLVENT=Toluene)
 #P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
 Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C74H41F30N4O7P   C1[X(C74H41F30N4O7P)]  #Atoms= 157
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -6920.22890162       Predicted Change= -1.481149D-08
===========================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00003 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00360 ||  0.00180   [ NO ]       0.00360 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
      Atomic              Coordinates (Angstroms)
       Type              X              Y         Z
---------------------------------------------------------------------------
      C       -3.335358      -4.902524      -0.881305
      C       -4.620895      -4.969170      -1.427032
      C       -4.773432      -5.760836      -2.572443
      C       -3.684084      -6.453312      -3.140417
      C       -2.400296      -6.369142      -2.584145
      C       -2.221072      -5.580177      -1.438824
      C       -1.026423      -5.194652      -0.667392
      C        0.234091      -6.038624      -0.543625
      C        1.412104      -5.303670      -1.226213
      O        0.814727      -4.625293      -2.352288
      C       -0.109031      -3.766965      -1.892940
      C       -1.529799      -4.365194       0.377742
      N       -2.857322      -4.157320       0.228590
      C       -3.704903      -3.325626       1.094124
      N       -3.000131      -2.269141       1.571892
      C       -3.510770      -1.247416       2.407330
      O       -4.868808      -3.644510       1.300008
      C       -4.838402      -0.795444       2.345682
      C       -5.206491       0.332670       3.092206
      C       -6.600490       0.874593       2.904881
      F       -7.545940      -0.081566       3.102176
      F       -6.875583       1.910858       3.735990
```

F	-6.780337	1.335023	1.621726
C	-4.290038	0.992915	3.921975
C	-2.980580	0.503420	4.002866
C	-1.955801	1.144588	4.904598
F	-1.548470	0.278733	5.877419
F	-0.832885	1.498556	4.212228
F	-2.425821	2.257684	5.521551
C	-2.586974	-0.607560	3.249061
C	-1.031236	-3.182327	-2.897381
H	0.207587	-3.111250	-1.071258
H	1.865867	-4.565018	-0.544517
H	2.190690	-5.970898	-1.618036
H	-1.365009	-3.918846	-3.642267
H	-0.501052	-2.359846	-3.414405
H	-1.892209	-2.727976	-2.385438
H	-5.458744	-4.435704	-0.978371
H	-5.763041	-5.839124	-3.032467
H	-3.844405	-7.065292	-4.033271
H	-1.555862	-6.897191	-3.038634
H	0.481486	-6.237554	0.511526
H	0.059152	-7.008693	-1.036764
H	-0.986941	-3.928160	1.214523
H	-2.152651	-1.979037	1.015377
H	-5.557661	-1.294269	1.692727
H	-4.586091	1.881410	4.481706
H	-1.564054	-0.989721	3.311220
C	-3.738065	3.311787	1.158061
C	-4.151166	2.497448	0.073461
C	-3.256211	1.699215	-0.628492
C	-3.751137	0.715109	-1.622651
C	-1.873193	1.775150	-0.270141
O	-0.970934	1.013648	-1.012319
C	-1.393917	2.592437	0.755267
C	0.054483	2.597490	1.112855
C	-2.348156	3.340965	1.536906
C	0.682798	1.389158	1.415912
O	-0.046329	0.215120	1.230428
P	-0.250015	-0.327731	-0.329692
C	2.014172	1.293345	1.940399
C	2.635789	-0.007405	2.301572
C	2.713329	2.489159	2.089039
C	2.172769	3.740540	1.695149
C	0.823969	3.810914	1.193396
C	-1.990101	4.061773	2.712341
C	-2.945019	4.743879	3.449976
C	-4.306589	4.744425	3.052652
C	-4.694263	4.034512	1.929733
C	2.954652	4.930448	1.763631
C	2.440551	6.141229	1.335093
C	1.118591	6.206122	0.824328
C	0.325923	5.071201	0.757932
C	-3.083099	0.453524	-2.836923
C	-3.546430	-0.547946	-3.697494
C	-2.821529	-0.821056	-4.991356
F	-1.518901	-0.424269	-4.941805
F	-3.395010	-0.179131	-6.045414

F	-2.826554	-2.153780	-5.292038
C	-4.693451	-1.294580	-3.388848
C	-5.383297	-1.007337	-2.206083
C	-6.649399	-1.747956	-1.860007
F	-6.663923	-2.139031	-0.548699
F	-6.812756	-2.872393	-2.612826
F	-7.753418	-0.975121	-2.046631
C	-4.916985	-0.018382	-1.328373
C	1.860017	-1.126981	2.672650
C	2.456207	-2.361496	2.947049
C	1.579661	-3.566666	3.145119
F	1.454828	-4.282588	1.969449
F	0.306043	-3.235916	3.512961
F	2.066467	-4.430291	4.066883
C	3.848198	-2.509623	2.935396
C	4.630839	-1.390877	2.621470
C	6.134134	-1.513280	2.688398
F	6.764691	-0.604438	1.900813
F	6.555317	-2.754578	2.311000
F	6.585094	-1.318764	3.961668
C	4.038890	-0.167672	2.279972
O	-1.186280	-1.514685	-0.201643
O	1.040587	-0.495659	-1.109290
H	-5.212699	2.477957	-0.191592
H	3.721173	2.480092	2.517152
H	-0.953261	4.048691	3.052064
H	-2.644376	5.276183	4.357926
H	-5.049493	5.287312	3.645637
H	-5.747190	3.987013	1.632748
H	3.981401	4.859958	2.139147
H	3.057815	7.044118	1.362447
H	0.732723	7.158550	0.448724
H	-0.673744	5.127826	0.321530
H	-2.198588	1.030737	-3.107468
H	-5.034925	-2.093675	-4.050817
H	-5.448919	0.169123	-0.391177
H	0.778341	-1.037806	2.732685
H	4.313962	-3.474818	3.146366
H	4.681483	0.658661	1.966213
C	3.728910	1.549118	-1.589915
N	3.724015	0.205973	-1.221763
H	2.790932	-0.218248	-1.087994
C	4.799572	-0.666789	-1.114787
N	2.419327	1.985653	-1.775266
H	1.689599	1.261423	-1.693989
C	1.974899	3.263383	-2.106869
C	6.149821	-0.291209	-1.277104
H	6.393717	0.747082	-1.503799
C	7.150243	-1.259353	-1.133535
C	8.594353	-0.829815	-1.180389
F	8.781618	0.273798	-1.952149
F	9.400696	-1.814009	-1.669888
F	9.056465	-0.527040	0.068439
C	6.854332	-2.594498	-0.827620
H	7.650554	-3.329778	-0.697801
C	5.510231	-2.954156	-0.661162

C	5.140024	-4.376643	-0.339624
F	4.104980	-4.445053	0.559511
F	6.173763	-5.078483	0.186109
F	4.713924	-5.057208	-1.449497
C	4.491905	-2.008915	-0.801078
H	3.445735	-2.295620	-0.654549
C	0.614633	3.386900	-2.456817
H	-0.013589	2.493495	-2.474570
C	0.065258	4.638542	-2.739134
C	-1.418028	4.736630	-2.975106
F	-2.111481	4.825627	-1.795734
F	-1.909286	3.639776	-3.623655
F	-1.752901	5.829811	-3.709675
C	0.852867	5.796112	-2.689980
H	0.419005	6.777709	-2.892303
C	2.205568	5.663379	-2.344413
C	3.058374	6.903766	-2.263005
F	2.345153	7.969837	-1.789200
F	3.545815	7.273057	-3.481923
F	4.128368	6.740561	-1.438183
C	2.780522	4.419698	-2.057180
H	3.828710	4.336144	-1.771293
O	4.738854	2.248416	-1.727609

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -6920.22890162	Predicted Change= -1.481149D-08	
Zero-point correction (ZPE)=	-6919.2023	1.02654
Internal Energy (U)=	-6919.1370	1.09186
Enthalpy (H)=	-6919.1363	1.09260
Gibbs Free Energy (G)=	-6919.3025	0.92634

Frequencies -- -199.7633 7.3824 8.8960

PBE-D3BJ/6-311++G(2df,p) = -6922.424226
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -6922.472199
PBE/def2-TZVPP = -6921.71127898996

Minor-TS

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#pbepbe/6-31G(d)/auto EmpiricalDispersion=GD3BJ
scf=(maxcycle=300,direct,tight) density=current
opt=(maxcycle=250,modredundant) iop(1/8=18) Temperature=233.15
SCRF=(SMD,SOLVENT=Toluene)
Modredundant Input: B 76 80 F
Modredundant Input:
--link 1--
#pbepbe/6-31G(d)/auto EmpiricalDispersion=GD3BJ
scf=(direct,tight,maxcycle=300,xqc)
opt=(nofreeze,maxcycle=250,ts,calcfc,noeigentest) iop(1/8=18) freq=noraman
Temperature=233.15 geom=check guess=read SCRF=(SMD,SOLVENT=Toluene)
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto

Freq

Pointgroup= C1 Stoichiometry= C74H41F30N4O7P C1[X(C74H41F30N4O7P)] #Atoms= 157
Charge = 0 Multiplicity = 1

SCF Energy= -6920.21944687 Predicted Change= -4.220356D-09

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Optimization completed. {Found 3 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00138	0.00180	[YES]	0.00138	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.360549	-3.378982	1.522752
C	3.841983	-2.541234	0.486507
C	3.031591	-1.614198	-0.165287
C	3.618129	-0.725523	-1.202838
C	1.648168	-1.583833	0.216376
O	0.804049	-0.693530	-0.446861
C	1.087476	-2.472721	1.136122
C	-0.390832	-2.534700	1.329456
C	1.966165	-3.339915	1.877445
C	-1.109920	-1.390880	1.677192
O	-0.414588	-0.183275	1.783729
C	-2.503576	-1.407756	2.005713
C	-3.208070	-0.235739	2.590684
C	-3.173055	-2.619716	1.861768
C	-2.525034	-3.795640	1.403851
C	-1.108649	-3.771419	1.141266
C	1.523032	-4.144955	2.965029
C	2.406042	-4.971468	3.641002
C	3.772573	-5.038078	3.264739
C	4.239928	-4.250956	2.227968
C	-3.258755	-4.997825	1.184535
C	-2.628118	-6.137956	0.720146
C	-1.235519	-6.111872	0.450751
C	-0.493295	-4.959160	0.652169
C	4.985647	-0.377785	-1.130758
C	5.578484	0.442962	-2.098127
C	7.021049	0.864614	-1.953547
F	7.640697	0.951270	-3.161365
F	7.734867	0.006117	-1.180808
F	7.117509	2.100082	-1.374520
C	4.824853	0.964234	-3.157000
C	3.468386	0.624124	-3.237645
C	2.649990	1.193441	-4.367565
F	2.805900	2.551973	-4.445817
F	1.313222	0.960733	-4.206513
F	3.006785	0.687921	-5.574823
C	2.873063	-0.218338	-2.290780
C	-3.023668	1.086429	2.139859
C	-3.680851	2.151728	2.769370
C	-3.356830	3.564459	2.360298
F	-2.265322	4.035894	3.045355

F	-4.374644	4.424115	2.608391
F	-3.039748	3.664332	1.034012
C	-4.560543	1.931442	3.835670
C	-4.770549	0.616542	4.269526
C	-5.758069	0.350007	5.378178
F	-5.807676	1.379885	6.267640
F	-5.449780	-0.778348	6.074015
F	-7.022033	0.184810	4.893307
P	0.012219	0.544094	0.356616
O	-1.164535	0.840211	-0.562142
C	-4.095795	-0.451336	3.665766
O	0.927715	1.683491	0.761319
H	4.892450	-2.642699	0.196395
H	-4.246111	-2.667079	2.076926
H	0.476494	-4.093714	3.274858
H	2.046188	-5.573569	4.481396
H	4.456022	-5.699503	3.806496
H	5.296945	-4.270448	1.939961
H	-4.336948	-4.992811	1.378530
H	-3.202254	-7.049873	0.530360
H	-0.748983	-7.003708	0.044663
H	0.566525	-4.945790	0.391354
H	5.597181	-0.733132	-0.299355
H	5.283241	1.625575	-3.897691
H	1.819899	-0.469575	-2.400959
H	-2.383270	1.288466	1.280951
H	-5.066010	2.767378	4.324988
H	-4.233657	-1.462584	4.057516
C	2.958845	5.455772	-0.965454
C	3.801248	6.488511	-0.543294
C	3.428976	7.788085	-0.912167
C	2.260727	8.036512	-1.661368
C	1.422917	6.988741	-2.067673
C	1.779926	5.679498	-1.718630
C	1.106280	4.380305	-1.903923
C	0.128638	4.090042	-3.035282
C	-1.298376	3.962182	-2.439967
O	-1.289872	4.801108	-1.264075
C	-0.307078	4.363511	-0.452886
H	-0.299969	3.279800	-0.266557
C	2.014962	3.428468	-1.347349
N	3.041110	4.054460	-0.730972
C	4.063848	3.425471	0.116777
N	3.537242	2.392017	0.825402
C	4.226188	1.518471	1.690378
O	5.205482	3.866814	0.129165
C	3.435290	0.792340	2.602373
C	4.028208	-0.162021	3.432429
C	3.176853	-0.884933	4.448435
F	3.157860	-0.219277	5.639717
F	3.647344	-2.135116	4.700990
F	1.885377	-1.000408	4.037818
C	5.400995	-0.427775	3.351048
C	6.174706	0.302749	2.438572
C	7.611775	-0.097937	2.223082
F	8.214099	-0.490036	3.377534

F	8.356794	0.897276	1.682488
F	7.680951	-1.165710	1.363083
C	5.611020	1.289270	1.618246
C	0.020267	5.239971	0.705149
H	0.400177	3.171224	-3.575735
H	0.169651	4.923264	-3.755576
H	-2.094712	4.336477	-3.096936
H	-1.507980	2.918918	-2.143500
H	-0.756682	5.088034	1.476131
H	0.049631	6.304537	0.428737
H	0.980073	4.939600	1.154310
H	1.928483	2.344213	-1.319232
H	4.709451	6.286916	0.027052
H	4.064779	8.626636	-0.612730
H	2.005660	9.065542	-1.931985
H	0.510364	7.186683	-2.638830
H	2.507921	2.218496	0.790129
H	2.355831	0.961867	2.638693
H	5.856642	-1.200941	3.974155
H	6.227443	1.839329	0.907090
C	-3.475301	-1.543524	-1.807193
N	-3.642628	-0.252099	-1.322132
H	-2.787394	0.236715	-1.007381
C	-4.790012	0.535085	-1.421596
N	-2.131330	-1.918883	-1.756739
H	-1.458862	-1.196947	-1.474962
C	-1.586028	-3.135720	-2.171369
C	-6.068934	0.028239	-1.730190
H	-6.194199	-1.039217	-1.912189
C	-7.153770	0.910252	-1.821974
C	-8.521834	0.335367	-2.094264
F	-9.083449	-0.172922	-0.958736
F	-8.474517	-0.682176	-2.997056
F	-9.384019	1.271183	-2.579167
C	-7.005665	2.287335	-1.617875
H	-7.857964	2.963353	-1.710799
C	-5.729421	2.780531	-1.308382
C	-5.548724	4.255130	-1.054176
F	-4.284639	4.677325	-1.347600
F	-5.781284	4.578376	0.249477
F	-6.407251	5.002924	-1.802925
C	-4.633534	1.921502	-1.202221
H	-3.646136	2.319729	-0.956379
C	-0.185162	-3.206992	-2.306612
H	0.417439	-2.319235	-2.108003
C	0.434282	-4.406687	-2.666479
C	1.937278	-4.481193	-2.664990
F	2.514306	-3.293620	-3.006921
F	2.407135	-5.426037	-3.521878
F	2.419017	-4.803357	-1.422713
C	-0.319914	-5.562276	-2.902264
H	0.166551	-6.505222	-3.162273
C	-1.712908	-5.483339	-2.763132
C	-2.529256	-6.734135	-2.969696
F	-2.705558	-7.019953	-4.290995
F	-1.913449	-7.822565	-2.415138

F	-3.764966	-6.645770	-2.409962
C	-2.356558	-4.293714	-2.408464
H	-3.437619	-4.256643	-2.285922
O	-4.384816	-2.266916	-2.226519

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy=	-6920.21944687	Predicted Change= -4.220356D-09
Zero-point correction (ZPE)=	-6919.1915	1.02793
Internal Energy (U)=	-6919.1263	1.09310
Enthalpy (H)=	-6919.1256	1.09384
Gibbs Free Energy (G)=	-6919.2913	0.92807

Frequencies -- -254.2220 8.5187 9.4926

PBE-D3BJ/6-311++G(2df,p) = -6922.416415
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -6922.464816
PBE/def2-TZVPP = -6921.70843617253

Urea•••Phosphate Stacking/Urea•••Phosphate

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(verytight,maxcycle=250,gdiis)
freq=noraman iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C37H20F12N2O5P(1-) C1[X(C37H20F12N2O5P)] #Atoms= 77
Charge = -1 Multiplicity = 1

SCF Energy= -3444.05547806 Predicted Change= -1.295514D-12

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00000	[YES]	0.00000	0.00000	[YES]
Displ	0.00006	0.00000	[NO]	0.00006	0.00000	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.000833	-2.895170	0.829497
C	-4.973632	-3.271065	-0.543564
C	-3.832153	-3.092453	-1.297837
C	-2.685063	-2.492228	-0.719065
O	-1.611791	-2.257944	-1.552219
C	-2.672137	-2.035579	0.604401
C	-1.468277	-1.337992	1.127985
C	-3.830456	-2.293644	1.422609
C	-0.214184	-1.945831	0.996799
O	-0.100103	-3.159470	0.343065
P	-0.136144	-3.081847	-1.345101

C	0.962907	-1.370142	1.537262
C	0.905690	-0.139040	2.159440
C	-0.321930	0.579523	2.231622
C	-1.526710	-0.019202	1.709124
C	-3.866474	-1.996533	2.817175
C	-5.001631	-2.238402	3.574278
C	-6.163130	-2.794061	2.979392
C	-6.153941	-3.120717	1.634144
C	-0.371155	1.903243	2.756088
C	-1.549837	2.628148	2.754918
C	-2.730935	2.048538	2.224654
C	-2.721131	0.760108	1.717069
O	-0.194547	-4.486692	-1.857370
O	0.868957	-2.042805	-1.845477
H	-5.868934	-3.719540	-0.988525
H	1.815671	0.321698	2.559701
H	-2.975420	-1.577921	3.291504
H	-4.998191	-2.002497	4.643844
H	-7.056557	-2.975553	3.586163
H	-7.035854	-3.570318	1.162849
H	0.557256	2.346039	3.134668
H	-1.568271	3.656328	3.129295
H	-3.651521	2.638682	2.182289
H	-3.625155	0.347532	1.264710
C	1.556590	1.140451	-0.984109
N	2.433689	0.061017	-1.038458
H	2.005557	-0.854213	-1.295148
C	3.758882	0.030982	-0.629802
N	0.278253	0.739971	-1.362805
H	0.180348	-0.260482	-1.621832
C	-0.886996	1.502127	-1.333365
C	4.493002	1.171449	-0.233138
H	4.006890	2.146893	-0.245033
C	5.826410	1.028566	0.170810
C	6.567141	2.243397	0.666811
F	6.154469	3.385758	0.052591
F	7.913052	2.139485	0.467933
F	6.386346	2.432721	2.008408
C	6.463560	-0.218578	0.191540
H	7.503897	-0.313474	0.509898
C	5.727649	-1.345368	-0.205389
C	6.411933	-2.686755	-0.253897
F	5.535765	-3.719727	-0.136451
F	7.335025	-2.819302	0.743073
F	7.084351	-2.868574	-1.429315
C	4.395998	-1.233259	-0.611619
H	3.834323	-2.122606	-0.914886
C	-2.080207	0.867267	-1.741225
H	-2.044764	-0.173876	-2.072620
C	-3.297824	1.550291	-1.689788
C	-4.565690	0.797706	-1.991970
F	-5.053272	0.164499	-0.878859
F	-4.387101	-0.164669	-2.937390
F	-5.559801	1.622566	-2.432211
C	-3.364783	2.881614	-1.258211
H	-4.319237	3.412163	-1.221743

C	-2.172188	3.509663	-0.871043
C	-2.244927	4.917980	-0.344471
F	-2.802523	4.965888	0.907193
F	-3.027517	5.712744	-1.134384
F	-1.026676	5.512241	-0.254019
C	-0.941950	2.844065	-0.894555
H	-0.027654	3.339104	-0.571178
O	1.867995	2.289796	-0.642125
H	-3.780194	-3.390170	-2.348666
H	1.903699	-1.917358	1.428553

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -3444.05547806 Predicted Change= -1.295514D-12

Zero-point correction (ZPE)=	-3443.5509	0.50450
Internal Energy (U)=	-3443.5202	0.53518
Enthalpy (H)=	-3443.5195	0.53592
Gibbs Free Energy (G)=	-3443.6095	0.44597

Frequencies -- 4.9414 13.5685 18.5358

Urea•••Phosphate No Stacking

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C37H20F12N2O5P(1-) C1[X(C37H20F12N2O5P)] #Atoms= 77
Charge = -1 Multiplicity = 1

SCF Energy= -3444.04847692 Predicted Change= -6.451807D-09

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00180	0.00180	[YES]	0.00180	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.008987	-3.390678	-0.890500
C	3.837688	-3.998846	-0.355951
C	2.862210	-3.235269	0.253361
C	3.046043	-1.836038	0.387226
O	2.065424	-1.116998	1.048375
C	4.192725	-1.181367	-0.078426
C	4.307411	0.290618	0.107534
C	5.182692	-1.961572	-0.777326
C	3.257999	1.110645	-0.325077

O	2.144412	0.543464	-0.921268
P	1.032485	-0.186455	0.106844
C	3.303815	2.523159	-0.217487
C	4.407325	3.131228	0.347122
C	5.484035	2.353547	0.860486
C	5.429893	0.913983	0.761731
C	6.321804	-1.375447	-1.405317
C	7.260011	-2.154960	-2.062770
C	7.108403	-3.563487	-2.134346
C	5.998501	-4.162782	-1.564147
C	6.601125	2.968085	1.495809
C	7.620298	2.207829	2.043348
C	7.549348	0.792247	1.985244
C	6.482745	0.162971	1.363705
O	0.159395	-1.054712	-0.781887
O	0.410314	0.824372	1.054401
H	3.708717	-5.082058	-0.459281
H	4.452785	4.222776	0.431596
H	6.445687	-0.290290	-1.369885
H	8.123173	-1.676314	-2.537581
H	7.858705	-4.169660	-2.652800
H	5.853480	-5.247386	-1.631549
H	6.628321	4.062574	1.553371
H	8.470602	2.693702	2.533317
H	8.340406	0.188833	2.443338
H	6.434057	-0.928567	1.339085
H	1.936334	-3.679364	0.630335
H	2.453784	3.106752	-0.582400
C	-3.146819	0.338029	0.109334
N	-2.503614	-0.890592	0.007568
C	-3.063835	-2.159007	0.080488
N	-2.203319	1.351579	0.243715
C	-2.383177	2.717191	0.070574
C	-4.439209	-2.418694	0.271388
C	-4.881360	-3.745017	0.359901
C	-6.336638	-4.014980	0.637666
F	-7.146913	-3.020136	0.184737
F	-6.581078	-4.141999	1.977164
F	-6.759532	-5.176583	0.057339
C	-3.998673	-4.830545	0.262993
C	-2.636329	-4.559631	0.069800
C	-1.651788	-5.687639	-0.089336
F	-2.114233	-6.854603	0.443780
F	-0.459512	-5.413656	0.517928
F	-1.370319	-5.939416	-1.401113
C	-2.167142	-3.248148	-0.026350
C	-1.222327	3.519733	0.159430
C	-1.299533	4.898722	-0.047887
C	-0.023175	5.692956	0.034155
F	0.907700	5.241920	-0.865067
F	0.559658	5.600411	1.262730
F	-0.211902	7.016667	-0.223216
C	-2.521674	5.521391	-0.336159
C	-3.671214	4.719953	-0.406480
C	-4.982974	5.359576	-0.778558
F	-6.050995	4.692409	-0.262326

F	-5.161513	5.397550	-2.133698
F	-5.064151	6.651189	-0.342501
C	-3.623384	3.334164	-0.208704
O	-4.375218	0.506974	0.082417
H	-1.485142	-0.883326	-0.237643
H	-1.229752	1.076293	0.514415
H	-5.137122	-1.583325	0.336932
H	-4.362356	-5.857603	0.334975
H	-1.102825	-3.042134	-0.182023
H	-0.266106	3.037582	0.390935
H	-2.579390	6.599673	-0.495168
H	-4.524439	2.721649	-0.258580

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -3444.04847692	Predicted Change= -6.451807D-09	
Zero-point correction (ZPE)=	-3443.5446	0.50386
Internal Energy (U)=	-3443.5134	0.53501
Enthalpy (H)=	-3443.5127	0.53575
Gibbs Free Energy (G)=	-3443.6061	0.44233

Frequencies -- 10.0287 12.4657 16.7771

Spirocycle•••Phosphate Stacking/Spirocycle•••Phosphate

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C40H27F6N2O6P C1[X(C40H27F6N2O6P)] #Atoms= 82
Charge = 0 Multiplicity = 1

SCF Energy= -3038.88488633 Predicted Change= -2.177641D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00126	0.00180	[YES]	0.00126	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.481937	0.996877	-0.904431
C	-4.477222	1.893197	-1.974890
C	-5.429507	1.667334	-2.981209
C	-6.328771	0.589004	-2.910311
C	-6.303144	-0.306391	-1.827740
C	-5.369631	-0.092679	-0.812927
C	-5.051981	-0.868330	0.438134
C	-4.602812	-2.351962	0.196542

C	-4.827943	-3.022359	1.563536
O	-5.626713	-2.105654	2.355000
C	-6.179809	-1.143562	1.488628
C	-3.962981	-0.056071	1.041135
N	-3.633488	0.955899	0.255456
C	-2.522773	1.928302	0.470308
N	-1.475792	1.321565	1.061644
C	-0.195839	1.880186	1.252979
O	-2.663800	3.076592	0.064191
C	0.191905	3.131331	0.743779
C	1.522972	3.540383	0.890048
C	1.933926	4.885473	0.347418
F	1.739852	5.879185	1.262591
F	3.251182	4.915728	0.004875
F	1.216381	5.226876	-0.760066
C	2.466515	2.737733	1.543601
C	2.057046	1.503577	2.064733
C	3.062007	0.578994	2.705629
F	2.526242	-0.094798	3.758339
F	3.513827	-0.361508	1.825466
F	4.154317	1.252461	3.160595
C	0.736421	1.067904	1.925843
H	-5.271702	-2.760338	-0.578973
H	-3.885119	-3.199409	2.104258
H	-5.360991	-3.984739	1.447090
H	-7.070197	-1.508171	0.931948
H	-6.468328	-0.259863	2.081470
H	-3.566660	-2.431516	-0.160093
H	-3.502503	-0.214572	2.013507
H	-3.784159	2.734360	-2.012084
H	-5.468843	2.349215	-3.835643
H	-7.060255	0.443744	-3.710753
H	-6.998393	-1.150782	-1.785063
H	-1.517426	0.262696	1.214280
H	-0.528355	3.755021	0.214770
H	3.504619	3.063226	1.636356
H	0.432804	0.088349	2.304569
C	1.134444	1.236715	-2.141504
C	-0.265538	1.039538	-2.311987
C	-0.877130	-0.103848	-1.834766
C	-0.107147	-1.110635	-1.199694
O	-0.778229	-2.236417	-0.746448
C	1.286734	-1.023495	-1.096331
C	2.052612	-2.171739	-0.543624
C	1.922777	0.201714	-1.516494
C	1.698246	-2.702479	0.699329
O	0.647809	-2.145077	1.414989
P	-0.923354	-2.461309	0.918642
C	2.419618	-3.753542	1.313755
C	3.504166	-4.308884	0.665279
C	3.879168	-3.862844	-0.633906
C	3.136076	-2.796662	-1.262460
C	3.307920	0.458834	-1.291891
C	3.887763	1.652527	-1.690612
C	3.116179	2.655629	-2.330912
C	1.764380	2.448909	-2.544886

C	4.960772	-4.468206	-1.335721
C	5.293352	-4.068596	-2.618342
C	4.539003	-3.050077	-3.254390
C	3.488093	-2.432127	-2.595485
O	-1.701239	-1.276210	1.523630
O	-1.379785	-3.869147	1.143864
H	-0.854613	1.819157	-2.807840
H	4.076793	-5.116228	1.134846
H	3.907986	-0.290964	-0.772841
H	4.950679	1.828223	-1.494885
H	3.583553	3.599256	-2.628417
H	1.148643	3.227983	-3.008117
H	5.519075	-5.270052	-0.839020
H	6.124844	-4.545504	-3.147372
H	4.784205	-2.752520	-4.279371
H	2.909689	-1.657833	-3.104931
H	2.095657	-4.097319	2.299632
H	-1.953881	-0.266250	-1.941629

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy=	-3038.88488633	Predicted Change= -2.177641D-08
Zero-point correction (ZPE)=	-3038.2991	0.58577
Internal Energy (U)=	-3038.2703	0.61453
Enthalpy (H)=	-3038.2696	0.61527
Gibbs Free Energy (G)=	-3038.3539	0.53095

Frequencies -- 11.2682 22.0906 27.8642

Spirocycle•••Phosphate No Stacking

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C40H27F6N2O6P C1[X(C40H27F6N2O6P)] #Atoms= 82
Charge = 0 Multiplicity = 1

SCF Energy= -3038.88002972 Predicted Change= -3.474348D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00771	0.00180	[NO]	0.00771	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.943085	1.498021	-1.277439
C	-5.196082	2.685163	-1.029906

C	-3.922622	2.618622	-0.500425
C	-3.374933	1.358787	-0.158525
O	-2.104517	1.345054	0.404229
C	-4.077870	0.160102	-0.307532
C	-3.449407	-1.116151	0.128082
C	-5.375509	0.215174	-0.935337
C	-2.174513	-1.451411	-0.337561
O	-1.485475	-0.592736	-1.183358
P	-0.843513	0.810501	-0.549677
C	-1.557619	-2.689787	-0.043711
C	-2.192964	-3.598513	0.777659
C	-3.452904	-3.284656	1.361095
C	-4.086947	-2.024472	1.050348
C	-6.118092	-0.955485	-1.269563
C	-7.364188	-0.867933	-1.869258
C	-7.935926	0.394899	-2.168919
C	-7.231572	1.551605	-1.882945
C	-4.090835	-4.183122	2.263515
C	-5.294313	-3.857916	2.864601
C	-5.900446	-2.604945	2.590919
C	-5.312865	-1.712393	1.708583
O	-0.541049	1.702911	-1.732710
O	0.255190	0.531414	0.487968
H	-5.638929	3.652521	-1.292197
H	-1.716679	-4.557144	1.007600
H	-5.686777	-1.936261	-1.056075
H	-7.909165	-1.784355	-2.118720
H	-8.923267	0.450955	-2.638821
H	-7.649666	2.534710	-2.128909
H	-3.597632	-5.137595	2.480210
H	-5.771449	-4.556582	3.559502
H	-6.839150	-2.336323	3.086756
H	-5.785098	-0.745610	1.517223
H	-3.308274	3.507007	-0.327864
H	-0.586463	-2.905245	-0.493321
C	3.647799	1.383788	-0.272361
N	2.914810	2.649908	-0.002735
N	2.829093	0.315360	-0.170795
C	3.243950	-1.030263	-0.256503
C	2.344000	-2.002016	0.227207
C	2.712100	-3.352120	0.210276
C	1.747662	-4.394441	0.722237
F	0.890140	-4.812435	-0.260777
F	0.977799	-3.922564	1.738126
F	2.392120	-5.503295	1.173119
C	3.956019	-3.756256	-0.293511
C	4.834142	-2.780503	-0.780164
C	6.151806	-3.203200	-1.383365
F	7.094994	-2.228323	-1.279743
F	6.021310	-3.491838	-2.709505
F	6.647070	-4.319961	-0.782556
C	4.495943	-1.422098	-0.766579
O	4.850737	1.452107	-0.498306
C	3.478383	3.709792	0.790395
C	2.521058	4.739234	0.846636
C	1.299268	4.306062	0.071369

C	-0.002001	4.123001	1.007871
H	-0.206839	3.076136	1.279725
C	0.749546	5.264221	-1.036262
H	0.553810	4.692941	-1.957148
H	1.461316	6.073286	-1.260377
H	0.190732	4.718877	1.922999
C	1.720308	2.983396	-0.456096
C	4.716335	3.774743	1.430193
C	4.982225	4.947192	2.155234
C	4.042626	5.989886	2.229643
C	2.799981	5.894033	1.579164
H	1.797622	0.457968	0.089692
H	1.376364	-1.686161	0.630609
H	4.241929	-4.810410	-0.290091
H	5.200697	-0.674130	-1.128640
H	1.105689	2.357997	-1.131377
H	5.445656	2.966613	1.356092
H	5.942773	5.046378	2.669144
H	4.282728	6.891727	2.800670
H	2.072400	6.709365	1.644713
O	-1.087876	4.628062	0.273236
C	-0.582916	5.756175	-0.441944
H	-1.327818	6.035978	-1.202160
H	-0.419347	6.616934	0.241481

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3038.88002972 Predicted Change= -3.474348D-08
Zero-point correction (ZPE)= -3038.2943 0.58566
Internal Energy (U)= -3038.2653 0.61464
Enthalpy (H)= -3038.2646 0.61538
Gibbs Free Energy (G)= -3038.3530 0.52698

Frequencies -- 2.7265 6.5216 12.9262

Urea•••Spirocycle

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C37H23F18N4O3(1+) C1[X(C37H23F18N4O3)] #Atoms= 85
Charge = 1 Multiplicity = 1

SCF Energy= -3661.81664142 Predicted Change= -4.372931D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.07934	0.00180	[NO]	0.07934	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.005213	-2.526831	-1.413894
C	-2.841139	-1.685981	-2.518581
C	-3.996103	-1.420489	-3.267431
C	-5.240637	-1.977759	-2.918506
C	-5.373130	-2.833018	-1.812527
C	-4.235723	-3.109722	-1.053399
C	-4.042787	-3.929446	0.195093
C	-4.525672	-5.423385	0.193399
C	-5.290086	-5.576450	1.536434
O	-4.884361	-4.464539	2.350206
C	-4.832627	-3.374929	1.483559
C	-2.599349	-3.761463	0.456482
N	-2.035084	-2.966526	-0.448120
C	-0.691445	-2.385987	-0.349931
N	0.234462	-3.216919	0.173133
C	1.541118	-2.774519	0.551451
O	-0.530911	-1.219975	-0.704209
C	2.653706	-3.537309	0.180918
C	3.931645	-3.111880	0.574244
C	5.123359	-3.943754	0.151105
F	5.091751	-5.165303	0.755449
F	6.298091	-3.355246	0.465269
F	5.104625	-4.165970	-1.190284
C	4.098310	-1.939905	1.317601
C	2.969841	-1.185141	1.672709
C	3.152033	0.073354	2.494763
F	3.322280	-0.226326	3.810554
F	2.072669	0.894673	2.400868
F	4.244090	0.767256	2.091085
C	1.687263	-1.595320	1.300825
H	-5.044110	-6.496230	2.086990
H	-6.382619	-5.539998	1.361652
H	-5.827533	-3.064980	1.105287
H	-4.348338	-2.522488	1.983965
H	-3.672192	-6.116092	0.123549
H	-5.171733	-5.597254	-0.680794
H	-2.046473	-4.130039	1.323496
H	-1.878582	-1.244494	-2.780578
H	-3.924870	-0.757947	-4.134162
H	-6.122916	-1.736170	-3.517519
H	-6.345449	-3.261738	-1.552198
H	0.044112	-4.222159	0.192475
H	2.534194	-4.442328	-0.422903
H	5.098202	-1.597209	1.590641
H	0.817913	-0.998551	1.584319
C	-3.629594	1.222842	-0.104206
C	-2.554597	2.134906	-0.121364
N	-1.282381	1.604152	-0.348885
C	-2.814428	3.505470	0.088286
C	-4.131686	3.927333	0.303802
C	-4.408831	5.404625	0.465018
F	-3.346970	6.067689	0.990975

F	-5.479090	5.627238	1.276089
F	-4.692118	5.984926	-0.735497
C	-5.207407	3.027938	0.316889
C	-4.936594	1.669512	0.111020
C	-6.055443	0.663196	0.069076
F	-5.666777	-0.535964	0.620840
F	-6.443982	0.381820	-1.208505
F	-7.155302	1.075636	0.741600
C	-0.054944	2.269133	-0.342640
N	0.987984	1.389724	-0.629024
C	2.355950	1.676520	-0.708977
O	0.085787	3.472084	-0.113335
C	2.922549	2.915946	-0.353257
C	4.311304	3.080488	-0.434650
C	4.914404	4.427790	-0.112221
F	4.141031	5.142411	0.746169
F	5.069558	5.181555	-1.237188
F	6.146726	4.299959	0.452466
C	5.155147	2.044349	-0.852396
C	4.578610	0.817131	-1.208276
C	5.483833	-0.317126	-1.615265
F	6.279466	-0.709252	-0.574491
F	6.315585	0.035938	-2.628599
F	4.789252	-1.420528	-2.019198
C	3.196637	0.630732	-1.144537
H	-3.440335	0.155302	-0.256536
H	-1.266032	0.595795	-0.517634
H	-1.988716	4.216900	0.091656
H	-6.226645	3.376272	0.496581
H	0.745112	0.416809	-0.828528
H	2.279039	3.727932	-0.015546
H	6.237457	2.188095	-0.898657
H	2.763922	-0.332736	-1.428689

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3661.81664142 Predicted Change= -4.372931D-07
Zero-point correction (ZPE)= -3661.2566 0.55994
Internal Energy (U)= -3661.2208 0.59576
Enthalpy (H)= -3661.2201 0.59650
Gibbs Free Energy (G)= -3661.3225 0.49405

Frequencies -- 3.7583 14.9052 17.7685

Enol Ether

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#pbepbe/3-21G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,gdiis) iop(1/8=18) freq=noraman temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C21H16F6N2O2 C1[X(C21H16F6N2O2)] #Atoms= 47
Charge = 0 Multiplicity = 1

SCF Energy= -1658.16082559 Predicted Change= -2.800242D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00188	0.00180	[NO]	0.00188	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.697984	-1.697352	-0.656148
C	-2.639334	-3.094311	-0.744659
C	-3.821661	-3.790550	-1.017237
C	-5.045993	-3.106603	-1.199124
C	-5.121227	-1.712835	-1.107963
C	-3.935394	-1.007696	-0.832727
C	-3.674026	0.417629	-0.677487
C	-4.698845	1.515102	-0.692252
C	-5.497877	1.518455	0.620775
O	-6.491528	2.596004	0.458301
C	-7.335813	2.801925	1.548067
C	-7.364123	2.146226	2.720222
C	-2.326098	0.557640	-0.436683
N	-1.702557	-0.720804	-0.434965
C	-0.330430	-1.023686	-0.241988
N	0.484835	0.085314	-0.461450
C	1.870482	0.134802	-0.225166
O	0.065800	-2.165290	0.071506
C	2.547773	1.338984	-0.507922
C	3.921032	1.457574	-0.295818
C	4.614406	2.716395	-0.700203
F	3.748793	3.799551	-0.599547
F	5.061477	2.670432	-2.011532
F	5.719282	2.941348	0.106115
C	4.657970	0.390367	0.220379
C	3.993642	-0.803170	0.508880
C	4.744129	-1.934714	1.132661
F	6.075797	-1.898868	0.741797
F	4.192929	-3.150549	0.759304
F	4.718764	-1.875958	2.517539
C	2.624293	-0.943915	0.281459
H	-8.023450	3.621193	1.318991
H	-8.096296	2.436020	3.475113
H	-6.688948	1.325920	2.968695
H	-1.769757	1.455900	-0.185831
H	-4.841526	1.728613	1.485322
H	-6.006320	0.550470	0.785446
H	-1.693098	-3.605814	-0.578409
H	-3.795521	-4.881426	-1.083529
H	-5.950841	-3.682906	-1.412013
H	-6.067614	-1.184566	-1.250520
H	-5.409883	1.376826	-1.528116
H	-4.224429	2.505153	-0.816145

H	0.071741	0.897744	-0.928369
H	2.005271	2.210847	-0.882018
H	5.729843	0.486247	0.391821
H	2.127797	-1.892725	0.470529

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy=	-1658.16082559	Predicted Change= -2.800242D-09
Zero-point correction (ZPE)=	-1657.8214	0.33933
Internal Energy (U)=	-1657.8037	0.35702
Enthalpy (H)=	-1657.8030	0.35776
Gibbs Free Energy (G)=	-1657.8649	0.29589

Frequencies -- 14.9572 15.8048 31.2806

PBE-D3BJ = -0.05881225
PBE/6-311++G(2df,p) = -1667.598396
PBE/6-31+G(d,p) = -1667.148819
PBE/6-31+G(d,p)/SMD(Toluene) = -1667.173333

Chiral Phosphoric Acid (CPA)

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#pbepbe/3-21G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,gdiis) iop(1/8=18) freq=noraman temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C36H17F12O4P C1[X(C36H17F12O4P)] #Atoms= 70
Charge = 0 Multiplicity = 1

SCF Energy= -3202.35639762 Predicted Change= -8.538624D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00158	0.00180	[YES]	0.00158	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.595699	3.292480	1.377522
C	-3.427916	2.218785	0.955669
C	-2.898777	1.156493	0.231580
C	-3.775002	0.005743	-0.119368
C	-1.522416	1.174504	-0.147988
O	-0.999777	0.083210	-0.895559
P	-0.032311	-0.999475	-0.112063
O	0.539750	-2.000000	-1.049610
C	-0.693556	2.234260	0.210595
C	0.729187	2.220809	-0.243009
C	-1.198709	3.303768	1.027912

C	1.525297	1.119513	0.066931
O	0.969627	-0.007872	0.736563
C	2.914057	1.098217	-0.269273
C	3.777117	-0.063563	0.080104
C	3.478339	2.185715	-0.927224
C	2.675428	3.290876	-1.322969
C	1.273829	3.317113	-0.996490
C	-0.372992	4.345705	1.543583
C	-0.916313	5.347684	2.331759
C	-2.303990	5.359290	2.638783
C	-3.129205	4.349487	2.175344
C	3.244265	4.371682	-2.062470
C	2.448117	5.419409	-2.491578
C	1.055737	5.425268	-2.206104
C	0.478569	4.400441	-1.473305
C	-4.719588	-0.462090	0.815553
C	-5.601714	-1.494563	0.480526
C	-6.544307	-2.019555	1.513392
F	-5.982384	-3.042606	2.262310
F	-7.687363	-2.525812	0.912152
F	-6.903770	-1.011470	2.398110
C	-5.562398	-2.080773	-0.785183
C	-4.614571	-1.636082	-1.709647
C	-4.519416	-2.304061	-3.043516
F	-5.772790	-2.744441	-3.448726
F	-3.684726	-3.410114	-3.013573
F	-4.016652	-1.426940	-3.991745
C	-3.723142	-0.607566	-1.389257
C	3.673110	-0.712215	1.327966
C	4.558483	-1.741346	1.661101
C	4.405381	-2.446612	2.968937
F	5.638895	-2.899441	3.418914
F	3.571355	-3.549900	2.876956
F	3.861068	-1.594942	3.919904
C	5.552742	-2.150618	0.770186
C	5.644179	-1.529050	-0.475722
C	6.646093	-2.011258	-1.472820
F	6.156240	-3.037014	-2.263795
F	7.775497	-2.492555	-0.824083
F	7.018308	-0.976308	-2.322098
C	4.767149	-0.496849	-0.823122
O	-0.880984	-1.523093	1.150133
H	-4.492317	2.232311	1.209064
H	4.550341	2.194625	-1.146105
H	0.694700	4.337149	1.314300
H	-0.270715	6.136785	2.727900
H	-2.712813	6.163864	3.256524
H	-4.195340	4.336220	2.423751
H	4.313766	4.346569	-2.294889
H	2.884117	6.241835	-3.065726
H	0.433935	6.245963	-2.575192
H	-0.592901	4.403808	-1.261454
H	-4.776085	-0.022273	1.814010
H	-6.281089	-2.854501	-1.058540
H	-3.005049	-0.273338	-2.137214
H	2.918635	-0.405516	2.051301

H	6.266017	-2.925222	1.054830
H	4.863722	-0.031682	-1.806755
H	-1.270509	-2.434801	1.013587

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3202.35639762 Predicted Change= -8.538624D-09

Zero-point correction (ZPE)=	-3201.8931	0.46325
Internal Energy (U)=	-3201.8652	0.49110
Enthalpy (H)=	-3201.8645	0.49184
Gibbs Free Energy (G)=	-3201.9496	0.40674

Frequencies -- 10.0475 11.9360 14.1118

PBE-D3BJ = -0.11363749
PBE/6-311++G(2df,p) = -3220.310465
PBE/6-31+G(d,p) = -3219.471946
PBE/6-31+G(d,p)/SMD(Toluene) = -3219.504135

(R)-phosphate-acetal

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#pbepbe/3-21G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,gdiis) iop(1/8=18) freq=noraman temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4860.62396151 Predicted Change= -2.621671D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00005	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00367	0.00180	[NO]	0.00367	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.862477	3.138304	2.339430
C	1.753544	2.033668	2.399351
C	1.306244	0.743795	2.123064
C	2.310245	-0.354715	2.053491
C	-0.088150	0.518003	1.906773
O	-0.555372	-0.810024	1.586938
C	-1.003418	1.570875	1.935916
C	-2.471365	1.288084	1.889877
C	-0.533522	2.924700	2.069301
C	-3.024173	0.517654	0.869468
O	-2.246001	-0.011966	-0.192772
C	-4.431325	0.276488	0.809763

C	-4.970567	-0.691561	-0.188029
C	-5.279755	0.867143	1.731742
C	-4.749374	1.634675	2.806222
C	-3.325510	1.814291	2.927924
C	-1.376041	4.054107	1.866404
C	-0.863252	5.336399	1.972247
C	0.499307	5.547814	2.315834
C	1.351570	4.471465	2.490733
C	-5.614684	2.170728	3.806744
C	-5.092480	2.836448	4.901609
C	-3.686157	2.972983	5.047521
C	-2.820527	2.475279	4.086558
C	3.591044	-0.077149	1.533556
C	4.572115	-1.071649	1.489859
C	5.947085	-0.722935	1.018642
F	6.594290	-1.843692	0.530136
F	6.724102	-0.205760	2.047851
F	5.883443	0.250792	0.028371
C	4.290110	-2.368804	1.914668
C	3.019546	-2.655167	2.421844
C	2.735169	-4.034112	2.911981
F	3.144763	-4.996251	1.981686
F	1.380083	-4.215795	3.159557
F	3.416904	-4.323084	4.082336
C	2.038651	-1.663392	2.503493
C	-5.974073	-0.360529	-1.112402
C	-6.487292	-1.342630	-1.971584
C	-7.503044	-0.962149	-2.999265
F	-8.279248	0.094413	-2.542299
F	-8.327987	-2.042479	-3.282498
F	-6.920904	-0.562832	-4.190746
C	-6.015654	-2.657483	-1.924456
C	-5.018337	-2.986759	-1.003868
C	-4.447520	-4.362929	-0.946382
F	-3.249741	-4.481046	-1.657702
F	-5.327772	-5.290904	-1.470123
F	-4.145912	-4.717019	0.371066
P	-0.962493	-0.995250	0.001575
O	-1.590166	-2.448975	-0.081182
C	-4.508733	-2.016669	-0.139264
O	0.076767	-0.624723	-1.012406
C	4.916294	-1.560131	-2.178918
C	6.166697	-1.119383	-2.631876
C	7.169133	-2.069861	-2.852198
C	6.934796	-3.445046	-2.623265
C	5.693901	-3.903870	-2.167569
C	4.681817	-2.953412	-1.945644
C	3.304271	-3.089161	-1.493580
C	2.565893	-4.355104	-1.147084
C	1.041142	-4.218520	-1.244209
O	0.560626	-3.664895	0.078656
C	-0.833000	-3.780343	0.263242
C	-1.183060	-4.069246	1.709470
C	2.758378	-1.831146	-1.457118
N	3.715833	-0.877023	-1.880780
C	3.548726	0.532329	-1.995488

N	2.245875	0.948899	-1.751618
C	1.810355	2.283129	-1.793083
O	4.504235	1.281480	-2.302131
C	2.645564	3.400090	-2.008618
C	2.116099	4.692143	-1.996839
C	3.042775	5.854637	-2.119411
F	2.388910	6.937516	-2.695184
F	4.146077	5.529684	-2.892652
F	3.518126	6.278637	-0.884268
C	0.752952	4.917773	-1.798611
C	-0.084922	3.816336	-1.604961
C	-1.556762	4.020545	-1.490849
F	-1.839527	5.245447	-0.890650
F	-2.143574	3.011510	-0.722852
F	-2.200380	4.013934	-2.717577
C	0.428285	2.520856	-1.594992
H	2.807328	2.207662	2.634577
H	-6.356969	0.682355	1.677089
H	-2.406835	3.890682	1.554102
H	-1.507586	6.193717	1.761690
H	0.880604	6.568797	2.406106
H	2.413099	4.624630	2.708643
H	-6.695184	2.034047	3.695303
H	-5.757977	3.243958	5.667715
H	-3.282413	3.472224	5.933066
H	-1.741239	2.579717	4.209562
H	3.823114	0.906508	1.118374
H	5.045886	-3.148950	1.811114
H	1.062977	-1.915391	2.911301
H	-6.367342	0.656961	-1.169590
H	-6.444712	-3.419908	-2.575896
H	-3.749297	-2.301016	0.584957
H	-1.330308	-4.452017	-0.451101
H	0.564430	-5.206005	-1.380594
H	0.742893	-3.537667	-2.058934
H	-0.939892	-3.197861	2.334242
H	-2.259559	-4.287324	1.759176
H	-0.597161	-4.930659	2.058296
H	6.330921	-0.055374	-2.784135
H	8.150612	-1.738619	-3.202357
H	7.742469	-4.160646	-2.803968
H	5.513009	-4.966907	-1.986431
H	2.796092	-4.677553	-0.115731
H	2.883910	-5.161917	-1.835641
H	1.759407	-1.552020	-1.146671
H	1.493241	0.269099	-1.531599
H	3.703545	3.234597	-2.198717
H	0.351206	5.930556	-1.796898
H	-0.247385	1.683801	-1.413790

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -4860.62396151 Predicted Change= -2.621671D-08
Zero-point correction (ZPE)= -4859.8146 0.80928
Internal Energy (U)= -4859.7699 0.85402

Enthalpy (H)=	-4859.7692	0.85476
Gibbs Free Energy (G)=	-4859.8887	0.73525

Frequencies -- 8.3542 11.2910 13.9287

PBE-D3BJ = -0.214050
PBE/6-311++G(2df,p) = -4887.924556
PBE/6-31+G(d,p) = -4886.637592
PBE/6-31+G(d,p)/SMD(Toluene) = -4886.679043

Spirocyclization

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

#pbepbe/3-21G*/auto scf=(maxcycle=300,direct,tight) density=current
opt=(maxcycle=250,ts,calcfc,noeigentest,gdiis) iop(1/8=18) freq=noraman
temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4860.59272684 Predicted Change= -2.973827D-08

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00007	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00777	0.00180	[NO]	0.00777	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.405119	-3.805556	-0.381016
C	4.767459	-4.121672	-0.389159
C	5.137231	-5.444502	-0.107912
C	4.167539	-6.427722	0.183528
C	2.801329	-6.114010	0.226958
C	2.425592	-4.793514	-0.054342
C	1.114819	-4.128300	-0.057059
C	-0.196368	-4.562325	0.549041
C	-1.116177	-5.162099	-0.550022
O	-0.954658	-4.231207	-1.700668
C	0.351558	-4.124896	-2.076148
C	0.594429	-2.991156	-3.034980
C	1.376912	-2.774274	-0.371276
N	2.710254	-2.577838	-0.607029
C	3.346429	-1.353733	-1.096911
N	2.453741	-0.346249	-1.323343
C	2.810482	0.923615	-1.832050
O	4.581147	-1.348390	-1.282375
C	1.749345	1.811903	-2.117945
C	2.004105	3.079717	-2.636252
C	0.866636	4.017501	-2.872981
F	0.577455	4.785880	-1.755074

F	1.177094	4.895205	-3.905792
C	3.313701	3.501921	-2.879544
C	4.366797	2.637398	-2.577080
C	5.773957	3.107706	-2.736737
F	6.237276	3.761363	-1.602664
F	5.865666	4.007012	-3.791459
F	6.626783	2.041382	-2.974748
C	4.130096	1.361382	-2.060025
F	-0.282788	3.317221	-3.205053
H	-2.179210	-5.094317	-0.292463
H	-0.805001	-6.178941	-0.847246
H	0.937298	-5.047753	-2.203065
H	1.673505	-2.821305	-3.167821
H	0.167035	-3.267816	-4.018992
H	0.099128	-2.072349	-2.677171
H	5.497225	-3.333764	-0.562257
H	6.197404	-5.710631	-0.103278
H	4.492297	-7.448875	0.401113
H	2.054406	-6.867886	0.488740
H	-0.711482	-3.661747	0.932284
H	-0.032026	-5.289299	1.360544
H	0.643403	-1.971563	-0.461020
H	1.418796	-0.414883	-1.078003
H	0.720041	1.489528	-1.943583
H	3.506661	4.477608	-3.325305
H	4.961303	0.703908	-1.825220
C	-1.116948	2.569970	1.426256
C	-2.581003	2.263290	1.531431
C	-0.205650	1.530074	1.611791
O	-0.680846	0.202730	1.676700
C	1.200814	1.789593	1.731562
C	2.160741	0.676656	1.995186
C	1.666781	3.095846	1.614649
C	0.769456	4.160020	1.320412
C	-0.646035	3.910462	1.216477
C	-3.381032	2.949720	2.514064
C	-4.791573	2.665324	2.569693
C	-5.356263	1.691618	1.700696
C	-4.553863	0.981344	0.817207
C	-5.187175	-0.064752	-0.038948
C	-3.154553	1.272614	0.730101
O	-2.392619	0.559921	-0.215963
C	1.262355	5.486918	1.131168
C	0.392239	6.517436	0.822864
C	-0.999592	6.264638	0.684047
C	-1.510686	4.991766	0.878993
C	-2.831843	3.855070	3.470438
C	-3.647186	4.474340	4.404381
C	-5.045085	4.222100	4.431657
C	-5.606327	3.328411	3.536515
C	1.769259	-0.472883	2.717358
C	2.665645	-1.527969	2.914053
C	2.167145	-2.779840	3.554079
F	1.210972	-2.498413	4.514543
F	3.207743	-3.485633	4.136309
F	1.565137	-3.633919	2.622609

C	3.974579	-1.459872	2.437707
C	4.384266	-0.310685	1.755909
C	5.810448	-0.203654	1.320800
F	5.953826	0.693758	0.270532
F	6.299174	-1.447323	0.931605
F	6.628551	0.242330	2.348674
C	3.492095	0.743373	1.523969
C	-6.413117	0.215699	-0.673566
C	-7.073658	-0.766373	-1.419575
C	-8.411081	-0.465239	-2.007458
F	-8.643486	-1.259365	-3.122424
F	-8.491178	0.870651	-2.378244
F	-9.444869	-0.701894	-1.111999
C	-6.517526	-2.037535	-1.567100
C	-5.294927	-2.318142	-0.953163
C	-4.651956	-3.649324	-1.162150
F	-3.571391	-3.600832	-2.028526
F	-5.561236	-4.565947	-1.672781
F	-4.149573	-4.161459	0.043415
P	-1.214314	-0.503851	0.257806
C	-4.627522	-1.351513	-0.190107
O	-0.158501	-0.390912	-0.853783
O	-1.743502	-1.860427	0.649618
H	2.729146	3.318952	1.749354
H	-6.423013	1.458679	1.775923
H	2.338529	5.667537	1.220567
H	0.773336	7.531007	0.669081
H	-1.671191	7.084739	0.414103
H	-2.579449	4.795013	0.767625
H	-1.757266	4.046623	3.460515
H	-3.209485	5.160561	5.135411
H	-5.671004	4.725023	5.174297
H	-6.678147	3.105761	3.562005
H	0.757388	-0.561394	3.107285
H	4.662616	-2.293699	2.584088
H	3.830800	1.588754	0.920949
H	-6.846590	1.217555	-0.619594
H	-7.026324	-2.795867	-2.162168
H	-3.671255	-1.621980	0.273382

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -4860.59272684	Predicted Change= -2.973827D-08	
Zero-point correction (ZPE)=	-4859.7855	0.80720
Internal Energy (U)=	-4859.7410	0.85166
Enthalpy (H)=	-4859.7403	0.85240
Gibbs Free Energy (G)=	-4859.8591	0.73361

Frequencies -- -149.3618 7.2642 14.3787

PBE-D3BJ = -0.213688
PBE/6-311++G(2df,p) = -4887.902465
PBE/6-31+G(d,p) = -4886.616715
PBE/6-31+G(d,p)/SMD(Toluene) = -4886.659385

Spirocycle

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#pbepbe/3-21G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,gdiis) iop(1/8=18) freq=noraman temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4860.61239423 Predicted Change= -2.116080D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00703	0.00180	[NO]	0.00703	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.483347	-3.612050	-0.389039
C	4.849662	-3.648884	-0.099480
C	5.371676	-4.839872	0.429266
C	4.543144	-5.955038	0.653570
C	3.166334	-5.908191	0.371189
C	2.646191	-4.722567	-0.145031
C	1.238227	-4.373281	-0.563339
C	0.085314	-4.532059	0.491193
C	-1.089460	-5.170338	-0.318318
O	-0.705264	-5.062986	-1.750965
C	0.724890	-5.289939	-1.765032
C	1.267667	-4.943702	-3.144002
C	1.383350	-2.965294	-1.019405
N	2.645991	-2.551499	-0.911200
C	3.216562	-1.221356	-1.333909
N	2.252129	-0.289152	-1.470418
C	2.491266	1.034612	-1.909388
O	4.447245	-1.148493	-1.507427
C	1.358420	1.856648	-2.094906
C	1.506037	3.190435	-2.468246
C	0.293814	4.031638	-2.702045
F	0.570332	5.360965	-2.409019
F	-0.126131	3.982549	-4.023757
C	2.776249	3.738962	-2.665765
C	3.898945	2.928563	-2.490173
C	5.262858	3.485802	-2.732773
F	6.190835	2.882982	-1.895021
F	5.270223	4.856138	-2.501434
F	5.691179	3.284794	-4.034850
C	3.768726	1.587670	-2.118336
F	-0.761612	3.596693	-1.915634
H	-2.032780	-4.626708	-0.206196
H	-1.206524	-6.235214	-0.041738

H	0.988212	-6.326590	-1.461981
H	2.369828	-4.956529	-3.139299
H	0.903588	-5.677999	-3.882228
H	0.903176	-3.947789	-3.446387
H	5.471350	-2.770483	-0.247957
H	6.436827	-4.893664	0.667408
H	4.975574	-6.870416	1.066219
H	2.521700	-6.768995	0.565689
H	-0.242841	-3.554799	0.883434
H	0.434807	-5.163388	1.322408
H	0.568106	-2.304636	-1.340691
H	1.224234	-0.455823	-1.147455
H	0.364433	1.448112	-1.899509
H	2.888702	4.794886	-2.911016
H	4.651936	0.986787	-1.919026
C	-1.055232	2.490713	1.374730
C	-2.502157	2.164893	1.565335
C	-0.104943	1.480042	1.528431
O	-0.520202	0.137662	1.642587
C	1.294548	1.798551	1.594265
C	2.318402	0.741203	1.829679
C	1.705940	3.120806	1.449490
C	0.765461	4.144840	1.155804
C	-0.639613	3.839313	1.105789
C	-3.260212	2.881760	2.559794
C	-4.669515	2.613327	2.673100
C	-5.273203	1.633993	1.838001
C	-4.507880	0.895196	0.945057
C	-5.182197	-0.142111	0.114960
C	-3.105948	1.155571	0.814346
O	-2.373833	0.416910	-0.134149
C	1.203648	5.478669	0.891250
C	0.286471	6.460798	0.561308
C	-1.099803	6.153710	0.488967
C	-1.556109	4.873581	0.756683
C	-2.668454	3.807172	3.470154
C	-3.443407	4.456927	4.417711
C	-4.841166	4.217462	4.503551
C	-5.442761	3.307155	3.652428
C	3.628584	0.892622	1.322078
C	4.598028	-0.093254	1.536125
C	5.991867	0.121977	1.044068
F	6.018096	0.976787	-0.049775
F	6.582894	-1.091494	0.679096
F	6.809261	0.677164	2.014631
C	4.287250	-1.259898	2.240359
C	2.991800	-1.421844	2.732920
C	2.586932	-2.714351	3.357845
F	3.684823	-3.381438	3.876532
F	1.992110	-3.565075	2.417300
F	1.656071	-2.513786	4.360881
C	2.018470	-0.434367	2.552840
C	-4.653529	-1.440882	-0.023568
C	-5.350688	-2.401509	-0.765561
C	-4.735613	-3.748307	-0.946128
F	-5.673503	-4.675786	-1.374233

F	-4.181054	-4.196659	0.257621
F	-3.692901	-3.744163	-1.862262
C	-6.573052	-2.103347	-1.369803
C	-7.100001	-0.818142	-1.233519
C	-8.437729	-0.496153	-1.809289
F	-8.497066	0.838821	-2.187694
F	-9.466457	-0.708034	-0.901738
F	-8.696325	-1.292721	-2.916437
P	-1.182789	-0.646333	0.317176
C	-6.409508	0.158275	-0.507462
O	-0.220364	-0.609680	-0.880988
O	-1.707951	-1.965184	0.823107
H	2.761754	3.386739	1.553033
H	-6.341583	1.421405	1.943622
H	2.274919	5.700730	0.933424
H	0.624768	7.477579	0.342733
H	-1.809749	6.935883	0.205231
H	-2.619039	4.632628	0.688989
H	-1.593703	3.989619	3.414783
H	-2.973447	5.157811	5.113957
H	-5.434804	4.744306	5.256044
H	-6.514868	3.095844	3.722286
H	3.892349	1.754931	0.706131
H	5.032605	-2.041345	2.388891
H	1.020512	-0.591237	2.957869
H	-3.701094	-1.723902	0.438802
H	-7.105310	-2.860548	-1.945965
H	-6.820091	1.169980	-0.459608

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -4860.61239423 Predicted Change= -2.116080D-08
Zero-point correction (ZPE)= -4859.8052 0.80716
Internal Energy (U)= -4859.7602 0.85213
Enthalpy (H)= -4859.7595 0.85287
Gibbs Free Energy (G)= -4859.8805 0.73189

Frequencies -- 6.6691 8.1393 16.9051

PBE-D3BJ = -0.21397123
PBE/6-311++G(2df,p) = -4887.913510
PBE/6-31+G(d,p) = -4886.629437
PBE/6-31+G(d,p)/SMD(Toluene) = -4886.671302

1,2-shift

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#pbepbe/3-21G*/auto scf=(maxcycle=300,direct,tight) density=current
opt=(maxcycle=250,ts,calcfc,noeigentest,gdiis) iop(1/8=18) freq=noraman
temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4860.59172901 Predicted Change= -6.523902D-09

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00145	0.00180	[YES]	0.00145	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.833843	-3.913550	-0.122990
C	4.122707	-4.254557	0.303742
C	4.307375	-5.515270	0.887112
C	3.232162	-6.418331	1.044359
C	1.935544	-6.081080	0.638321
C	1.743529	-4.820898	0.051520
C	0.540717	-4.157487	-0.443606
C	-0.906404	-4.530756	-0.300977
C	-1.479411	-5.075231	-1.649371
O	-0.814844	-4.305065	-2.738651
C	0.539811	-4.395781	-2.648634
C	1.299399	-3.556343	-3.632339
C	0.956802	-2.881324	-0.906961
N	2.313960	-2.727978	-0.711058
C	3.138357	-1.579043	-1.101129
N	2.385975	-0.475399	-1.364503
C	2.910807	0.754531	-1.816994
O	4.378930	-1.715940	-1.158860
C	1.981096	1.793116	-2.051251
C	2.412514	3.056841	-2.446214
C	1.409959	4.131312	-2.710817
F	1.938188	5.371074	-2.364558
F	1.054002	4.201804	-4.050726
C	3.773569	3.322636	-2.626593
C	4.695254	2.298809	-2.405315
C	6.150552	2.547203	-2.625250
F	6.434504	3.901847	-2.496628
F	6.566847	2.156626	-3.889146
F	6.912339	1.839152	-1.707134
C	4.279997	1.026110	-2.002867
F	0.250667	3.910691	-1.985286
H	-2.545823	-4.850986	-1.758533
H	-1.250755	-6.146584	-1.780980
H	0.978975	-5.368044	-2.381132
H	2.339688	-3.423259	-3.296871
H	1.326378	-4.088074	-4.604950
H	0.811648	-2.580645	-3.778041
H	4.933319	-3.534078	0.214992
H	5.304787	-5.798397	1.233921
H	3.416425	-7.390475	1.509405
H	1.095935	-6.764274	0.789619
H	-1.466652	-3.621196	-0.002905

H	-1.031644	-5.309738	0.471179
H	0.325069	-2.059121	-1.252728
H	1.338193	-0.426940	-1.121648
H	0.919586	1.604926	-1.874383
H	4.113105	4.323349	-2.892688
H	5.010042	0.258557	-1.764066
C	-0.968512	2.657577	1.280557
C	-2.447741	2.454136	1.411182
C	-0.125762	1.568535	1.506190
O	-0.681998	0.270527	1.585738
C	1.293858	1.741599	1.620694
C	2.183110	0.590653	1.958241
C	1.843096	3.007135	1.433969
C	1.018096	4.107355	1.068586
C	-0.411962	3.949436	0.994148
C	-3.184746	3.227719	2.376705
C	-4.608097	3.032074	2.469973
C	-5.246325	2.055858	1.657148
C	-4.507182	1.267397	0.783608
C	-5.220780	0.214159	0.001773
C	-3.095244	1.473704	0.654909
O	-2.403087	0.700352	-0.289567
C	1.598534	5.375401	0.762531
C	0.796642	6.435423	0.376309
C	-0.612451	6.275342	0.287663
C	-1.206760	5.060766	0.590530
C	-2.564075	4.143682	3.277460
C	-3.322700	4.856687	4.192164
C	-4.732101	4.689227	4.256989
C	-5.362765	3.787224	3.418282
C	1.716503	-0.496367	2.731633
C	2.561934	-1.569491	3.027506
C	2.001201	-2.768879	3.716362
F	0.984072	-2.408174	4.585670
F	2.993928	-3.430733	4.427588
F	1.468108	-3.679300	2.810182
C	3.887342	-1.583634	2.595390
C	4.362246	-0.510954	1.837381
C	5.795808	-0.508628	1.418832
F	6.009089	0.316040	0.324772
F	6.219464	-1.801587	1.101559
F	6.630044	-0.064189	2.434157
C	3.524850	0.563280	1.513346
C	-4.721410	-1.102795	-0.114401
C	-5.494476	-2.089880	-0.737561
C	-4.971064	-3.480956	-0.861110
F	-4.342307	-3.713661	-2.097092
F	-5.999582	-4.407453	-0.770359
F	-4.017313	-3.772594	0.105378
C	-6.755337	-1.796725	-1.265595
C	-7.233377	-0.489140	-1.188642
C	-8.532438	-0.134758	-1.831666
F	-9.385388	-1.231212	-1.835183
F	-8.379375	0.270604	-3.148648
F	-9.143154	0.910165	-1.149704
P	-1.223184	-0.383289	0.143344

C	-6.478094	0.507996	-0.560662
O	-0.177924	-0.237884	-0.968115
O	-1.794201	-1.736855	0.479717
H	2.917855	3.168273	1.557328
H	-6.321402	1.885122	1.770722
H	2.686362	5.485914	0.817120
H	1.246365	7.399746	0.123883
H	-1.230625	7.117677	-0.036116
H	-2.288450	4.931278	0.508355
H	-1.480692	4.271271	3.238737
H	-2.830890	5.551973	4.878864
H	-5.312201	5.264701	4.984014
H	-6.445142	3.630670	3.473404
H	0.688507	-0.521849	3.087500
H	4.533357	-2.429827	2.831869
H	3.914470	1.348372	0.861883
H	-3.739805	-1.384808	0.282261
H	-7.372657	-2.580389	-1.707168
H	-6.885374	1.520448	-0.504768

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -4860.59172901 Predicted Change= -6.523902D-09

Zero-point correction (ZPE)=	-4859.7847	0.80697
Internal Energy (U)=	-4859.7402	0.85145
Enthalpy (H)=	-4859.7395	0.85219
Gibbs Free Energy (G)=	-4859.8581	0.73358

Frequencies -- -138.0899 9.9425 14.0987

PBE-D3BJ = -0.213480
PBE/6-311++G(2df,p) = -4887.903842
PBE/6-31+G(d,p) = -4886.617810
PBE/6-31+G(d,p)/SMD(Toluene) = -4886.661474

[6.5.6]-chair

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#pbepbe/3-21G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,gdiis) iop(1/8=18) freq=noraman temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4860.61696952 Predicted Change= -3.248928D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00123	0.00180	[YES]	0.00123	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.890137	-3.845258	-0.306507
C	4.207224	-4.108169	0.135388
C	4.424048	-5.248501	0.898792
C	3.366512	-6.144508	1.253730
C	2.061453	-5.893482	0.874249
C	1.810216	-4.737607	0.082784
C	0.615402	-4.201639	-0.419200
C	-0.775107	-4.690056	-0.439506
C	-1.163219	-4.921592	-1.948070
O	-0.900111	-3.706223	-2.714865
C	0.507225	-3.335138	-2.750226
C	0.568785	-2.106930	-3.650474
C	0.922009	-3.005401	-1.231967
N	2.373878	-2.806846	-1.044117
C	3.151288	-1.633528	-1.417067
N	2.363401	-0.522617	-1.542048
C	2.831515	0.747687	-1.936080
O	4.390956	-1.724254	-1.556173
C	1.869359	1.779280	-2.026825
C	2.246475	3.072030	-2.382805
C	1.205887	4.131627	-2.539520
F	1.722952	5.365356	-2.156533
F	0.781921	4.260217	-3.854470
C	3.585615	3.378708	-2.643872
C	4.540071	2.364889	-2.548961
C	5.987678	2.693250	-2.701376
F	6.573078	3.033368	-1.489475
F	6.150427	3.777313	-3.554302
F	6.687735	1.608889	-3.205776
C	4.177711	1.060323	-2.206447
F	0.091143	3.843676	-1.768882
H	-2.247296	-5.071279	-2.015261
H	-0.598862	-5.783755	-2.349922
H	1.148729	-4.170140	-3.093653
H	1.607525	-1.788172	-3.820557
H	0.103621	-2.361461	-4.616558
H	0.002430	-1.290361	-3.173707
H	5.001954	-3.401436	-0.091908
H	5.437748	-5.464807	1.248994
H	3.602441	-7.023764	1.858055
H	1.237794	-6.545828	1.172391
H	-1.432410	-3.877291	-0.060641
H	-0.919319	-5.622561	0.129937
H	0.334795	-2.089253	-0.968848
H	1.353086	-0.521664	-1.206218
H	0.826449	1.560082	-1.786962
H	3.881528	4.393849	-2.909072
H	4.933186	0.286656	-2.110411
C	-0.985907	2.483887	1.470999
C	-2.453681	2.236054	1.629830
C	-0.104784	1.413745	1.625180
O	-0.620435	0.097456	1.718085
C	1.313009	1.626505	1.660713

C	2.255839	0.499781	1.917035
C	1.817088	2.911621	1.481349
C	0.944798	4.000115	1.204510
C	-0.481481	3.801375	1.201195
C	-3.195736	2.959975	2.628279
C	-4.616403	2.745262	2.716013
C	-5.247785	1.810352	1.850624
C	-4.502320	1.068826	0.942035
C	-5.212286	0.083538	0.074846
C	-3.090674	1.280750	0.835642
O	-2.378946	0.540124	-0.125410
C	1.472780	5.295247	0.918527
C	0.621990	6.345124	0.619654
C	-0.784469	6.145059	0.597468
C	-1.327604	4.902145	0.881562
C	-2.580815	3.843863	3.564220
C	-3.343249	4.505763	4.513420
C	-4.750282	4.317615	4.576856
C	-5.375281	3.448116	3.700211
C	3.558433	0.517294	1.368865
C	4.459986	-0.518619	1.638840
C	5.858144	-0.456898	1.116673
F	6.311039	-1.732009	0.765051
F	6.745965	0.021820	2.067228
F	5.951899	0.373357	0.010473
C	4.088005	-1.596036	2.446607
C	2.798566	-1.628283	2.977990
C	2.348380	-2.825893	3.746323
F	1.767675	-3.783883	2.920264
F	1.402907	-2.476126	4.695844
F	3.426505	-3.432537	4.378748
C	1.889631	-0.595051	2.731388
C	-4.736331	-1.231227	-0.117488
C	-5.497036	-2.144335	-0.859154
C	-5.049861	-3.564446	-0.956771
F	-5.631894	-4.192967	-2.049623
F	-5.370734	-4.306765	0.167102
F	-3.660554	-3.639926	-1.103391
C	-6.709482	-1.770844	-1.443227
C	-7.167193	-0.463281	-1.279802
C	-8.404621	-0.016211	-1.982892
F	-9.283910	-1.080113	-2.138627
F	-8.143684	0.488730	-3.247366
F	-9.035826	0.989817	-1.261790
P	-1.219030	-0.565135	0.302754
C	-6.433026	0.454713	-0.522080
O	-0.183259	-0.434986	-0.829894
O	-1.783016	-1.916865	0.653601
H	2.893007	3.097236	1.547286
H	-6.324220	1.635345	1.943335
H	2.558452	5.435479	0.918856
H	1.029886	7.331948	0.383804
H	-1.442774	6.979920	0.340288
H	-2.407937	4.744005	0.851813
H	-1.499049	3.986172	3.524643
H	-2.856976	5.176272	5.228098

H	-5.333410	4.852505	5.331909
H	-6.455755	3.278143	3.751811
H	3.868854	1.313361	0.688921
H	4.787618	-2.406108	2.654318
H	0.892624	-0.650631	3.164988
H	-3.772030	-1.554990	0.289873
H	-7.290448	-2.490306	-2.020849
H	-6.817804	1.470640	-0.404817

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -4860.61696952 Predicted Change= -3.248928D-09
Zero-point correction (ZPE)= -4859.8085 0.80840
Internal Energy (U)= -4859.7640 0.85295
Enthalpy (H)= -4859.7632 0.85369
Gibbs Free Energy (G)= -4859.8826 0.73429

Frequencies -- 8.0383 15.0282 17.0079

PBE-D3BJ = -0.213657
PBE/6-311++G(2df,p) = -4887.924798
PBE/6-31+G(d,p) = -4886.641083
PBE/6-31+G(d,p)/SMD(Toluene) = -4886.684398

Product

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#pbepbe/3-21G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,gdiis) iop(1/8=18) freq=noraman temp=233.15
#P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/3-21G*/Auto
Freq

Pointgroup= C1 Stoichiometry= C21H16F6N2O2 C1[X(C21H16F6N2O2)] #Atoms= 47
Charge = 0 Multiplicity = 1

SCF Energy= -1658.20013650 Predicted Change= -5.807370D-09

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00191	0.00180	[NO]	0.00191	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.693659	2.712322	-0.427850
C	-3.950752	3.778207	-0.948081
C	-2.585040	3.626892	-1.267869
C	-1.922744	2.410416	-1.049584
C	-2.640858	1.342521	-0.487014
C	-4.037292	1.489981	-0.205555
N	-2.288622	0.004665	-0.163921
C	-0.989927	-0.573372	-0.111657

N	-0.004766	0.385507	0.095553
C	1.382272	0.146682	0.089554
O	-0.790250	-1.803193	-0.204203
C	-3.468797	-0.676031	0.258947
C	-4.523940	0.207206	0.258924
C	-3.587827	-2.129104	0.649353
C	-3.566531	-3.058606	-0.578625
O	-4.826411	-2.306155	1.445637
C	-5.996547	-1.718292	0.760223
C	-5.897549	-0.178935	0.730059
C	1.967449	-1.114808	-0.140119
C	3.355891	-1.255286	-0.162240
C	3.942382	-2.586763	-0.502572
F	3.131583	-3.608700	-0.034211
F	5.206189	-2.713734	0.058164
F	4.077598	-2.760831	-1.871048
C	4.198031	-0.165606	0.064163
C	3.624698	1.083319	0.312180
C	4.498036	2.249510	0.639646
F	5.691611	2.167529	-0.060856
F	4.814812	2.307454	1.987635
F	3.859960	3.440636	0.313210
C	2.239835	1.243243	0.318102
H	-5.758964	2.817435	-0.207582
H	-4.437616	4.740301	-1.130065
H	-2.033499	4.460965	-1.709397
H	-0.883784	2.298306	-1.365493
H	-0.314791	1.329926	0.353607
H	-2.776026	-2.422065	1.337445
H	-3.786484	-4.089777	-0.253474
H	-2.561451	-3.012827	-1.020083
H	-4.311962	-2.746505	-1.328693
H	-6.862010	-2.053548	1.353668
H	-6.092814	-2.101364	-0.273772
H	-6.073301	0.230552	1.744121
H	-6.675956	0.224062	0.054742
H	1.321917	-1.978802	-0.279402
H	5.280688	-0.289314	0.050677
H	1.834494	2.244069	0.484866

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy=	-1658.20013650	Predicted Change= -5.807370D-09
Zero-point correction (ZPE)=	-1657.8578	0.34223
Internal Energy (U)=	-1657.8412	0.35890
Enthalpy (H)=	-1657.8404	0.35964
Gibbs Free Energy (G)=	-1657.8991	0.30099

Frequencies -- 14.7517 21.1263 29.7457

PBE-D3BJ = -0.06302544
PBE/6-311++G(2df,p) = -1667.622795
PBE/6-31+G(d,p) = -1667.175630
PBE/6-31+G(d,p)/SMD(Toluene) = -1667.198865

Phosphate Acetal A

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4886.68643023 Predicted Change= -3.840268D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00500	0.00180	[NO]	0.00500	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.273007	3.854743	1.163838
C	2.053970	2.688414	1.353671
C	1.499262	1.411358	1.415080
C	2.385646	0.231667	1.598907
C	0.072477	1.333580	1.318029
O	-0.522895	0.054442	1.308126
C	-0.761788	2.452978	1.293715
C	-2.235818	2.299087	1.457206
C	-0.160904	3.751680	1.136156
C	-2.959631	1.464654	0.611640
O	-2.275411	0.809024	-0.421069
C	-4.369394	1.257264	0.709949
C	-5.080096	0.267937	-0.136853
C	-5.045443	1.964011	1.698561
C	-4.370610	2.811122	2.614602
C	-2.939181	2.960763	2.529271
C	-0.921948	4.931671	0.899155
C	-0.293451	6.152795	0.716477
C	1.121271	6.256826	0.765393
C	1.889821	5.127510	0.984263
C	-5.085695	3.486237	3.646040
C	-4.419817	4.254085	4.584241
C	-3.006773	4.363604	4.530357
C	-2.283559	3.734192	3.529617
C	3.723761	0.293552	1.154029
C	4.599361	-0.781441	1.338879
C	6.048615	-0.639468	0.940045
F	6.803986	-0.249867	2.011693
F	6.235324	0.299274	-0.027250
F	6.576474	-1.808720	0.495547

C	4.165589	-1.959585	1.959982
C	2.846062	-2.019748	2.429055
C	2.403623	-3.248032	3.184238
F	2.758374	-4.396628	2.544974
F	1.050972	-3.287744	3.367909
F	2.970317	-3.300658	4.423066
C	1.967217	-0.942221	2.262082
C	-6.075081	-0.542233	0.449079
C	-6.745378	-1.513395	-0.304036
C	-7.706812	-2.450405	0.381219
F	-7.050746	-3.545952	0.871908
F	-8.663579	-2.909003	-0.468050
F	-8.333940	-1.861762	1.434466
C	-6.424537	-1.721468	-1.652417
C	-5.438303	-0.919770	-2.237739
C	-4.981178	-1.188172	-3.649093
F	-4.712931	-0.040612	-4.324633
F	-5.897973	-1.888206	-4.365790
F	-3.825654	-1.924686	-3.646019
P	-1.269116	-0.430185	-0.067751
O	-2.107608	-1.639851	0.558501
C	-4.778776	0.073081	-1.499721
O	-0.461429	-0.713867	-1.294514
C	3.803613	-3.749361	-1.122790
C	5.185003	-3.880558	-1.327001
C	5.781980	-5.084373	-0.930922
C	5.031524	-6.127361	-0.347749
C	3.654772	-5.990708	-0.148240
C	3.026882	-4.794061	-0.539756
C	1.655455	-4.330838	-0.451635
C	0.503921	-5.106650	0.126971
C	-0.681523	-4.278957	0.616137
O	-1.274290	-3.604243	-0.519286
C	-2.413555	-2.855611	-0.290013
C	-3.550232	-3.538367	0.448771
C	1.632392	-3.062300	-0.971650
N	2.923496	-2.676366	-1.382798
C	3.336737	-1.406103	-1.847286
N	2.309293	-0.491602	-1.994678
C	2.453444	0.896898	-2.131457
O	4.523507	-1.155409	-2.071424
C	1.282716	1.645578	-2.374695
C	1.328481	3.042692	-2.393758
C	0.050734	3.791093	-2.674721
F	-0.309853	3.690575	-3.987314
F	0.151999	5.116362	-2.388374
F	-0.993285	3.292274	-1.949307
C	2.525480	3.730918	-2.161482
C	3.683970	2.977402	-1.931462
C	4.948608	3.667932	-1.498301
F	5.006268	4.962929	-1.905370
F	6.066809	3.041114	-1.940059
F	5.035950	3.689946	-0.119318
C	3.673096	1.576700	-1.941442
H	3.135639	2.814238	1.446524
H	-6.132546	1.860473	1.785385

H	-2.010455	4.862328	0.834320
H	-0.894920	7.045130	0.516220
H	1.601836	7.228469	0.613775
H	2.983768	5.181239	0.988242
H	-6.174421	3.370975	3.686999
H	-4.977197	4.763866	5.376264
H	-2.478868	4.947538	5.290976
H	-1.195330	3.822131	3.511428
H	4.091857	1.183993	0.641749
H	4.839937	-2.812461	2.073132
H	0.954868	-1.018800	2.658146
H	-6.303446	-0.433770	1.513028
H	-6.928685	-2.498124	-2.232459
H	-4.027596	0.694069	-1.991303
H	-2.726109	-2.495150	-1.283084
H	-0.358465	-3.533105	1.363037
H	-1.421295	-4.951628	1.086857
H	-3.291890	-3.742519	1.499732
H	-4.444446	-2.899415	0.435116
H	-3.792050	-4.487809	-0.056531
H	5.765918	-3.068498	-1.760713
H	6.859532	-5.211944	-1.077167
H	5.534785	-7.052422	-0.048122
H	3.072484	-6.798989	0.306997
H	0.865790	-5.678799	1.001847
H	0.136053	-5.858470	-0.598901
H	0.772661	-2.408967	-1.090738
H	1.337440	-0.787310	-1.846099
H	0.330968	1.126488	-2.513322
H	2.548451	4.821431	-2.136777
H	4.587303	1.010846	-1.765961

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -4886.68643023 Predicted Change= -3.840268D-08
Zero-point correction (ZPE)= -4885.8961 0.79029
Internal Energy (U)= -4885.8504 0.83599
Enthalpy (H)= -4885.8496 0.83673
Gibbs Free Energy (G)= -4885.9712 0.71515

Frequencies -- 9.1731 15.5979 19.2492

PBE-D3BJ/6-311++G(2df,p) = -4888.179618
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -4888.217163
PBE/def2-TZVPP = -4887.60587851624

Phosphate Acetal B

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)

#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto Freq

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Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4886.68579333 Predicted Change= -2.866680D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00404	0.00180	[NO]	0.00404	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.143440	-1.567532	2.072241
C	-3.627903	-0.267568	1.769744
C	-2.770046	0.807912	1.567298
C	-3.283420	2.125412	1.119320
C	-1.377183	0.570512	1.749447
O	-0.480011	1.614716	1.427496
C	-0.842277	-0.646583	2.161515
C	0.598687	-0.733821	2.524264
C	-1.729993	-1.778051	2.256730
C	1.611948	-0.316839	1.656918
O	1.321462	0.114149	0.355708
C	3.000032	-0.423214	1.982937
C	4.104672	0.067383	1.116907
C	3.336729	-0.986406	3.208437
C	2.359368	-1.373708	4.158010
C	0.966490	-1.203420	3.840821
C	-1.261908	-3.106738	2.463217
C	-2.149227	-4.170050	2.505569
C	-3.544810	-3.956524	2.366045
C	-4.031004	-2.679588	2.151790
C	2.738018	-1.871875	5.437968
C	1.782168	-2.167599	6.392851
C	0.410751	-1.954013	6.102440
C	0.011685	-1.483106	4.861546
C	-2.780870	3.340251	1.630642
C	-3.288828	4.562846	1.175745
C	-2.690696	5.850170	1.682192
F	-3.596962	6.863630	1.693896
F	-1.652582	6.264220	0.888329
F	-2.194029	5.724663	2.940974
C	-4.300096	4.609044	0.204166
C	-4.803394	3.405532	-0.298946
C	-5.891043	3.391084	-1.344538
F	-5.502178	2.701524	-2.453615
F	-6.240415	4.643340	-1.742487
F	-7.017579	2.780975	-0.879841
C	-4.304719	2.176429	0.153660
C	5.231450	-0.751452	0.913638
C	6.363302	-0.258237	0.252084
C	7.594544	-1.118974	0.122865

F	7.300460	-2.446593	0.125419
F	8.459007	-0.902029	1.157216
F	8.284116	-0.851462	-1.023152
C	6.391229	1.055786	-0.225247
C	5.264321	1.869544	-0.037855
C	5.327937	3.285546	-0.550044
F	4.191274	3.991534	-0.292777
F	5.522219	3.314219	-1.905040
F	6.364990	3.973644	0.000254
P	0.235743	1.283969	-0.017652
O	1.119195	2.595532	-0.239747
C	4.126010	1.386057	0.619762
O	-0.698097	0.852330	-1.108219
C	2.904420	-1.984406	-2.439327
C	3.608631	-3.099870	-1.963706
C	5.003516	-3.076374	-2.084853
C	5.677750	-1.979586	-2.664424
C	4.970643	-0.865251	-3.122292
C	3.567651	-0.858478	-3.012042
C	2.554418	0.103318	-3.396262
C	2.798444	1.478126	-3.951346
C	2.645118	2.559595	-2.881151
O	1.233581	2.749462	-2.621117
C	0.964081	3.468049	-1.478574
C	-0.424348	4.063642	-1.541581
C	1.341460	-0.442932	-3.058401
N	1.524740	-1.703615	-2.460769
C	0.517158	-2.578207	-1.988675
N	-0.689184	-1.938054	-1.773247
C	-1.934623	-2.553699	-1.594736
O	0.733040	-3.779201	-1.810827
C	-2.102501	-3.941071	-1.415205
C	-3.394300	-4.467937	-1.285894
C	-3.542487	-5.947275	-1.034473
F	-2.652175	-6.677401	-1.758008
F	-4.789586	-6.397338	-1.342357
F	-3.324527	-6.259936	0.280329
C	-4.528743	-3.651533	-1.325271
C	-4.349963	-2.270517	-1.497966
C	-5.567037	-1.384881	-1.501790
F	-6.036312	-1.163932	-0.228912
F	-6.595378	-1.936599	-2.196343
F	-5.321053	-0.156170	-2.040126
C	-3.073525	-1.718206	-1.627726
H	-4.706128	-0.121845	1.656288
H	4.394195	-1.076639	3.478875
H	-0.187818	-3.285372	2.557825
H	-1.768988	-5.188330	2.631794
H	-4.228988	-4.809238	2.392149
H	-5.100047	-2.505341	1.992565
H	3.804632	-1.999295	5.653481
H	2.081058	-2.545532	7.375591
H	-0.343898	-2.154784	6.869619
H	-1.049101	-1.313871	4.667245
H	-1.998857	3.332486	2.392979
H	-4.688513	5.565985	-0.151314

H	-4.701093	1.249620	-0.266354
H	5.218429	-1.785930	1.266508
H	7.275964	1.441200	-0.739529
H	3.269923	2.046068	0.774446
H	1.741613	4.221709	-1.263479
H	3.076916	3.521392	-3.216989
H	3.149822	2.239996	-1.956634
H	-0.663954	4.587570	-0.604634
H	-0.455855	4.794328	-2.366714
H	-1.174627	3.281878	-1.736528
H	3.083043	-3.952951	-1.533550
H	5.583489	-3.930863	-1.722395
H	6.768503	-1.995977	-2.736808
H	5.497080	-0.007673	-3.555581
H	2.115521	1.710475	-4.788306
H	3.826105	1.545471	-4.350085
H	0.347016	-0.030793	-3.201652
H	-0.679252	-0.910527	-1.655333
H	-1.225942	-4.587826	-1.382775
H	-5.530020	-4.078525	-1.235485
H	-2.947739	-0.641499	-1.773160

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy=	-4886.68579333	Predicted Change= -2.866680D-08
Zero-point correction (ZPE)=	-4885.8956	0.79009
Internal Energy (U)=	-4885.8501	0.83559
Enthalpy (H)=	-4885.8494	0.83633
Gibbs Free Energy (G)=	-4885.9706	0.71514

Frequencies -- 9.7251 14.1752 16.7634

PBE-D3BJ/6-311++G(2df,p) = -4888.177993
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -4888.215866
PBE/def2-TZVPP = -4887.60449602910

Phosphate Acetal C

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) freq=noraman
iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4886.67982265 Predicted Change= -3.242316D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?

Force	0.00004	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00476	0.00180	[NO]	0.00476	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.957627	-0.446586	3.666514
C	2.982343	0.832189	3.049296
C	1.989910	1.234378	2.163236
C	2.046315	2.565548	1.501473
C	0.982627	0.282920	1.820489
O	-0.023208	0.690368	0.919674
C	0.996528	-1.040231	2.266096
C	0.103065	-2.029842	1.603032
C	1.946630	-1.399510	3.285419
C	-1.261686	-1.768522	1.485649
O	-1.811062	-0.669020	2.155816
C	-2.151511	-2.585589	0.728284
C	-3.581797	-2.230896	0.554721
C	-1.622777	-3.693861	0.080168
C	-0.247358	-4.027997	0.167362
C	0.644730	-3.189090	0.929464
C	1.914769	-2.658656	3.949688
C	2.854418	-2.972750	4.917892
C	3.873557	-2.048304	5.264854
C	3.920262	-0.808757	4.652066
C	0.265493	-5.167229	-0.517939
C	1.609730	-5.484981	-0.459115
C	2.490336	-4.658855	0.283090
C	2.028085	-3.531955	0.943712
C	0.951195	3.448751	1.501920
C	1.032216	4.671932	0.823892
C	-0.180397	5.568354	0.817619
F	-1.294124	4.888836	0.413085
F	-0.033408	6.631609	-0.019635
F	-0.451910	6.061386	2.057276
C	2.197768	5.042859	0.145279
C	3.294008	4.170622	0.155665
C	4.504736	4.496637	-0.677577
F	5.636342	3.924519	-0.188800
F	4.721072	5.835301	-0.768261
F	4.352953	4.034030	-1.961288
C	3.222812	2.940957	0.823092
C	-4.438873	-1.985029	1.642296
C	-5.786386	-1.664190	1.419269
C	-6.675571	-1.349318	2.597246
F	-6.386642	-2.133970	3.669162
F	-7.991458	-1.522371	2.300268
F	-6.527533	-0.052853	3.003280
C	-6.291359	-1.545318	0.118024
C	-5.433950	-1.782462	-0.966205
C	-5.960975	-1.614070	-2.368458
F	-6.680125	-0.457538	-2.486375
F	-6.786407	-2.629506	-2.735662
F	-4.957028	-1.554454	-3.290582
P	-1.493590	0.869250	1.662446

O	-2.430545	1.175094	0.405497
C	-4.098076	-2.139002	-0.752250
O	-1.558141	1.820478	2.811115
C	-0.203934	1.816019	-2.858510
C	1.029431	2.487805	-2.824211
C	1.002447	3.887176	-2.780411
C	-0.214842	4.599452	-2.762875
C	-1.438151	3.927252	-2.824612
C	-1.442452	2.522412	-2.902015
C	-2.503856	1.545929	-3.053651
C	-3.977455	1.827878	-3.006450
C	-4.498034	1.762088	-1.565742
O	-3.742342	2.706477	-0.773010
C	-3.437640	2.323671	0.512027
C	-4.604219	1.863997	1.365831
C	-1.905654	0.311997	-3.095321
N	-0.516173	0.444024	-2.945595
C	0.315702	-0.684392	-2.765279
N	1.431064	-0.386852	-2.002389
C	2.545592	-1.196819	-1.762232
O	0.027234	-1.789775	-3.221507
C	3.457879	-0.760833	-0.781116
C	4.611821	-1.504561	-0.518537
C	5.512760	-1.113681	0.622675
F	6.813931	-1.413664	0.372393
F	5.168869	-1.776019	1.769110
F	5.449615	0.219918	0.906760
C	4.880272	-2.686621	-1.220493
C	3.953131	-3.121043	-2.177515
C	4.219119	-4.413554	-2.908905
F	4.722774	-5.365155	-2.065435
F	5.134964	-4.253915	-3.905073
F	3.096005	-4.930025	-3.471878
C	2.791054	-2.396356	-2.459024
H	3.781242	1.533268	3.313377
H	-2.285079	-4.335337	-0.511454
H	1.131143	-3.375757	3.690744
H	2.807708	-3.942827	5.422922
H	4.614495	-2.315236	6.024956
H	4.692318	-0.079587	4.920708
H	-0.430937	-5.780617	-1.099916
H	2.000907	-6.352678	-0.998954
H	3.556904	-4.897738	0.310964
H	2.742554	-2.897929	1.468973
H	0.039600	3.185423	2.047673
H	2.248294	5.992061	-0.392158
H	4.078448	2.259685	0.801825
H	-4.058380	-2.055027	2.664453
H	-7.334481	-1.263517	-0.047527
H	-3.433457	-2.312264	-1.602082
H	-2.894920	3.165051	0.964740
H	-4.353979	0.742647	-1.174721
H	-5.573410	2.016655	-1.517490
H	-5.341092	2.682914	1.429171
H	-5.097484	0.978694	0.940835
H	-4.267672	1.626613	2.386759

H	1.988245	1.963533	-2.863549
H	1.953213	4.425996	-2.756512
H	-0.199242	5.691328	-2.692464
H	-2.381952	4.480548	-2.813402
H	-4.545688	1.089427	-3.597925
H	-4.194830	2.824119	-3.430901
H	-2.331440	-0.684087	-3.194776
H	1.383071	0.475773	-1.456437
H	3.252388	0.153320	-0.215658
H	5.776747	-3.272320	-1.002949
H	2.061368	-2.765007	-3.179210

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -4886.67982265	Predicted Change= -3.242316D-08	
Zero-point correction (ZPE)=	-4885.8893	0.79044
Internal Energy (U)=	-4885.8438	0.83594
Enthalpy (H)=	-4885.8431	0.83668
Gibbs Free Energy (G)=	-4885.9633	0.71642

Frequencies -- 14.8830 17.3626 20.3428

PBE-D3BJ/6-311++G(2df,p) = -4888.171483
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -4888.210835
PBE/def2-TZVPP = -4887.59293040622

Major-TS w/o urea

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========

# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) freq=noraman
SCRF=(SMD,SOLVENT=Toluene) iop(1/8=18) Temperature=233.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C57H33F18N2O6P C1[X(C57H33F18N2O6P)] #Atoms= 117
Charge = 0 Multiplicity = 1

SCF Energy= -4886.65573618 Predicted Change= -5.508857D-10
==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00116 ||	0.00180	[YES]	0.00116 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.977512	-4.057644	1.040751
C	-1.948986	-3.039039	1.186424
C	-1.612208	-1.712376	1.442152

C	-2.703387	-0.711271	1.550351
C	-0.218469	-1.392961	1.594469
O	0.125175	-0.076091	1.834879
C	0.769425	-2.385605	1.589143
C	2.192463	-2.043979	1.861570
C	0.409801	-3.736749	1.241730
C	2.822419	-1.093417	1.064607
O	2.057363	-0.392772	0.143933
C	4.222779	-0.817727	1.138103
C	4.858018	0.126287	0.188660
C	4.961687	-1.476316	2.113192
C	4.357440	-2.385276	3.022966
C	2.950849	-2.681214	2.905850
C	1.372004	-4.767745	1.031788
C	0.978400	-6.045337	0.667422
C	-0.393314	-6.362026	0.488655
C	-1.352794	-5.381787	0.669419
C	5.118405	-3.016308	4.049046
C	4.520931	-3.886850	4.943999
C	3.131170	-4.154990	4.848086
C	2.364902	-3.568649	3.853238
C	-3.883589	-0.903717	0.800584
C	-4.967944	-0.028823	0.916727
C	-6.231014	-0.288305	0.135961
F	-7.193789	-0.849534	0.921642
F	-6.033663	-1.130232	-0.913545
F	-6.766273	0.868215	-0.359991
C	-4.910098	1.066497	1.786849
C	-3.739260	1.270326	2.531087
C	-3.699470	2.442641	3.478458
F	-4.024542	3.607079	2.839269
F	-2.475148	2.621194	4.042091
F	-4.596120	2.295861	4.494150
C	-2.648244	0.397846	2.423055
C	5.828607	1.043742	0.631504
C	6.443832	1.921326	-0.271674
C	7.433184	2.939734	0.234506
F	6.819452	4.102203	0.600367
F	8.356692	3.264298	-0.713552
F	8.109737	2.489646	1.326881
C	6.095296	1.911859	-1.628254
C	5.128062	0.999451	-2.071569
C	4.781005	0.929124	-3.536430
F	3.489837	0.541899	-3.733506
F	5.567687	0.035527	-4.201546
F	4.943341	2.133759	-4.154320
P	1.102045	0.828271	0.787270
O	1.842363	1.822799	1.630449
C	4.518412	0.109810	-1.179787
O	0.304807	1.299483	-0.432565
H	-3.001715	-3.322120	1.095664
H	6.041413	-1.301908	2.182971
H	2.434554	-4.536524	1.131852
H	1.738391	-6.815010	0.497939
H	-0.686549	-7.374332	0.192624
H	-2.414209	-5.593169	0.498176

H	6.188047	-2.789004	4.120169
H	5.115014	-4.361163	5.731696
H	2.657530	-4.828386	5.569873
H	1.293178	-3.775131	3.794272
H	-3.954379	-1.741171	0.104994
H	-5.753756	1.756408	1.874812
H	-1.753715	0.573635	3.021315
H	6.089964	1.084851	1.692650
H	6.568598	2.605109	-2.327951
H	3.778941	-0.605225	-1.546563
C	-3.328966	3.641617	-1.049360
C	-4.668554	3.533999	-0.664432
C	-5.246266	4.671013	-0.084706
C	-4.512255	5.860354	0.099923
C	-3.171141	5.952017	-0.295391
C	-2.571558	4.828730	-0.882922
C	-1.200700	4.558176	-1.346844
C	-0.136867	4.217797	0.420509
O	0.315203	5.479878	0.481182
C	0.902008	5.816754	-0.793254
C	-0.239238	5.633618	-1.828669
C	-1.247974	3.227686	-1.849899
N	-2.462557	2.672248	-1.623161
C	-2.845926	1.287774	-1.926044
N	-1.779712	0.461242	-1.795478
C	-1.722675	-0.910870	-2.095595
O	-4.002995	1.031757	-2.245334
C	-0.433811	-1.480906	-2.120521
C	-0.282983	-2.851723	-2.344268
C	1.112036	-3.417504	-2.456856
F	1.655359	-3.144740	-3.679413
F	1.133044	-4.766667	-2.302179
F	1.957720	-2.881043	-1.530264
C	-1.402659	-3.679521	-2.503713
C	-2.677461	-3.098881	-2.467410
C	-3.897054	-3.981305	-2.444843
F	-3.685650	-5.180131	-3.046615
F	-4.971413	-3.399861	-3.036558
F	-4.266634	-4.253007	-1.146109
C	-2.854604	-1.718735	-2.298237
C	-0.991027	3.764054	1.542486
H	1.747743	5.135907	-0.997250
H	1.267438	6.850254	-0.718396
H	-0.798011	6.576667	-1.943227
H	0.185070	5.379637	-2.813704
H	-0.452556	2.654911	-2.323456
H	-5.234119	2.615409	-0.818898
H	-6.294509	4.631298	0.227108
H	-4.999434	6.726854	0.557268
H	-2.603332	6.875480	-0.143215
H	0.543864	3.472434	-0.014767
H	-1.676396	4.544995	1.900258
H	-0.317436	3.447590	2.361212
H	-1.555702	2.868736	1.239933
H	-0.937070	0.808330	-1.247764
H	0.440822	-0.847006	-1.949000

```
      H       -1.283244     -4.757305     -2.628544
      H       -3.852028     -1.278246     -2.277737
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 233.150 Kelvin       Pressure= 1.00000 Atm
===========================================================================
 SCF Energy=     -4886.65573618   Predicted Change= -5.508857D-10
 Zero-point correction (ZPE)=            -4885.8675      0.78815
 Internal Energy (U)=                    -4885.8219      0.83375
 Enthalpy (H)=                           -4885.8212      0.83448
 Gibbs Free Energy (G)=                  -4885.9428      0.71287
---------------------------------------------------------------------------
 Frequencies --   -199.2367               9.0986              12.7596

PBE-D3BJ/6-311++G(2df,p) = -4888.150191
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -4888.194974
PBE/def2-TZVPP = -4887.58867816919
```

Major-TS-Hbond-Substrate

```
---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
===========================================================================
 #pbepbe/6-31G(d)/auto EmpiricalDispersion=GD3BJ
 scf=(maxcycle=300,direct,tight) density=current
 opt=(maxcycle=250,modredundant) iop(1/8=18) Temperature=233.15
 SCRF=(SMD,SOLVENT=Toluene)
 Modredundant Input:  B       7      11 F
 Modredundant Input:
--link 1--
#pbepbe/6-31G(d)/auto EmpiricalDispersion=GD3BJ
 scf=(direct,tight,maxcycle=300,xqc)
 opt=(nofreeze,maxcycle=250,ts,calcfc,noeigentest) iop(1/8=18) freq=noraman
 Temperature=233.15 geom=check guess=read SCRF=(SMD,SOLVENT=Toluene)
 #P Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
 Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C74H41F30N4O7P   C1[X(C74H41F30N4O7P)]  #Atoms= 157
 Charge = 0         Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -6920.20377045       Predicted Change= -1.879718D-09
===========================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00253 ||  0.00180   [ NO ]       0.00253 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
      Atomic              Coordinates (Angstroms)
       Type              X             Y         Z
---------------------------------------------------------------------------
      C       -1.732883      2.169814      1.173436
      C       -2.964646      1.634830      1.561627
      C       -3.749733      2.426280      2.410951
      C       -3.307079      3.686215      2.861369
      C       -2.047295      4.184884      2.501178
```

C	-1.245569	3.413975	1.649972
C	0.133081	3.586446	1.148821
C	0.810157	4.935886	0.939062
C	1.863163	5.163583	2.055984
O	1.404482	4.380515	3.179047
C	1.280559	3.101737	2.781684
H	2.134561	2.692231	2.220547
C	0.332096	2.476937	0.281142
N	-0.731068	1.636190	0.316639
C	-0.847918	0.445777	-0.510917
N	0.334150	-0.170318	-0.645027
C	0.572982	-1.277549	-1.498870
O	-1.933895	0.150365	-1.032510
C	-0.213185	-2.434230	-1.451564
C	0.163696	-3.547741	-2.213813
C	-0.655655	-4.802831	-2.061518
F	-1.966902	-4.573998	-2.359629
F	-0.222212	-5.813796	-2.851402
F	-0.622773	-5.253222	-0.767587
C	1.298964	-3.513866	-3.034293
C	2.058717	-2.338091	-3.089599
C	3.269794	-2.222456	-3.981220
F	3.029933	-1.386506	-5.031669
F	4.332913	-1.693094	-3.303628
F	3.658808	-3.416490	-4.493628
C	1.700930	-1.220882	-2.326908
C	0.609143	2.185569	3.736648
H	2.865547	4.816169	1.751187
H	1.924233	6.206456	2.396799
H	-0.257294	2.650417	4.229654
H	1.354180	1.900973	4.502808
H	0.324250	1.258721	3.217674
H	-3.302188	0.652282	1.230116
H	-4.729358	2.053890	2.724676
H	-3.955205	4.280533	3.512252
H	-1.694313	5.150224	2.876188
H	1.287273	4.982044	-0.052121
H	0.038147	5.719753	0.964572
H	1.170420	2.279138	-0.381866
H	1.074949	0.032510	0.116340
H	-1.076948	-2.474806	-0.785171
H	1.598466	-4.394887	-3.604448
H	2.288250	-0.301220	-2.366764
C	2.988276	-4.780239	0.043953
C	2.113244	-4.371302	1.081607
C	2.305837	-3.187985	1.786958
C	1.232957	-2.665856	2.669909
C	3.473113	-2.411952	1.488714
O	3.716070	-1.262173	2.227553
C	4.369575	-2.763933	0.474067
C	5.459718	-1.811964	0.117785
C	4.114195	-3.949832	-0.302839
C	5.105828	-0.496199	-0.182123
O	3.780307	-0.101439	-0.044533
P	3.303714	0.217591	1.545945
C	6.048993	0.488290	-0.607712

C	5.548402	1.850301	-0.918863
C	7.385219	0.127731	-0.692569
C	7.817241	-1.184999	-0.354897
C	6.852068	-2.170424	0.070439
C	4.882673	-4.308727	-1.448241
C	4.580677	-5.444846	-2.183175
C	3.496361	-6.282081	-1.814114
C	2.712589	-5.949676	-0.722954
C	9.195390	-1.541145	-0.410474
C	9.619511	-2.805357	-0.039082
C	8.675811	-3.762773	0.413856
C	7.326198	-3.453467	0.468071
C	1.481551	-1.985624	3.879812
C	0.424571	-1.416345	4.600508
C	0.706944	-0.715239	5.905292
F	1.946895	-0.149970	5.921871
F	0.645674	-1.567633	6.965709
F	-0.194249	0.282119	6.145674
C	-0.896887	-1.490747	4.134150
C	-1.147529	-2.185156	2.946254
C	-2.532550	-2.253176	2.362818
F	-2.544913	-1.702585	1.090320
F	-3.449409	-1.566235	3.086448
F	-2.975714	-3.526761	2.220787
C	-0.099969	-2.780997	2.231415
C	4.492457	2.006420	-1.838504
C	3.933081	3.266398	-2.071755
C	2.745355	3.419613	-2.983897
F	1.628350	3.810812	-2.273999
F	2.415154	2.259878	-3.610835
F	2.941069	4.367253	-3.933775
C	4.437354	4.401957	-1.418447
C	5.499350	4.250492	-0.518511
C	5.968285	5.448784	0.266458
F	7.241806	5.306778	0.711888
F	5.180789	5.655869	1.369965
F	5.910003	6.592675	-0.468982
C	6.049756	2.984515	-0.261016
O	1.780699	0.333855	1.429017
O	4.102908	1.296121	2.216062
H	1.239093	-4.994165	1.299140
H	8.127635	0.861956	-1.025330
H	5.704090	-3.662825	-1.764138
H	5.177841	-5.688301	-3.067686
H	3.269484	-7.176070	-2.403826
H	1.845269	-6.560138	-0.450245
H	9.915734	-0.786279	-0.745213
H	10.682211	-3.064565	-0.081704
H	9.016831	-4.754162	0.729317
H	6.607883	-4.194759	0.828087
H	2.504515	-1.880972	4.244524
H	-1.709567	-1.004746	4.678704
H	-0.313873	-3.306335	1.296052
H	4.121550	1.130336	-2.374710
H	4.008991	5.390303	-1.610033
H	6.844604	2.873478	0.481339

C	-5.413826	0.552032	-1.151366
N	-4.852386	-0.717576	-0.996578
C	-5.519293	-1.920525	-0.736968
H	-3.833965	-0.790323	-1.072450
N	-4.425019	1.504663	-1.375339
H	-3.449989	1.176106	-1.325047
C	-4.570982	2.890929	-1.412823
O	-6.623208	0.795765	-1.093632
C	-4.742047	-3.097805	-0.698671
H	-3.670078	-3.052490	-0.908183
C	-5.337872	-4.328295	-0.405919
C	-4.486188	-5.574057	-0.401702
F	-4.258704	-6.035394	-1.664690
F	-5.072683	-6.587501	0.291881
F	-3.265070	-5.350522	0.161241
C	-6.714348	-4.422453	-0.163385
H	-7.176953	-5.384386	0.064704
C	-7.481110	-3.252015	-0.221583
C	-8.954294	-3.312204	0.100012
F	-9.671556	-2.414420	-0.628216
F	-9.189714	-3.031897	1.415191
F	-9.477417	-4.546237	-0.140699
C	-6.907151	-2.005921	-0.501034
H	-7.515440	-1.102715	-0.544984
C	-3.378409	3.646421	-1.466839
H	-2.413886	3.134980	-1.511873
C	-3.421765	5.039202	-1.453529
C	-2.140882	5.829483	-1.427017
F	-1.966567	6.450357	-0.216849
F	-2.124436	6.810624	-2.366881
F	-1.038895	5.049325	-1.632347
C	-4.646623	5.723528	-1.411993
H	-4.680157	6.815497	-1.400785
C	-5.824353	4.967895	-1.379498
C	-7.160390	5.669855	-1.401244
F	-7.637680	5.797737	-2.672713
F	-7.083852	6.925543	-0.878777
F	-8.101755	4.989776	-0.692360
C	-5.807115	3.565633	-1.376318
H	-6.733063	2.992438	-1.331095

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy=	-6920.20377045	Predicted Change= -1.879718D-09
Zero-point correction (ZPE)=	-6919.1769	1.02678
Internal Energy (U)=	-6919.1118	1.09195
Enthalpy (H)=	-6919.1110	1.09269
Gibbs Free Energy (G)=	-6919.2769	0.92678

Frequencies -- -261.3007 7.3033 10.0497

PBE-D3BJ/6-311++G(2df,p) = -6922.395297
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -6922.448691
PBE/def2-TZVPP = -6921.70241879243

Major Interaction

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,modredundant,gdiis)
freq=noraman iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
Modredundant Input: X * B
Modredundant Input: X * F
Modredundant Input: X 50 A
Modredundant Input: X 51 A
Modredundant Input: X 52 A
Modredundant Input:
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C26H14F12 C1[X(C26H14F12)] #Atoms= 52
Charge = 0 Multiplicity = 1

SCF Energy= -2195.10705501 Predicted Change= -4.405008D-07
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00008	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00511	0.00180	[NO]	0.00511	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.070048	0.754271	2.392784
C	1.026576	1.734348	1.388660
C	2.089635	1.821287	0.478840
C	1.956001	2.791699	-0.666780
F	1.674200	4.049062	-0.234722
F	3.073795	2.854687	-1.432837
F	0.922989	2.429957	-1.499152
C	3.205125	0.977991	0.572906
C	3.250269	0.033503	1.605734
C	4.437584	-0.878823	1.785553
F	5.060839	-0.643543	2.976438
F	4.060710	-2.191557	1.803277
F	5.363835	-0.730659	0.805440
C	2.189803	-0.084532	2.510669
H	0.156679	2.388240	1.298015
H	4.015657	1.044359	-0.154424
H	2.224197	-0.822708	3.317015
C	1.580293	-1.144278	-1.912450
C	0.231243	-0.753460	-1.718840
C	-0.607503	-1.421268	-0.834866
C	-1.945540	-0.868364	-0.509726
C	-0.088747	-2.575703	-0.167709
C	1.214511	-3.041847	-0.350343
C	2.101427	-2.281220	-1.196899
C	3.493176	-2.563012	-1.311013

C	4.314868	-1.787789	-2.114201
C	3.790991	-0.692298	-2.847139
C	2.448237	-0.374591	-2.740914
C	-3.084088	-1.680371	-0.326667
C	-4.301767	-1.113008	0.065193
C	-5.511352	-1.991958	0.261455
F	-5.167724	-3.282059	0.534038
F	-6.311650	-2.015525	-0.838974
F	-6.282507	-1.551482	1.299664
C	-4.426742	0.270775	0.259862
C	-3.310258	1.083697	0.036329
C	-3.412317	2.580225	0.182207
F	-2.350206	3.094150	0.875376
F	-4.541432	2.959209	0.844956
F	-3.426179	3.205456	-1.026041
C	-2.081068	0.523119	-0.338779
H	-0.143342	0.120261	-2.260849
H	3.921661	-3.382419	-0.731710
H	5.383639	-2.017211	-2.170718
H	4.452400	-0.088834	-3.476930
H	2.034849	0.493877	-3.264353
H	-3.017170	-2.756703	-0.487194
H	-5.372321	0.705168	0.592363
H	-1.209545	1.169824	-0.475349
H	0.239809	0.657567	3.098302
H	-0.745806	-3.106301	0.531996
H	1.586815	-3.914730	0.193470

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy=	-2195.10705501	Predicted Change= -4.405008D-07
Zero-point correction (ZPE)=	-2194.7678	0.33918
Internal Energy (U)=	-2194.7463	0.36074
Enthalpy (H)=	-2194.7455	0.36148
Gibbs Free Energy (G)=	-2194.8186	0.28842

Frequencies -- 2.4717 12.6234 19.9477

PBE-D3BJ/6-311++G(2df,p) = -2195.831779
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -2195.849950
PBE/def2-TZVPP = -2195.64538813388

Minor Interaction

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

# pbepbe/6-31G*/auto EmpiricalDispersion=GD3BJ gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,modredundant,gdiis)
freq=noraman iop(1/8=18) Temperature=233.15 SCRF=(SMD,SOLVENT=Toluene)
Modredundant Input: X * B
Modredundant Input: X * F
Modredundant Input: X 50 A
Modredundant Input: X 51 A
Modredundant Input: X 52 A

Modredundant Input:
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto Freq

---

Pointgroup= C1 Stoichiometry= C26H14F12 C1[X(C26H14F12)] #Atoms= 52
Charge = 0 Multiplicity = 1

SCF Energy= -2195.10522033 Predicted Change= -6.117143D-06

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00031	0.00045	[YES]	0.00009	0.00030	[YES]
Displ	0.01570	0.00180	[NO]	0.01570	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.278463	-1.599708	-1.602385
C	0.929608	-1.184045	-1.485279
C	0.031437	-1.791706	-0.611144
C	-1.345347	-1.247691	-0.474736
C	0.512634	-2.928325	0.124522
C	1.790183	-3.466029	-0.045162
C	2.736747	-2.740928	-0.854976
C	4.114450	-3.090509	-0.937720
C	4.981442	-2.374464	-1.747372
C	4.518191	-1.276256	-2.516989
C	3.191715	-0.893531	-2.438585
C	-1.587732	0.121612	-0.730771
C	-2.872168	0.666519	-0.611528
C	-3.091765	2.146946	-0.810838
F	-4.287609	2.398850	-1.408204
F	-2.120730	2.717017	-1.568485
F	-3.108094	2.808506	0.387356
C	-3.952782	-0.122957	-0.197665
C	-3.721226	-1.479354	0.060707
C	-4.866788	-2.341082	0.522011
F	-5.601444	-1.703925	1.485214
F	-4.429503	-3.514266	1.075069
F	-5.723704	-2.663551	-0.478317
C	-2.449325	-2.042943	-0.097227
H	0.597253	-0.352057	-2.113977
H	4.490297	-3.925110	-0.341684
H	6.038785	-2.655260	-1.786367
H	5.215216	-0.724455	-3.155483
H	2.821164	-0.031330	-3.004183
H	-0.762842	0.784030	-1.000706
H	-4.947510	0.312982	-0.070151
H	-2.319116	-3.105109	0.097683
C	0.106497	0.792023	2.273534
C	1.339474	0.111325	2.272522
C	2.412265	0.619140	1.535050
C	3.752523	-0.071794	1.605929
F	4.538001	0.477434	2.577683
F	4.436682	0.037332	0.436046
F	3.630195	-1.394890	1.895586

C	2.268150	1.782095	0.768278
C	1.032601	2.444585	0.775236
C	0.830549	3.597997	-0.174198
F	1.904500	4.433002	-0.198823
F	-0.265444	4.337405	0.124894
F	0.668975	3.133280	-1.454397
C	-0.047584	1.977435	1.534557
H	1.444839	-0.821081	2.833525
H	3.098865	2.157431	0.165339
H	-1.003535	2.499917	1.520466
H	-0.733366	0.394313	2.850282
H	2.110431	-4.345313	0.520716
H	-0.180178	-3.434815	0.807312

Statistical Thermodynamic Analysis
Temperature= 233.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy=	-2195.10522033	Predicted Change=	-6.117143D-06
Zero-point correction (ZPE)=		-2194.7658	0.33934
Internal Energy (U)=		-2194.7451	0.36009
Enthalpy (H)=		-2194.7443	0.36083
Gibbs Free Energy (G)=		-2194.8137	0.29146

Frequencies -- -14.0970 4.3534 13.4108

PBE-D3BJ/6-311++G(2df,p) = -2195.828480
PBE-D3BJ/6-311++G(2df,p)/SMD(Toluene) = -2195.846926
PBE/def2-TZVPP = -2195.63800322790

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