Supporting Information

for

# Presence or absence of a novel charge-transfer complex in the base-catalyzed hydrolysis of *N*-ethylbenzamide or ethyl benzoate

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## Detailed geometric data along with those of complementary calculations

**Figure S1** Geometric changes by an ADMP dynamical calculation from the TS1(es) geometry in  the reaction of Ph-C(=O)-O-Et + $OH^-(H_2O)_{16}$. XYZ coordinates are in ESI VII [5].
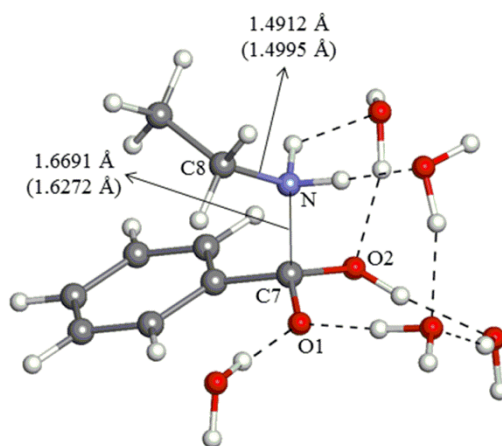


**Figure S2** The geometry optimized by B3LYP/6-31(+)G(d) SCRF = PCM and (B3PW91/6-311+G(d,p) SCRF = PCM). Can the geometry of the Mulliken charge-transfer complex of benzoic acid (Ph-C(=O)OH) and ethylamine ($H_5C_2$-$NH_2$) be expressed by the aid of $(H_2O)_5$ and SCRF = PCM solvent effect? The answer is yes. XYZ coordinates are in ESI VII [6].
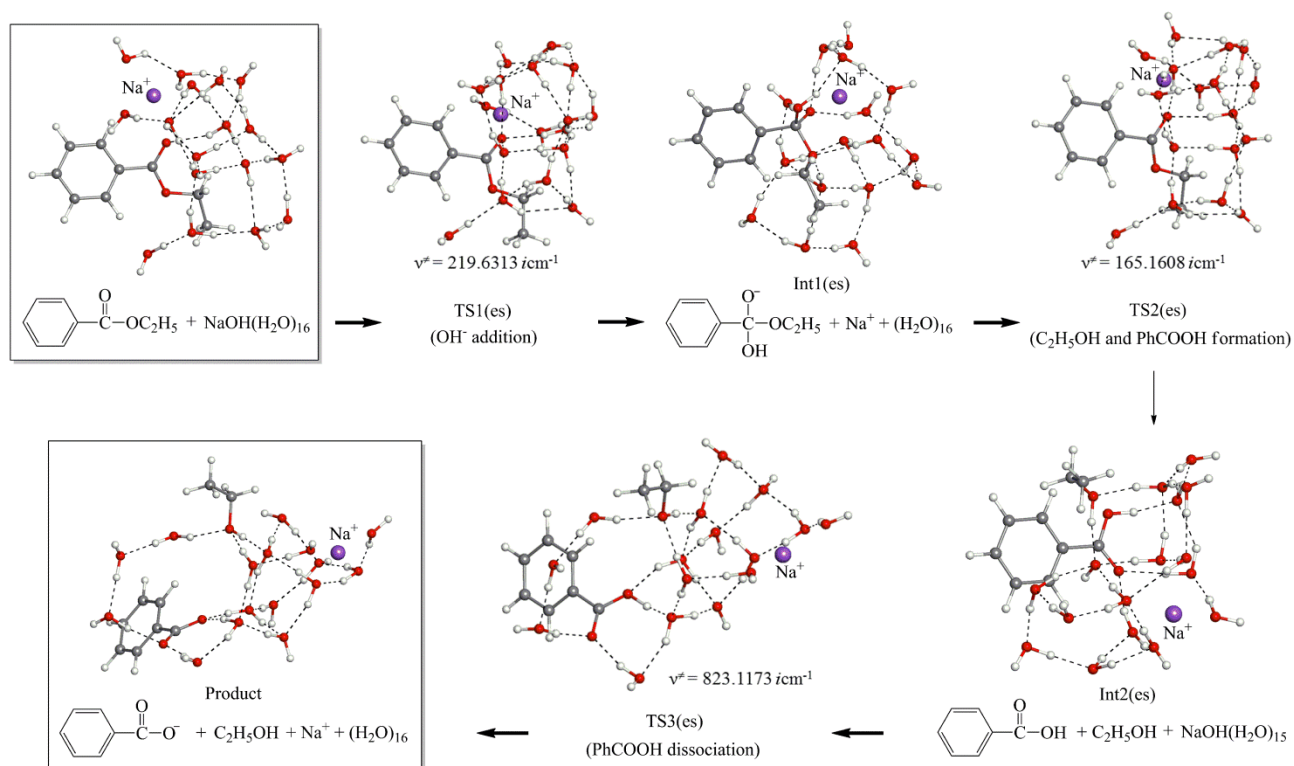
**Figure S3** Reaction paths of the hydrolysis in Ph-C(=O)-O-Et + NaOH($H_2O$)$_{16}$. XYZ coordinates are in ESI VII [7].
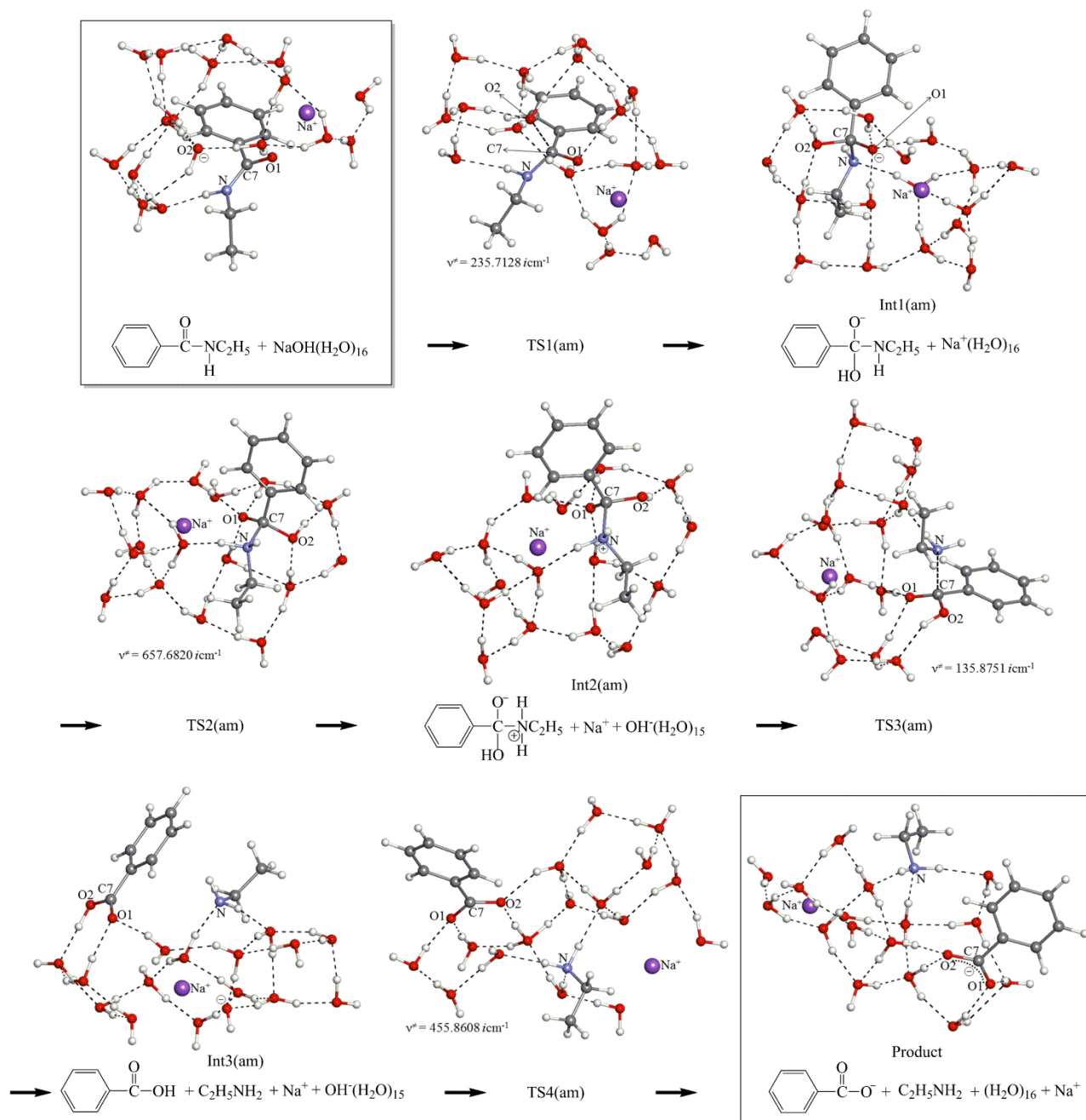
**Figure S4** Reaction paths of the hydrolysis in Ph-C(=O)-NH-Et + NaOH$(H_2O)_{16}$. XYZ coordinates are in ESI VII [8].

**Table S1** Dependence of computational methods on TS1(es) geometries in the $n$ =16 ester hydrolysis.[a]

| method | $v^{\neq}$ ($i$cm$^{-1}$) | $C_7\cdots O_3$ (Å) | $O_3\cdots H_2$ (Å) | $O_5\cdots H_2$ (Å) |
|---|---|---|---|---|
| B3LYP/6-31(+)G(d) | 200.41 | 1.990 | 1.544 | 1.038 |
| B3LYP/6-311+G(d,p) | 192.01 | 1.955 | 1.570 | 1.023 |
| B3PW91/6-31(+)G(d) | 183.61 | 2.066 | 1.467 | 1.060 |
| PCM/B3PW91/6-31(+)G(d) | 249.05 | 2.014 | 1.565 | 1.032 |
| B3PW91/6-311+G(d,p) | 197.65 | 1.997 | 1.497 | 1.041 |
| M06-2X/6-31(+)G(d) | 278.88 | 2.041 | 1.522 | 1.033 |

a) The numbering of atoms is shown in Figure 1.

**Table S2** Dependence of computational methods on TS1(am) geometries in the $n$ =16 amide hydrolysis.[a]

| method | $v^{\neq}$ ($i$cm$^{-1}$) | $C_7\cdots O_2$ (Å) | $O_2\cdots H_2$ (Å) | $O_3\cdots H_2$ (Å) |
|---|---|---|---|---|
| B3LYP/6-31(+)G(d) | 152.25 | 1.723 | 1.617 | 1.018 |
| B3LYP/6-311+G(d,p) | 113.80 | 1.697 | 1.645 | 1.006 |
| B3PW91/6-31(+)G(d) | 227.51 | 1.867 | 1.576 | 1.027 |
| PCM/B3PW91/6-31(+)G(d) | 289.16 | 1.882 | 1.563 | 1.028 |
| B3PW91/6-311+G(d,p) | 215.21 | 1.761 | 1.574 | 1.018 |
| M06-2X/6-31(+)G(d) | 271.49 | 1.889 | 1.656 | 1.007 |

a) The numbering of atoms is shown in Figure 2.

Cartesian Coordinates of B3LYP/6-31(+)G(d) and B3LYP/6-311+G(d,p) geometry optimizations

[1] TS1(es) geometries in Figure 1. Hereafter, n denotes the number of water molecules around Ph-COO-Et and OH⁻

 n=3  TS

ethyl benzoate(C6H5-COO-C2H5) and HO-(H2O)3, HO-, addition TS
zuka03aa.chk

               Standard orientation:
---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|-------|-------|-------|
| Number | Number | Type | X | Y | Z |

---------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.728327 | -0.592871 | -0.389120 |
| 2 | 6 | 0 | -0.511088 | 0.261283 | -0.588849 |
| 3 | 8 | 0 | -0.517536 | 1.223134 | -1.391341 |
| 4 | 8 | 0 | -0.585852 | 1.003929 | 1.104238 |
| 5 | 1 | 0 | -1.038267 | 1.829453 | 0.861533 |
| 6 | 6 | 0 | 1.845269 | -0.341286 | -1.190251 |
| 7 | 6 | 0 | 2.998526 | -1.117829 | -1.060244 |
| 8 | 6 | 0 | 0.779497 | -1.630564 | 0.550105 |
| 9 | 8 | 0 | -1.643156 | -0.587092 | -0.537163 |
| 10 | 6 | 0 | -2.870805 | 0.027511 | -0.925427 |
| 11 | 1 | 0 | -3.133839 | 0.812045 | -0.202694 |
| 12 | 1 | 0 | -2.749077 | 0.502127 | -1.904450 |
| 13 | 6 | 0 | -3.945021 | -1.049177 | -0.961851 |
| 14 | 1 | 0 | 0.609092 | 2.753086 | -1.100161 |
| 15 | 8 | 0 | 1.194357 | 3.485434 | -0.805908 |
| 16 | 1 | 0 | 1.527247 | 3.170954 | 0.059298 |
| 17 | 1 | 0 | -2.442648 | -1.183515 | 1.850487 |
| 18 | 8 | 0 | -2.214787 | -0.607065 | 2.595601 |
| 19 | 1 | 0 | -1.597485 | 0.042708 | 2.155660 |
| 20 | 1 | 0 | 0.917052 | 1.656884 | 1.576863 |
| 21 | 8 | 0 | 1.722347 | 2.215201 | 1.802937 |
| 22 | 1 | 0 | 1.442228 | 2.741493 | 2.565831 |
| 23 | 1 | 0 | -3.675452 | -1.842499 | -1.668081 |
| 24 | 1 | 0 | -4.087112 | -1.504216 | 0.025287 |
| 25 | 1 | 0 | -4.903265 | -0.616334 | -1.275543 |
| 26 | 6 | 0 | 1.931181 | -2.405695 | 0.679520 |
| 27 | 6 | 0 | 3.044460 | -2.154351 | -0.127274 |
| 28 | 1 | 0 | 1.795792 | 0.471892 | -1.907118 |
| 29 | 1 | 0 | 3.862716 | -0.908767 | -1.687201 |
| 30 | 1 | 0 | -0.078091 | -1.813083 | 1.188482 |
| 31 | 1 | 0 | 1.962363 | -3.204383 | 1.417732 |
| 32 | 1 | 0 | 3.943690 | -2.758294 | -0.022497 |

----------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) = -804.632753111     A.U. after    1 cycles

Convg  =    0.1662D-08          -V/T =  2.0094

S**2  =   0.0000

Zero-point correction=                        0.258592 (a.u.)
Thermal correction to Energy=                 0.278339
Thermal correction to Enthalpy=               0.279283
Thermal correction to Gibbs Free Energy=      0.208811
Sum of electronic and zero-point Energies=        -804.374161
Sum of electronic and thermal Energies=           -804.354414
Sum of electronic and thermal Enthalpies=         -804.353470
Sum of electronic and thermal Free Energies=      -804.423942


n=5 TS


ethyl benzoate and HO-(H2O)5, HO- addition TS1(es)
zuka05a.chk

Standard orientation:

--------------------------------------------------------------------------
| 1  | 6 | 0 | 0.600624 | -0.780942 | -0.664532 |
| 2  | 6 | 0 | -0.789370 | -0.190240 | -0.659086 |
| 3  | 8 | 0 | -1.099653 | 0.761281 | -1.409456 |
| 4  | 8 | 0 | -0.660679 | 0.616081 | 1.151754 |
| 5  | 1 | 0 | -1.337170 | 1.312738 | 1.064544 |
| 6  | 6 | 0 | 1.482174 | -0.399055 | -1.680628 |
| 7  | 6 | 0 | 2.766917 | -0.942415 | -1.743213 |
| 8  | 6 | 0 | 1.017355 | -1.713401 | 0.294353 |
| 9  | 8 | 0 | -1.716188 | -1.180540 | -0.375215 |
| 10 | 6 | 0 | -3.092369 | -0.794796 | -0.488615 |
| 11 | 1 | 0 | -3.308041 | -0.012796 | 0.249247 |
| 12 | 1 | 0 | -3.271029 | -0.382743 | -1.487143 |
| 13 | 6 | 0 | -3.945288 | -2.027973 | -0.240266 |
| 14 | 1 | 0 | -0.031149 | 2.413693 | -1.257499 |
| 15 | 8 | 0 | 0.263342 | 3.292104 | -0.935891 |
| 16 | 1 | 0 | 0.787736 | 3.072830 | -0.135334 |
| 17 | 1 | 0 | -1.863412 | -1.909431 | 2.160696 |
| 18 | 8 | 0 | -1.521889 | -1.328218 | 2.856315 |
| 19 | 1 | 0 | -1.185733 | -0.548566 | 2.327189 |
| 20 | 1 | 0 | 0.633115 | 1.470606 | 1.338222 |
| 21 | 8 | 0 | 1.415846 | 2.140087 | 1.432876 |
| 22 | 1 | 0 | 1.275295 | 2.567557 | 2.290789 |
| 23 | 1 | 0 | -3.708954 | -2.817905 | -0.961741 |
| 24 | 1 | 0 | -3.786939 | -2.424197 | 0.768881 |
| 25 | 1 | 0 | -5.006946 | -1.772702 | -0.340404 |
| 26 | 6 | 0 | 2.300601 | -2.255017 | 0.231788 |

| 27 | 6 | 0 | 3.179779 | -1.874386 | -0.788560 |
|----|---|---|----------|-----------|-----------|
| 28 | 1 | 0 | 1.150443 | 0.326593 | -2.416093 |
| 29 | 1 | 0 | 3.445587 | -0.634660 | -2.534832 |
| 30 | 1 | 0 | 0.345988 | -1.984667 | 1.101108 |
| 31 | 1 | 0 | 2.619712 | -2.968997 | 0.987064 |
| 32 | 1 | 0 | 4.180073 | -2.299206 | -0.835262 |
| 33 | 1 | 0 | -2.354436 | 2.159263 | -0.753496 |
| 34 | 8 | 0 | -2.520897 | 2.960124 | -0.217814 |
| 35 | 1 | 0 | -1.668038 | 3.431795 | -0.321215 |
| 36 | 1 | 0 | 3.105899 | 1.376397 | 1.398509 |
| 37 | 8 | 0 | 3.974029 | 0.911508 | 1.365319 |
| 38 | 1 | 0 | 3.784176 | 0.114324 | 0.846228 |

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SCF Done:  E(RB+HF-LYP) = -957.521199563    A.U. after   1 cycles

Convg  =   0.2048D-08         -V/T = 2.0093

S**2  =  0.0000

Zero-point correction=                         0.309377 (a.u.)

Thermal correction to Energy=                 0.334313

Thermal correction to Enthalpy=               0.335257

Thermal correction to Gibbs Free Energy=      0.253374

Sum of electronic and zero-point Energies=        -957.211822

Sum of electronic and thermal Energies=           -957.186887

Sum of electronic and thermal Enthalpies=         -957.185943

Sum of electronic and thermal Free Energies=      -957.267825

n=8 TS

ethyl benzoate and HO-(H2O)8, HO- addtion TS

zuka03cc.log

Standard orientation:

------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|-----|-----|-----|
| Number | Number | Type | X | Y | Z |

------------------------------------------------------------------

| 1 | 6 | 0 | -1.073567 | -0.895704 | -0.625382 |
|---|---|---|-----------|-----------|-----------|
| 2 | 6 | 0 | -1.793402 | 0.408425 | -0.291537 |
| 3 | 8 | 0 | -1.334862 | 1.511745 | -0.718983 |
| 4 | 8 | 0 | -1.635750 | 0.424046 | 1.434157 |
| 5 | 1 | 0 | -1.761439 | 1.375504 | 1.593949 |
| 6 | 6 | 0 | -0.098352 | -0.877172 | -1.626124 |
| 7 | 6 | 0 | 0.576375 | -2.047622 | -1.983592 |
| 8 | 6 | 0 | -1.372906 | -2.104943 | 0.016980 |
| 9 | 8 | 0 | -3.182115 | 0.167471 | -0.454536 |
| 10 | 6 | 0 | -4.004193 | 1.336830 | -0.497305 |
| 11 | 1 | 0 | -3.994129 | 1.833901 | 0.483403 |

| 12 | 1 | 0 | -3.599734 | 2.038862 | -1.232472 |
|----|---|---|-----------|----------|-----------|
| 13 | 6 | 0 | -5.415839 | 0.902311 | -0.859323 |
| 14 | 1 | 0 | 0.190741 | 2.072760 | -0.189854 |
| 15 | 8 | 0 | 1.066981 | 2.341163 | 0.214288 |
| 16 | 1 | 0 | 1.186752 | 1.712777 | 0.958133 |
| 17 | 1 | 0 | -4.292065 | -1.001827 | 1.540633 |
| 18 | 8 | 0 | -3.873784 | -0.933442 | 2.412761 |
| 19 | 1 | 0 | -3.042994 | -0.445100 | 2.193733 |
| 20 | 1 | 0 | -0.081249 | 0.199837 | 1.898997 |
| 21 | 8 | 0 | 0.909861 | 0.218151 | 2.116011 |
| 22 | 1 | 0 | 0.983646 | 0.288655 | 3.079200 |
| 23 | 1 | 0 | 1.940578 | -1.058635 | 1.358326 |
| 24 | 8 | 0 | 2.510877 | -1.713603 | 0.889800 |
| 25 | 1 | 0 | 1.898862 | -2.228205 | 0.337169 |
| 26 | 1 | 0 | 1.824678 | 4.192662 | 0.451091 |
| 27 | 8 | 0 | 2.539759 | 4.849123 | 0.333473 |
| 28 | 1 | 0 | 3.203378 | 4.337511 | -0.161351 |
| 29 | 1 | 0 | 2.481789 | 2.252747 | -0.781142 |
| 30 | 8 | 0 | 3.370153 | 2.328010 | -1.226264 |
| 31 | 1 | 0 | 3.179389 | 2.410253 | -2.172358 |
| 32 | 1 | 0 | 3.618797 | -0.746570 | -0.350175 |
| 33 | 8 | 0 | 4.371651 | -0.364679 | -0.848556 |
| 34 | 1 | 0 | 4.158859 | 0.587206 | -0.945454 |
| 35 | 1 | 0 | 4.525879 | -2.146995 | 1.425518 |
| 36 | 8 | 0 | 5.480516 | -2.008099 | 1.290382 |
| 37 | 1 | 0 | 5.487364 | -1.365848 | 0.552756 |
| 38 | 1 | 0 | -5.426979 | 0.394418 | -1.829828 |
| 39 | 1 | 0 | -5.827396 | 0.216739 | -0.109588 |
| 40 | 1 | 0 | -6.075748 | 1.776444 | -0.917315 |
| 41 | 6 | 0 | -0.696091 | -3.273583 | -0.334006 |
| 42 | 6 | 0 | 0.281148 | -3.250512 | -1.335938 |
| 43 | 1 | 0 | 0.124919 | 0.065817 | -2.114375 |
| 44 | 1 | 0 | 1.338607 | -2.017681 | -2.757870 |
| 45 | 1 | 0 | -2.124573 | -2.125282 | 0.799243 |
| 46 | 1 | 0 | -0.929497 | -4.204683 | 0.176776 |
| 47 | 1 | 0 | 0.806235 | -4.162542 | -1.610031 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1186.84664368    A.U. after    1 cycles

Convg  =   0.2672D-08        -V/T =  2.0093

S**2  =  0.0000

Zero-point correction=                          0.385558 (a.u.)

Thermal correction to Energy=                   0.418605

Thermal correction to Enthalpy=                 0.419550

Thermal correction to Gibbs Free Energy=        0.316946

Sum of electronic and zero-point Energies=          -1186.461085

Sum of electronic and thermal Energies=             -1186.428038

Sum of electronic and thermal Enthalpies=        -1186.427094
Sum of electronic and thermal Free Energies=      -1186.529697


  n=12 TS


ethyl benzoate and HO-(H2O)8+4, HO- addition TS
zuka03dd.chk
                  Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic       Coordinates (Angstroms)
Number   Number   Type       X        Y        Z
-----------------------------------------------------------------------
   1       6       0     -0.414011  -0.492230  -1.266906
   2       6       0     -0.935588   0.764169  -0.597454
   3       8       0     -0.134895   1.680437  -0.230856
   4       8       0     -1.537625   0.034866   0.964587
   5       1       0     -1.508808   0.830098   1.524497
   6       6       0      0.944209  -0.566339  -1.587916
   7       6       0      1.461469  -1.694325  -2.232460
   8       6       0     -1.255953  -1.564744  -1.592771
   9       8       0     -2.135412   1.136008  -1.198301
  10       6       0     -2.626848   2.447038  -0.871164
  11       1       0     -2.854870   2.492585   0.201727
  12       1       0     -1.851352   3.188531  -1.082246
  13       6       0     -3.872704   2.696006  -1.704164
  14       1       0      1.031594   1.365259   1.053926
  15       8       0      1.658493   1.182243   1.800979
  16       1       0      1.359077   0.326699   2.173228
  17       1       0     -4.215009  -0.185096  -0.307764
  18       8       0     -4.100582  -0.580909   0.570568
  19       1       0     -3.131527  -0.396961   0.777287
  20       1       0     -0.400972  -0.920889   1.704727
  21       8       0      0.369086  -1.334187   2.212446
  22       1       0     -0.011830  -1.751372   2.999432
  23       1       0      1.483507  -2.459399   1.293842
  24       8       0      2.082144  -3.043897   0.773897
  25       1       0      1.620227  -3.184283  -0.068751
  26       1       0      2.501174   2.697169   2.460575
  27       8       0      3.125118   3.447048   2.588488
  28       1       0      3.977431   3.012093   2.749641
  29       1       0      3.355075   0.953815   0.988086
  30       8       0      4.237346   0.994749   0.561168
  31       1       0      4.223885   1.864386   0.099269
  32       1       0      3.596398  -1.974214   0.080876
  33       8       0      4.458500  -1.703474  -0.292624

| 34 | 1 | 0 | 4.546029 | -0.751094 | -0.062897 |
|----|---|---|----------|-----------|-----------|
| 35 | 1 | 0 | 3.896266 | -4.136325 | 1.178577 |
| 36 | 8 | 0 | 4.856520 | -4.246693 | 1.062964 |
| 37 | 1 | 0 | 5.106092 | -3.414751 | 0.612383 |
| 38 | 1 | 0 | -3.644556 | 2.626249 | -2.772868 |
| 39 | 1 | 0 | -4.663738 | 1.973232 | -1.473438 |
| 40 | 1 | 0 | -4.263022 | 3.699006 | -1.497820 |
| 41 | 6 | 0 | -0.741545 | -2.693199 | -2.228505 |
| 42 | 6 | 0 | 0.618498 | -2.761125 | -2.552689 |
| 43 | 1 | 0 | 1.601078 | 0.255209 | -1.320812 |
| 44 | 1 | 0 | 2.523259 | -1.740156 | -2.457025 |
| 45 | 1 | 0 | -2.309236 | -1.518428 | -1.338851 |
| 46 | 1 | 0 | -1.401822 | -3.522333 | -2.469751 |
| 47 | 1 | 0 | 1.017737 | -3.640558 | -3.052095 |
| 48 | 1 | 0 | 0.730163 | 2.869154 | -1.215726 |
| 49 | 8 | 0 | 1.279567 | 3.517427 | -1.721760 |
| 50 | 1 | 0 | 1.482372 | 3.077295 | -2.560433 |
| 51 | 1 | 0 | 2.884250 | 3.698604 | -0.755681 |
| 52 | 8 | 0 | 3.716904 | 3.667113 | -0.235048 |
| 53 | 1 | 0 | 3.455000 | 3.840791 | 0.694014 |
| 54 | 1 | 0 | -5.341055 | -2.289549 | 0.836411 |
| 55 | 8 | 0 | -6.196348 | -2.627320 | 1.159526 |
| 56 | 1 | 0 | -6.556875 | -1.850146 | 1.626339 |
| 57 | 1 | 0 | -5.374127 | 0.014434 | 1.717166 |
| 58 | 8 | 0 | -6.185326 | 0.124965 | 2.269264 |
| 59 | 1 | 0 | -5.874901 | 0.152414 | 3.185963 |

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SCF Done:  E(RB+HF-LYP) =  -1492.61180227     A.U. after    1 cycles
            Convg  =    0.3406D-08          -V/T =  2.0093
            S**2  =   0.0000

Zero-point correction=                           0.487061 (a.u.)
Thermal correction to Energy=                    0.531069
Thermal correction to Enthalpy=                  0.532013
Thermal correction to Gibbs Free Energy=         0.400716
Sum of electronic and zero-point Energies=          -1492.124742
Sum of electronic and thermal Energies=             -1492.080733
Sum of electronic and thermal Enthalpies=           -1492.079789
Sum of electronic and thermal Free Energies=        -1492.211086


 n=16 TS

ethyl benzoate + HO-(H2O)16 TS1(es)
 molecular formula: C9H43O19(1-)
zuka02aa.chk
               Standard orientation:

```
---------------------------------------------------------------------
Center     Atomic    Atomic          Coordinates (Angstroms)
Number     Number     Type         X          Y          Z
---------------------------------------------------------------------
   1          6         0      -0.029063   2.670394  -0.007977
   2          6         0      -0.333003   1.442850   0.812460
   3          8         0      -1.376670   0.754484   0.605280
   4          8         0       0.171988   1.585091   2.066932
   5          6         0      -0.139275   0.572461   3.039007
   6          6         0      -1.002168   3.171408  -0.877904
   7          6         0      -0.749097   4.321731  -1.629854
   8          6         0       1.198353   3.337491   0.111139
   9          6         0       0.566257   0.950146   4.329589
  10          1         0      -1.223399   0.524903   3.180571
  11          1         0       0.203927  -0.397340   2.667420
  12          8         0       1.112393   0.292708   0.071213
  13          1         0       0.932669   0.320348  -0.890057
  14          1         0       1.114067  -1.184518   0.519889
  15          8         0       1.192987  -2.180322   0.801716
  16          1         0       1.845657  -2.191722   1.527157
  17          1         0       2.282543  -2.529205  -0.575781
  18          8         0       3.048589  -2.485507  -1.207847
  19          1         0       3.408064  -1.583854  -1.018809
  20          1         0       4.170642  -3.491734  -0.329493
  21          8         0       4.696286  -3.933476   0.394713
  22          1         0       4.341013  -4.832240   0.461187
  23          1         0       2.010705  -2.321772  -2.810826
  24          8         0       1.402411  -2.060926  -3.535093
  25          1         0       0.524611  -2.466652  -3.319601
  26          1         0       1.016843  -0.447951  -3.233872
  27          8         0       0.682451   0.445165  -2.919219
  28          1         0       1.211674   1.125550  -3.359063
  29          1         0       4.222380  -2.794697   1.660728
  30          8         0       3.807768  -2.051158   2.172094
  31          1         0       4.304338  -1.966378   2.999044
  32          1         0      -1.780425   0.266555  -1.176166
  33          8         0      -1.957116   0.073115  -2.124303
  34          1         0      -1.149027   0.394229  -2.581711
  35          1         0      -1.491720  -1.730337  -2.649809
  36          8         0      -1.210496  -2.637471  -2.894836
  37          1         0      -1.749771  -3.194595  -2.285945
  38          1         0      -3.752133  -0.711160  -2.126512
  39          8         0      -4.520913  -1.258597  -1.870622
  40          1         0      -5.010333  -0.733016  -1.199075
  41          1         0      -1.479635  -1.082881   0.892639
  42          8         0      -1.537605  -2.041667   1.114426
```

| 43 | 1 | 0 | -0.594979 | -2.336076 | 1.095771 |
|----|---|---|-----------|-----------|----------|
| 44 | 1 | 0 | -2.722830 | -2.085136 | 2.424479 |
| 45 | 8 | 0 | -3.492898 | -1.889416 | 3.015905 |
| 46 | 1 | 0 | -4.215209 | -2.436026 | 2.670742 |
| 47 | 1 | 0 | -2.530443 | -3.008100 | -0.197370 |
| 48 | 8 | 0 | -3.023201 | -3.456601 | -0.916608 |
| 49 | 1 | 0 | -3.672187 | -2.781392 | -1.227886 |
| 50 | 1 | 0 | 2.757130 | 0.240645 | 0.083527 |
| 51 | 8 | 0 | 3.733753 | -0.035893 | 0.041959 |
| 52 | 1 | 0 | 3.882110 | -0.538171 | 0.868944 |
| 53 | 1 | 0 | 4.855338 | 1.390809 | -0.064081 |
| 54 | 8 | 0 | 5.487433 | 2.140200 | -0.180177 |
| 55 | 1 | 0 | 5.722263 | 2.112831 | -1.118899 |
| 56 | 1 | 0 | -3.796555 | -0.141584 | 2.455045 |
| 57 | 8 | 0 | -3.878579 | 0.723874 | 1.990145 |
| 58 | 1 | 0 | -3.022635 | 0.840248 | 1.523462 |
| 59 | 1 | 0 | -5.125077 | 0.487778 | 0.813224 |
| 60 | 8 | 0 | -5.812308 | 0.299351 | 0.117364 |
| 61 | 1 | 0 | -6.118306 | 1.164679 | -0.190050 |
| 62 | 6 | 0 | 1.449119 | 4.483124 | -0.640012 |
| 63 | 6 | 0 | 0.475828 | 4.978745 | -1.514168 |
| 64 | 1 | 0 | -1.953836 | 2.658323 | -0.964538 |
| 65 | 1 | 0 | -1.512870 | 4.701300 | -2.304012 |
| 66 | 1 | 0 | 1.955900 | 2.940920 | 0.777266 |
| 67 | 1 | 0 | 2.408934 | 4.984545 | -0.546915 |
| 68 | 1 | 0 | 0.674130 | 5.872185 | -2.101826 |
| 69 | 1 | 0 | 1.650787 | 0.994343 | 4.183860 |
| 70 | 1 | 0 | 0.226743 | 1.928073 | 4.686954 |
| 71 | 1 | 0 | 0.347041 | 0.204541 | 5.102382 |

-------------------------------------------------------------------

SCF Done: E(RB+HF-LYP) = -1798.39889531    A.U. after    1 cycles

Convg =   0.2155D-08          -V/T = 2.0093

S**2  =  0.0000

Zero-point correction=                      0.595360 (a.u.)

Thermal correction to Energy=              0.646200

Thermal correction to Enthalpy=             0.647145

Thermal correction to Gibbs Free Energy=      0.506737

Sum of electronic and zero-point Energies=        -1797.803536

Sum of electronic and thermal Energies=           -1797.752695

Sum of electronic and thermal Enthalpies=         -1797.751751

Sum of electronic and thermal Free Energies=       -1797.892158

n=24 TS

ethyl benzoate + HO-(H2O)16+8 TS1(es) n=24

molecular formula: C9H59O27(1-)
zuka02jj.chk

Standard orientation:
-----------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number     Type         X            Y            Z
-----------------------------------------------------------------------
| 1 | 6 | 0 | 0.231153 | -2.101990 | 2.247982 |
| 2 | 6 | 0 | -0.240438 | -2.091777 | 0.815798 |
| 3 | 8 | 0 | -1.197209 | -1.321989 | 0.455577 |
| 4 | 8 | 0 | -0.102901 | -3.320129 | 0.265703 |
| 5 | 6 | 0 | -0.723599 | -3.580083 | -1.011287 |
| 6 | 6 | 0 | -0.488075 | -1.393435 | 3.215261 |
| 7 | 6 | 0 | -0.076800 | -1.407582 | 4.550700 |
| 8 | 6 | 0 | 1.360033 | -2.839215 | 2.632113 |
| 9 | 6 | 0 | -0.443431 | -5.024520 | -1.378149 |
| 10 | 1 | 0 | -1.799038 | -3.402566 | -0.936764 |
| 11 | 1 | 0 | -0.311729 | -2.889657 | -1.754423 |
| 12 | 8 | 0 | 1.336591 | -1.232019 | 0.044905 |
| 13 | 1 | 0 | 1.334708 | -0.375930 | 0.517617 |
| 14 | 1 | 0 | 1.322312 | -0.944645 | -1.427901 |
| 15 | 8 | 0 | 1.320102 | -0.682757 | -2.448945 |
| 16 | 1 | 0 | 1.552087 | -1.483604 | -2.943220 |
| 17 | 1 | 0 | 2.732326 | 0.434606 | -2.365037 |
| 18 | 8 | 0 | 3.503142 | 0.920410 | -1.978729 |
| 19 | 1 | 0 | 3.789866 | 0.311573 | -1.240823 |
| 20 | 1 | 0 | 4.993376 | 1.070126 | -2.923689 |
| 21 | 8 | 0 | 5.905135 | 1.074115 | -3.311413 |
| 22 | 1 | 0 | 6.055825 | 1.975289 | -3.631172 |
| 23 | 1 | 0 | 2.797781 | 2.266346 | -1.078030 |
| 24 | 8 | 0 | 2.480091 | 2.934748 | -0.416395 |
| 25 | 1 | 0 | 1.578943 | 3.226308 | -0.694743 |
| 26 | 1 | 0 | 2.074491 | 1.931546 | 0.995405 |
| 27 | 8 | 0 | 1.676902 | 1.318416 | 1.665021 |
| 28 | 1 | 0 | 2.351195 | 1.154773 | 2.341063 |
| 29 | 1 | 0 | 6.113145 | -2.737728 | -1.800379 |
| 30 | 8 | 0 | 6.143228 | -2.345061 | -0.915963 |
| 31 | 1 | 0 | 6.708848 | -1.525432 | -1.006502 |
| 32 | 1 | 0 | -1.062856 | 0.405150 | 0.884262 |
| 33 | 8 | 0 | -0.996019 | 1.365457 | 1.120476 |
| 34 | 1 | 0 | -0.163455 | 1.431132 | 1.639242 |
| 35 | 1 | 0 | -0.485193 | 2.612644 | -0.129860 |
| 36 | 8 | 0 | -0.258874 | 3.359399 | -0.735855 |
| 37 | 1 | 0 | -0.855062 | 3.204520 | -1.499665 |
| 38 | 1 | 0 | -2.622228 | 2.131759 | 0.990407 |

| 39 | 8 | 0 | -3.439917 | 2.567485 | 0.653383 |
|----|---|---|-----------|-----------|-----------|
| 40 | 1 | 0 | -4.141192 | 1.857116 | 0.627390 |
| 41 | 1 | 0 | -1.274490 | -0.649169 | -1.185385 |
| 42 | 8 | 0 | -1.357402 | -0.235296 | -2.081361 |
| 43 | 1 | 0 | -0.440479 | -0.299506 | -2.444533 |
| 44 | 1 | 0 | -2.909267 | -1.013056 | -2.669683 |
| 45 | 8 | 0 | -3.860527 | -1.267440 | -2.649263 |
| 46 | 1 | 0 | -4.322137 | -0.477201 | -3.016846 |
| 47 | 1 | 0 | -2.098357 | 1.384019 | -2.021264 |
| 48 | 8 | 0 | -2.538403 | 2.270228 | -2.069947 |
| 49 | 1 | 0 | -2.938315 | 2.422927 | -1.182230 |
| 50 | 1 | 0 | 3.120145 | -1.206007 | 0.144393 |
| 51 | 8 | 0 | 4.038726 | -0.831662 | 0.045230 |
| 52 | 1 | 0 | 4.650561 | -1.540458 | -0.270794 |
| 53 | 1 | 0 | 5.201889 | 0.408121 | 0.914472 |
| 54 | 8 | 0 | 5.951310 | 1.022875 | 1.061264 |
| 55 | 1 | 0 | 5.573317 | 1.928462 | 1.042223 |
| 56 | 1 | 0 | -4.029139 | -1.475559 | -0.886374 |
| 57 | 8 | 0 | -4.002729 | -1.660386 | 0.090139 |
| 58 | 1 | 0 | -3.047659 | -1.628826 | 0.326971 |
| 59 | 1 | 0 | -4.901877 | -0.241470 | 0.795767 |
| 60 | 8 | 0 | -5.307293 | 0.641876 | 0.965038 |
| 61 | 1 | 0 | -5.357724 | 0.783514 | 1.928690 |
| 62 | 6 | 0 | 1.768608 | -2.851777 | 3.963035 |
| 63 | 6 | 0 | 1.052654 | -2.133690 | 4.926735 |
| 64 | 1 | 0 | -1.372989 | -0.837909 | 2.923523 |
| 65 | 1 | 0 | -0.644475 | -0.852756 | 5.293022 |
| 66 | 1 | 0 | 1.916856 | -3.383395 | 1.877701 |
| 67 | 1 | 0 | 2.650921 | -3.418064 | 4.249535 |
| 68 | 1 | 0 | 1.375787 | -2.142656 | 5.964741 |
| 69 | 1 | 0 | 0.631169 | -5.204986 | -1.492069 |
| 70 | 1 | 0 | -0.828643 | -5.697400 | -0.605354 |
| 71 | 1 | 0 | -0.951591 | -5.258166 | -2.319147 |
| 72 | 1 | 0 | 6.985690 | 0.470367 | -1.896483 |
| 73 | 8 | 0 | 7.411240 | 0.052505 | -1.115968 |
| 74 | 1 | 0 | 7.017762 | 0.504243 | -0.329484 |
| 75 | 1 | 0 | 3.926598 | 3.569631 | 0.433295 |
| 76 | 8 | 0 | 4.759566 | 3.630658 | 0.957050 |
| 77 | 1 | 0 | 5.291918 | 4.321884 | 0.538063 |
| 78 | 1 | 0 | -1.351277 | 4.735394 | 0.131468 |
| 79 | 8 | 0 | -2.107816 | 5.164138 | 0.584198 |
| 80 | 1 | 0 | -2.785931 | 4.462966 | 0.619201 |
| 81 | 1 | 0 | -3.967110 | -3.221330 | -3.024355 |
| 82 | 8 | 0 | -3.900687 | -4.191698 | -2.936898 |
| 83 | 1 | 0 | -4.252146 | -4.374834 | -2.042116 |
| 84 | 1 | 0 | -3.941616 | 1.766770 | -3.084115 |

| 85 | 8 | 0 | -4.656848 | 1.263092 | -3.548758 |
|----|---|---|-----------|----------|-----------|
| 86 | 1 | 0 | -4.593099 | 1.504896 | -4.483944 |
| 87 | 1 | 0 | -2.601001 | 6.878876 | 0.158399 |
| 88 | 8 | 0 | -2.812105 | 7.837345 | 0.079594 |
| 89 | 1 | 0 | -2.427503 | 8.228224 | 0.877386 |
| 90 | 1 | 0 | -4.282606 | 2.746552 | 2.490549 |
| 91 | 8 | 0 | -4.818145 | 2.371916 | 3.220629 |
| 92 | 1 | 0 | -5.445695 | 3.066933 | 3.467505 |
| 93 | 1 | 0 | -4.591780 | -3.380903 | 0.044066 |
| 94 | 8 | 0 | -4.886318 | -4.295433 | -0.182493 |
| 95 | 1 | 0 | -5.853212 | -4.275368 | -0.132879 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -2409.92783513    A.U. after    1 cycles

      Convg  =    0.3469D-08          -V/T =  2.0092

      S**2  =   0.0000

Zero-point correction=                       0.799991 (a.u.)

Thermal correction to Energy=              0.871243

Thermal correction to Enthalpy=            0.872187

Thermal correction to Gibbs Free Energy=        0.684917

Sum of electronic and zero-point Energies=         -2409.127844

Sum of electronic and thermal Energies=            -2409.056592

Sum of electronic and thermal Enthalpies=          -2409.055648

Sum of electronic and thermal Free Energies=       -2409.242918


  n=32 TS


 ethyl benzoate and HO-(H2O)32, TS1(es)

zuka02ww.g09.chk    Stoichiometry: C9H75O35(1-)

           Standard orientation:

---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|------|------|------|
| Number | Number | Type | X | Y | Z |

---------------------------------------------------------------------

| 1 | 6 | 0 | -0.732364 | -1.234766 | 2.884903 |
|----|---|---|-----------|-----------|----------|
| 2 | 6 | 0 | -1.020399 | -1.308196 | 1.403009 |
| 3 | 8 | 0 | -1.897030 | -0.533649 | 0.878609 |
| 4 | 8 | 0 | -0.901938 | -2.594485 | 0.977416 |
| 5 | 6 | 0 | -1.389196 | -2.944300 | -0.334236 |
| 6 | 6 | 0 | -1.525368 | -0.426985 | 3.705031 |
| 7 | 6 | 0 | -1.287154 | -0.370067 | 5.080585 |
| 8 | 6 | 0 | 0.293631 | -1.999132 | 3.458419 |
| 9 | 6 | 0 | -1.205561 | -4.439966 | -0.511885 |
| 10 | 1 | 0 | -2.445951 | -2.672698 | -0.409616 |
| 11 | 1 | 0 | -0.830966 | -2.376661 | -1.087668 |
| 12 | 8 | 0 | 0.624594 | -0.628838 | 0.755042 |

| 13 | 1 | 0 | 0.707238 | 0.259244 | 1.164311 |
|----|---|---|----------|----------|----------|
| 14 | 1 | 0 | 0.769308 | -0.345309 | -0.727551 |
| 15 | 8 | 0 | 0.940585 | -0.064924 | -1.717274 |
| 16 | 1 | 0 | 1.413617 | -0.803162 | -2.134948 |
| 17 | 1 | 0 | 2.110603 | 1.175986 | -1.317040 |
| 18 | 8 | 0 | 2.815092 | 1.848072 | -1.127309 |
| 19 | 1 | 0 | 3.088258 | 1.739819 | -0.176498 |
| 20 | 1 | 0 | 4.138968 | 1.453544 | -2.014384 |
| 21 | 8 | 0 | 4.974793 | 1.090767 | -2.441080 |
| 22 | 1 | 0 | 4.778180 | 0.931806 | -3.389673 |
| 23 | 1 | 0 | 1.857788 | 3.431206 | -0.755832 |
| 24 | 8 | 0 | 1.533549 | 4.120411 | -0.137363 |
| 25 | 1 | 0 | 0.611751 | 4.336518 | -0.409368 |
| 26 | 1 | 0 | 1.118318 | 2.912402 | 1.212357 |
| 27 | 8 | 0 | 0.969004 | 2.194960 | 1.874658 |
| 28 | 1 | 0 | 1.879766 | 2.012634 | 2.184649 |
| 29 | 1 | 0 | 4.243675 | -0.689106 | -2.107747 |
| 30 | 8 | 0 | 3.841875 | -1.576765 | -2.234540 |
| 31 | 1 | 0 | 4.587037 | -2.198722 | -2.060475 |
| 32 | 1 | 0 | -1.814043 | 1.261333 | 1.270265 |
| 33 | 8 | 0 | -1.770613 | 2.213886 | 1.528978 |
| 34 | 1 | 0 | -0.917190 | 2.281852 | 2.010300 |
| 35 | 1 | 0 | -1.410165 | 3.523692 | 0.232701 |
| 36 | 8 | 0 | -1.245509 | 4.235379 | -0.429639 |
| 37 | 1 | 0 | -1.815988 | 3.973260 | -1.180205 |
| 38 | 1 | 0 | -3.533594 | 2.880296 | 1.340565 |
| 39 | 8 | 0 | -4.294182 | 3.180300 | 0.797739 |
| 40 | 1 | 0 | -5.061971 | 2.613726 | 1.037844 |
| 41 | 1 | 0 | -1.799188 | -0.006170 | -0.798431 |
| 42 | 8 | 0 | -1.804913 | 0.351312 | -1.725130 |
| 43 | 1 | 0 | -0.859481 | 0.302031 | -1.995059 |
| 44 | 1 | 0 | -3.197122 | -0.495349 | -2.543799 |
| 45 | 8 | 0 | -4.142083 | -0.762887 | -2.635516 |
| 46 | 1 | 0 | -4.594164 | 0.017449 | -3.026695 |
| 47 | 1 | 0 | -2.751726 | 1.921286 | -1.689377 |
| 48 | 8 | 0 | -3.325850 | 2.722114 | -1.754521 |
| 49 | 1 | 0 | -3.727207 | 2.857625 | -0.855119 |
| 50 | 1 | 0 | 2.092125 | -1.399508 | 0.775444 |
| 51 | 8 | 0 | 3.010821 | -1.780836 | 0.581378 |
| 52 | 1 | 0 | 3.098575 | -1.765536 | -0.393653 |
| 53 | 1 | 0 | 4.228121 | -3.028499 | 1.234685 |
| 54 | 8 | 0 | 5.175172 | -3.252394 | 1.400506 |
| 55 | 1 | 0 | 5.507074 | -2.435380 | 1.832209 |
| 56 | 1 | 0 | -4.416835 | -0.754509 | -0.836345 |
| 57 | 8 | 0 | -4.567199 | -0.831918 | 0.137589 |
| 58 | 1 | 0 | -3.668315 | -0.856031 | 0.542035 |

| 59  | 1 | 0 | -5.579039 | 0.475946  | 0.771416  |
| 60  | 8 | 0 | -6.226294 | 1.190198  | 0.998440  |
| 61  | 1 | 0 | -6.945584 | 0.729004  | 1.486264  |
| 62  | 6 | 0 | 0.530538  | -1.939610 | 4.829132  |
| 63  | 6 | 0 | -0.258285 | -1.122417 | 5.644901  |
| 64  | 1 | 0 | -2.330548 | 0.153156  | 3.268252  |
| 65  | 1 | 0 | -1.909450 | 0.263611  | 5.706745  |
| 66  | 1 | 0 | 0.902528  | -2.631002 | 2.821153  |
| 67  | 1 | 0 | 1.333799  | -2.529741 | 5.262838  |
| 68  | 1 | 0 | -0.069625 | -1.074531 | 6.714462  |
| 69  | 1 | 0 | -0.143860 | -4.710805 | -0.510652 |
| 70  | 1 | 0 | -1.701567 | -4.980427 | 0.300726  |
| 71  | 1 | 0 | -1.665112 | -4.760248 | -1.452670 |
| 72  | 1 | 0 | 6.237282  | 0.295090  | -1.423710 |
| 73  | 8 | 0 | 6.832623  | -0.134510 | -0.765700 |
| 74  | 1 | 0 | 6.870517  | -1.083633 | -1.014804 |
| 75  | 1 | 0 | 3.854405  | -0.984060 | -4.119406 |
| 76  | 8 | 0 | 4.116051  | -0.284298 | -4.755237 |
| 77  | 1 | 0 | 3.340691  | -0.108332 | -5.308336 |
| 78  | 1 | 0 | -2.569335 | 5.658939  | 0.296994  |
| 79  | 8 | 0 | -3.424513 | 6.012151  | 0.607307  |
| 80  | 1 | 0 | -3.957415 | 5.206796  | 0.743358  |
| 81  | 1 | 0 | -5.095526 | -2.388329 | -2.859942 |
| 82  | 8 | 0 | -5.690263 | -3.164059 | -2.788415 |
| 83  | 1 | 0 | -6.312314 | -2.927565 | -2.069533 |
| 84  | 1 | 0 | -4.597899 | 2.212332  | -2.753114 |
| 85  | 8 | 0 | -5.293153 | 1.711941  | -3.275270 |
| 86  | 1 | 0 | -5.408832 | 2.180293  | -4.115052 |
| 87  | 1 | 0 | 5.770598  | -2.947519 | -0.265496 |
| 88  | 8 | 0 | 6.113364  | -2.840574 | -1.189776 |
| 89  | 1 | 0 | 6.550020  | -3.699570 | -1.342172 |
| 90  | 1 | 0 | 4.396548  | -0.738686 | 1.218331  |
| 91  | 8 | 0 | 5.246147  | -0.416431 | 1.605464  |
| 92  | 1 | 0 | 5.834859  | -0.240968 | 0.837538  |
| 93  | 1 | 0 | -6.219700 | -1.755753 | -0.159170 |
| 94  | 8 | 0 | -7.110930 | -1.840660 | -0.559379 |
| 95  | 1 | 0 | -7.228084 | -0.992566 | -1.060025 |
| 96  | 1 | 0 | 6.151187  | -4.809989 | 0.824634  |
| 97  | 8 | 0 | 6.681134  | -5.303040 | 0.163770  |
| 98  | 1 | 0 | 6.459417  | -6.238164 | 0.277440  |
| 99  | 1 | 0 | 4.414665  | 1.300008  | 1.737479  |
| 100 | 8 | 0 | 3.702646  | 1.929525  | 1.493108  |
| 101 | 1 | 0 | 4.090805  | 2.839927  | 1.377566  |
| 102 | 1 | 0 | -7.050129 | 1.132943  | -0.689195 |
| 103 | 8 | 0 | -7.383013 | 0.753358  | -1.534220 |
| 104 | 1 | 0 | -6.786901 | 1.114055  | -2.222005 |

| 105 | 1 | 0 | 5.806990 | 2.936183 | -1.863730 |
|-----|---|---|----------|----------|-----------|
| 106 | 8 | 0 | 6.166629 | 3.662253 | -1.321180 |
| 107 | 1 | 0 | 6.973823 | 3.279021 | -0.912189 |
| 108 | 1 | 0 | 3.488343 | 4.672655 | 0.392248 |
| 109 | 8 | 0 | 4.371549 | 4.434409 | 0.735512 |
| 110 | 1 | 0 | 4.958385 | 4.287566 | -0.042500 |
| 111 | 1 | 0 | 8.014109 | 1.241888 | -0.431297 |
| 112 | 8 | 0 | 8.381916 | 2.149313 | -0.340712 |
| 113 | 1 | 0 | 9.170667 | 2.175759 | -0.901557 |
| 114 | 1 | 0 | -4.613998 | -4.607638 | -2.610894 |
| 115 | 8 | 0 | -3.991033 | -5.373897 | -2.622718 |
| 116 | 1 | 0 | -4.305321 | -5.929852 | -3.350097 |
| 117 | 1 | 0 | -8.005223 | -1.213489 | 0.947414 |
| 118 | 8 | 0 | -8.274874 | -0.640282 | 1.706798 |
| 119 | 1 | 0 | -9.178957 | -0.355968 | 1.506968 |

-------------------------------------------------------------------

SCF Done:  E(RB3LYP) = -3021.46919438    A.U. after    1 cycles

       Convg  =    0.1651D-08        -V/T = 2.0092

Zero-point correction=                    1.010357 (a.u.)

Thermal correction to Energy=              1.099222

Thermal correction to Enthalpy=            1.100167

Thermal correction to Gibbs Free Energy=      0.877552

Sum of electronic and zero-point Energies=       -3020.458837

Sum of electronic and thermal Energies=          -3020.369972

Sum of electronic and thermal Enthalpies=        -3020.369028

Sum of electronic and thermal Free Energies=       -3020.591642

=========================================================================

[2] TS1(am) geometries in Figure 2. Hereafter, n denotes the number of water molecules around Ph-CO-NH-Et and OH-

n=3 TS
N-ethyl benzamide(C6H5-C(=O)-NHC2H5) and HO-(H2O)3, HO- addition TS1(am)
tuka03aa.chk    Stoichiometry: C9H18NO5(1-)
                Standard orientation:

---------------------------------------------------------------------
Center    Atomic    Atomic          Coordinates (Angstroms)
Number    Number    Type       X         Y         Z
---------------------------------------------------------------------
| 1 | 6 | 0 | 0.708812 | -0.588882 | -0.364345 |
| 2 | 6 | 0 | -0.536797 | 0.266755 | -0.537381 |
| 3 | 8 | 0 | -0.536664 | 1.244188 | -1.333203 |
| 4 | 8 | 0 | -0.499883 | 1.066827 | 1.182326 |
| 5 | 1 | 0 | -0.934259 | 1.893742 | 0.913961 |
| 6 | 6 | 0 | 1.764560 | -0.424831 | -1.266695 |
| 7 | 6 | 0 | 2.905266 | -1.224411 | -1.173991 |
| 8 | 6 | 0 | 0.811885 | -1.561976 | 0.640443 |
| 9 | 7 | 0 | -1.740404 | -0.550894 | -0.428235 |
| 10 | 6 | 0 | -2.955327 | 0.059799 | -0.970550 |
| 11 | 1 | 0 | -3.164482 | 0.955563 | -0.376369 |
| 12 | 1 | 0 | -2.814370 | 0.399190 | -2.006761 |
| 13 | 6 | 0 | -4.133210 | -0.909304 | -0.878856 |
| 14 | 1 | 0 | 0.715493 | 2.667542 | -1.135889 |
| 15 | 8 | 0 | 1.372784 | 3.361936 | -0.903853 |
| 16 | 1 | 0 | 1.705173 | 3.067392 | -0.031255 |
| 17 | 1 | 0 | -2.332987 | -0.944320 | 1.684526 |
| 18 | 8 | 0 | -2.172292 | -0.582537 | 2.575950 |
| 19 | 1 | 0 | -1.529947 | 0.128586 | 2.313208 |
| 20 | 1 | 0 | 1.027121 | 1.665929 | 1.565115 |
| 21 | 8 | 0 | 1.875778 | 2.181075 | 1.749321 |
| 22 | 1 | 0 | 1.641483 | 2.773769 | 2.478227 |
| 23 | 1 | 0 | -3.940600 | -1.827837 | -1.450952 |
| 24 | 1 | 0 | -4.334097 | -1.194868 | 0.159971 |
| 25 | 1 | 0 | -5.041564 | -0.451810 | -1.289909 |
| 26 | 6 | 0 | 1.951390 | -2.362074 | 0.729527 |
| 27 | 6 | 0 | 3.000347 | -2.198981 | -0.179250 |
| 28 | 1 | 0 | 1.677862 | 0.342642 | -2.029225 |
| 29 | 1 | 0 | 3.722145 | -1.082561 | -1.878456 |
| 30 | 1 | 0 | 0.011125 | -1.661563 | 1.366834 |
| 31 | 1 | 0 | 2.025778 | -3.106032 | 1.519968 |
| 32 | 1 | 0 | 3.890470 | -2.820593 | -0.104586 |
| 33 | 1 | 0 | -1.560869 | -1.456984 | -0.858505 |

---------------------------------------------------------------------
SCF Done:  E(RB+HF-LYP) =  -784.753767799    A.U. after   1 cycles

Convg  =   0.2480D-08          -V/T  =  2.0095
S**2   =   0.0000

Zero-point correction=                0.271480 (a.u.)
Thermal correction to Energy=              0.291173
Thermal correction to Enthalpy=            0.292117
Thermal correction to Gibbs Free Energy=        0.222385
Sum of electronic and zero-point Energies=        -784.482288
Sum of electronic and thermal Energies=          -784.462595
Sum of electronic and thermal Enthalpies=        -784.461651
Sum of electronic and thermal Free Energies=       -784.531383


n=5 TS
N-ethyl benzamide and HO-(H2O)5 HO- addition TS1(am)
tuka05a.chk   Stoichiometry  C9H22NO7(1-)
                Standard orientation:
-----------------------------------------------------------------------
Center    Atomic    Atomic           Coordinates (Angstroms)
Number   Number    Type          X          Y          Z
-----------------------------------------------------------------------
  1        6        0      0.585987  -0.786118  -0.586881
  2        6        0     -0.796340  -0.158222  -0.527575
  3        8        0     -1.087206   0.797095  -1.310431
  4        8        0     -0.574539   0.676786   1.173720
  5        1        0     -1.249803   1.375895   1.089372
  6        6        0      1.406892  -0.496239  -1.682068
  7        6        0      2.667259  -1.085523  -1.797838
  8        6        0      1.043266  -1.673626   0.398488
  9        7        0     -1.805294  -1.138027  -0.222638
 10        6        0     -3.181149  -0.795793  -0.583512
 11        1        0     -3.461285   0.098139  -0.016886
 12        1        0     -3.270321  -0.535158  -1.648405
 13        6        0     -4.128486  -1.942516  -0.235422
 14        1        0     -0.016743   2.373700  -1.266311
 15        8        0      0.330022   3.264043  -1.029459
 16        1        0      0.886502   3.081880  -0.243746
 17        1        0     -1.930686  -1.643460   2.075721
 18        8        0     -1.527600  -1.253434   2.870185
 19        1        0     -1.114328  -0.452760   2.450785
 20        1        0      0.756756   1.527089   1.309220
 21        8        0      1.558820   2.169357   1.355835
 22        1        0      1.459058   2.636176   2.198797
 23        1        0     -3.860475  -2.861643  -0.774933
 24        1        0     -4.109061  -2.162553   0.838023
 25        1        0     -5.157586  -1.686572  -0.513261
 26        6        0      2.302591  -2.264053   0.280287

| 27 | 6 | 0 | 3.118334 | -1.974749 | -0.818955 |
|---|---|---|---|---|---|
| 28 | 1 | 0 | 1.044363 | 0.199347 | -2.432106 |
| 29 | 1 | 0 | 3.298894 | -0.847490 | -2.650318 |
| 30 | 1 | 0 | 0.426034 | -1.866551 | 1.270747 |
| 31 | 1 | 0 | 2.653472 | -2.940703 | 1.055780 |
| 32 | 1 | 0 | 4.099937 | -2.434961 | -0.907836 |
| 33 | 1 | 0 | -1.529178 | -2.053181 | -0.569278 |
| 34 | 1 | 0 | -2.286071 | 2.186671 | -0.707098 |
| 35 | 8 | 0 | -2.463287 | 3.017865 | -0.217965 |
| 36 | 1 | 0 | -1.617446 | 3.491488 | -0.354601 |
| 37 | 1 | 0 | 3.220428 | 1.343512 | 1.289452 |
| 38 | 8 | 0 | 4.069785 | 0.847018 | 1.238899 |
| 39 | 1 | 0 | 3.836489 | 0.048509 | 0.739923 |

-----------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -937.643011233     A.U. after    1 cycles

Convg  =    0.2280D-08          -V/T =  2.0094

S**2  =  0.0000

Zero-point correction=                    0.322152 (a.u.)

Thermal correction to Energy=             0.347208

Thermal correction to Enthalpy=           0.348152

Thermal correction to Gibbs Free Energy=       0.265947

Sum of electronic and zero-point Energies=        -937.320859

Sum of electronic and thermal Energies=           -937.295803

Sum of electronic and thermal Enthalpies=         -937.294859

Sum of electronic and thermal Free Energies=       -937.377064


 n=8 TS

N-ethyl benzamide and HO-(H2O)8, HO- addition TS1(am)

tuka03cc.chk    Stoichiometry: C9H28NO10(1-)

Standard orientation:

-----------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| Number | Number | Type | X | Y | Z |

-----------------------------------------------------------------------

| 1 | 6 | 0 | -1.037207 | -0.909048 | -0.613492 |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -1.818637 | 0.360519 | -0.286756 |
| 3 | 8 | 0 | -1.375714 | 1.488666 | -0.674703 |
| 4 | 8 | 0 | -1.594693 | 0.358990 | 1.510894 |
| 5 | 1 | 0 | -1.772361 | 1.302681 | 1.665436 |
| 6 | 6 | 0 | -0.045803 | -0.849282 | -1.598436 |
| 7 | 6 | 0 | 0.670230 | -1.994106 | -1.957385 |
| 8 | 6 | 0 | -1.311807 | -2.136313 | 0.009151 |
| 9 | 7 | 0 | -3.252419 | 0.109252 | -0.403369 |
| 10 | 6 | 0 | -4.086703 | 1.305174 | -0.566950 |
| 11 | 1 | 0 | -3.989788 | 1.903944 | 0.345090 |

| 12 | 1 | 0 | -3.732335 | 1.935765 | -1.393611 |
|----|---|---|-----------|-----------|-----------|
| 13 | 6 | 0 | -5.548489 | 0.913486 | -0.774224 |
| 14 | 1 | 0 | 0.144752 | 2.069968 | -0.165648 |
| 15 | 8 | 0 | 1.024112 | 2.354373 | 0.222678 |
| 16 | 1 | 0 | 1.161032 | 1.731923 | 0.970112 |
| 17 | 1 | 0 | -4.028993 | -0.862092 | 1.350220 |
| 18 | 8 | 0 | -3.867977 | -1.061896 | 2.294001 |
| 19 | 1 | 0 | -2.998267 | -0.611446 | 2.377601 |
| 20 | 1 | 0 | -0.068044 | 0.218457 | 1.916746 |
| 21 | 8 | 0 | 0.936137 | 0.256174 | 2.126177 |
| 22 | 1 | 0 | 1.017148 | 0.359946 | 3.085712 |
| 23 | 1 | 0 | 1.983556 | -1.003198 | 1.407583 |
| 24 | 8 | 0 | 2.562898 | -1.658995 | 0.947524 |
| 25 | 1 | 0 | 1.955560 | -2.195625 | 0.411632 |
| 26 | 1 | 0 | 1.745988 | 4.207767 | 0.457775 |
| 27 | 8 | 0 | 2.446512 | 4.881122 | 0.343779 |
| 28 | 1 | 0 | 3.123883 | 4.384904 | -0.147812 |
| 29 | 1 | 0 | 2.429822 | 2.286755 | -0.778044 |
| 30 | 8 | 0 | 3.313907 | 2.371995 | -1.231637 |
| 31 | 1 | 0 | 3.112342 | 2.474757 | -2.173409 |
| 32 | 1 | 0 | 3.610779 | -0.692576 | -0.341565 |
| 33 | 8 | 0 | 4.335182 | -0.315876 | -0.884415 |
| 34 | 1 | 0 | 4.116129 | 0.634946 | -0.979164 |
| 35 | 1 | 0 | 4.595736 | -2.079970 | 1.393626 |
| 36 | 8 | 0 | 5.543666 | -1.956719 | 1.205380 |
| 37 | 1 | 0 | 5.519643 | -1.317411 | 0.465717 |
| 38 | 1 | 0 | -5.672714 | 0.299604 | -1.676971 |
| 39 | 1 | 0 | -5.933412 | 0.342730 | 0.078292 |
| 40 | 1 | 0 | -6.171055 | 1.807455 | -0.897822 |
| 41 | 6 | 0 | -0.595041 | -3.280122 | -0.347202 |
| 42 | 6 | 0 | 0.398023 | -3.214074 | -1.331303 |
| 43 | 1 | 0 | 0.158809 | 0.106643 | -2.069865 |
| 44 | 1 | 0 | 1.447422 | -1.931046 | -2.714449 |
| 45 | 1 | 0 | -2.069539 | -2.183769 | 0.785226 |
| 46 | 1 | 0 | -0.807352 | -4.224037 | 0.149072 |
| 47 | 1 | 0 | 0.955474 | -4.106013 | -1.607510 |
| 48 | 1 | 0 | -3.406925 | -0.545899 | -1.168231 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1166.96917346    A.U. after    1 cycles

Convg  =    0.3693D-08             -V/T =  2.0094

S**2  =   0.0000

Zero-point correction=                       0.398417 (a.u.)

Thermal correction to Energy=                0.431309

Thermal correction to Enthalpy=              0.432253

Thermal correction to Gibbs Free Energy=     0.330715

Sum of electronic and zero-point Energies=          -1166.570757

Sum of electronic and thermal Energies=       -1166.537864
Sum of electronic and thermal Enthalpies=      -1166.536920
Sum of electronic and thermal Free Energies=    -1166.638458


n=12 TS
N-ethyl benzamide and HO-(H2O)12, HO- addtion TS, TS1(am)
tuka03dd.chk   Stoichiometry  C9H36NO14(1-)
                Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number    Type       X        Y        Z
-----------------------------------------------------------------------
   1       6        0     0.157672  -1.035726  -1.168732
   2       6        0    -0.962084  -0.024549  -0.960683
   3       8        0    -0.718930   1.215678  -1.183615
   4       8        0    -1.071149  -0.152129   0.887198
   5       1        0    -1.602918   0.640954   1.114640
   6       6        0     1.258200  -0.663056  -1.949717
   7       6        0     2.287236  -1.570362  -2.208860
   8       6        0     0.095935  -2.340036  -0.655906
   9       7        0    -2.224464  -0.556847  -1.374470
  10       6        0    -3.265021   0.383662  -1.802075
  11       1        0    -3.525004   1.018259  -0.950185
  12       1        0    -2.901316   1.049655  -2.597563
  13       6        0    -4.505509  -0.373504  -2.270727
  14       1        0     0.593626   1.924783  -0.373116
  15       8        0     1.293194   2.384295   0.181699
  16       1        0     1.404495   1.779918   0.953599
  17       1        0    -3.272489  -1.838256   0.332469
  18       8        0    -2.991649  -1.939773   1.259739
  19       1        0    -2.197298  -1.318456   1.261792
  20       1        0     0.292155   0.057838   1.604569
  21       8        0     1.210127   0.298464   2.014954
  22       1        0     1.080485   0.364270   2.972611
  23       1        0     2.594822  -0.731409   1.536360
  24       8        0     3.368135  -1.257492   1.216579
  25       1        0     2.989923  -1.916560   0.611607
  26       1        0     0.561204   3.919155   0.578203
  27       8        0     0.011989   4.742463   0.672424
  28       1        0     0.534835   5.452073   0.271781
  29       1        0     2.866984   2.647225  -0.598323
  30       8        0     3.756373   2.798921  -1.007598
  31       1        0     3.624424   2.674271  -1.958726
  32       1        0     4.461559  -0.115697   0.123396
  33       8        0     5.197657   0.411783  -0.252409

| 34 | 1 | 0 | 4.810220 | 1.291044 | -0.448033 |
| 35 | 1 | 0 | 5.290315 | -1.165324 | 2.177022 |
| 36 | 8 | 0 | 6.184676 | -0.781410 | 2.210176 |
| 37 | 1 | 0 | 6.185596 | -0.205535 | 1.419146 |
| 38 | 1 | 0 | -4.274930 | -1.039399 | -3.113699 |
| 39 | 1 | 0 | -4.933201 | -0.978983 | -1.463636 |
| 40 | 1 | 0 | -5.273840 | 0.331329 | -2.606186 |
| 41 | 6 | 0 | 1.124074 | -3.248823 | -0.915527 |
| 42 | 6 | 0 | 2.223585 | -2.867162 | -1.691910 |
| 43 | 1 | 0 | 1.295509 | 0.345711 | -2.347925 |
| 44 | 1 | 0 | 3.142892 | -1.262919 | -2.803739 |
| 45 | 1 | 0 | -0.739969 | -2.643756 | -0.035598 |
| 46 | 1 | 0 | 1.062470 | -4.253053 | -0.504570 |
| 47 | 1 | 0 | 3.024928 | -3.574142 | -1.892147 |
| 48 | 1 | 0 | -1.735124 | 2.691809 | -0.887553 |
| 49 | 8 | 0 | -2.216245 | 3.469722 | -0.512301 |
| 50 | 1 | 0 | -1.508000 | 4.070530 | -0.190125 |
| 51 | 1 | 0 | -2.736641 | 2.683286 | 0.923791 |
| 52 | 8 | 0 | -2.875280 | 2.082331 | 1.710646 |
| 53 | 1 | 0 | -2.548350 | 2.575128 | 2.477613 |
| 54 | 1 | 0 | -2.542819 | -3.666458 | 1.521796 |
| 55 | 8 | 0 | -2.270595 | -4.610605 | 1.622730 |
| 56 | 1 | 0 | -2.329997 | -4.786020 | 2.572826 |
| 57 | 1 | 0 | -4.308130 | -0.730310 | 2.106990 |
| 58 | 8 | 0 | -4.864399 | 0.032962 | 2.363199 |
| 59 | 1 | 0 | -4.312488 | 0.806807 | 2.137732 |
| 60 | 1 | 0 | -2.098434 | -1.324197 | -2.028092 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1472.74204120    A.U. after   1 cycles
       Convg  =    0.2594D-08          -V/T =  2.0093
       S**2  =  0.0000

Zero-point correction=                    0.500557 (a.u.)
Thermal correction to Energy=             0.543788
Thermal correction to Enthalpy=           0.544732
Thermal correction to Gibbs Free Energy=       0.418220
Sum of electronic and zero-point Energies=        -1472.241484
Sum of electronic and thermal Energies=           -1472.198253
Sum of electronic and thermal Enthalpies=         -1472.197309
Sum of electronic and thermal Free Energies=       -1472.323821


 n=16 TS
N-ethyl benzamide + HO-(H2O)16 TS1, TS1(am)
tuka02aa.chk     Stoichiometry:C9H44NO18(1-)
             Standard orientation:
---------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.470652 | 2.399800 | -0.844394 |
| 2 | 6 | 0 | -0.180315 | 1.366931 | 0.254620 |
| 3 | 8 | 0 | -1.118661 | 0.470879 | 0.459457 |
| 4 | 7 | 0 | 0.342700 | 2.010664 | 1.397317 |
| 5 | 6 | 0 | 0.645579 | 1.245170 | 2.603188 |
| 6 | 6 | 0 | -1.799864 | 2.635945 | -1.211927 |
| 7 | 6 | 0 | -2.113841 | 3.598584 | -2.173143 |
| 8 | 6 | 0 | 0.540684 | 3.151935 | -1.458527 |
| 9 | 1 | 0 | 1.076941 | 2.683243 | 1.182820 |
| 10 | 6 | 0 | 0.885925 | 2.186439 | 3.783055 |
| 11 | 1 | 0 | -0.202787 | 0.591747 | 2.814586 |
| 12 | 1 | 0 | 1.528264 | 0.597069 | 2.466522 |
| 13 | 8 | 0 | 1.157664 | 0.509965 | -0.411976 |
| 14 | 1 | 0 | 0.896889 | 0.227086 | -1.314410 |
| 15 | 1 | 0 | 1.587771 | -0.852260 | 0.345443 |
| 16 | 8 | 0 | 1.952299 | -1.713037 | 0.748674 |
| 17 | 1 | 0 | 2.700652 | -1.434461 | 1.313807 |
| 18 | 1 | 0 | 2.706877 | -2.407177 | -0.567744 |
| 19 | 8 | 0 | 3.249789 | -2.785737 | -1.325315 |
| 20 | 1 | 0 | 3.390337 | -2.037032 | -1.927494 |
| 21 | 1 | 0 | 4.767183 | -3.037333 | -0.478314 |
| 22 | 8 | 0 | 5.544084 | -3.023980 | 0.142972 |
| 23 | 1 | 0 | 5.564892 | -3.901335 | 0.552826 |
| 24 | 1 | 0 | 1.612379 | -3.375996 | -2.394466 |
| 25 | 8 | 0 | 0.918694 | -3.204272 | -3.058986 |
| 26 | 1 | 0 | 0.050873 | -3.504101 | -2.664685 |
| 27 | 1 | 0 | 0.661174 | -1.532679 | -3.126138 |
| 28 | 8 | 0 | 0.461399 | -0.551175 | -3.066459 |
| 29 | 1 | 0 | 0.752093 | -0.153017 | -3.899660 |
| 30 | 1 | 0 | 5.065508 | -1.649753 | 1.162312 |
| 31 | 8 | 0 | 4.574746 | -0.895313 | 1.578999 |
| 32 | 1 | 0 | 5.059210 | -0.636911 | 2.376590 |
| 33 | 1 | 0 | -1.776876 | -0.345121 | -0.967672 |
| 34 | 8 | 0 | -2.108694 | -0.773240 | -1.803528 |
| 35 | 1 | 0 | -1.432968 | -0.526168 | -2.465828 |
| 36 | 1 | 0 | -1.815175 | -2.628230 | -2.039072 |
| 37 | 8 | 0 | -1.576407 | -3.579154 | -2.121011 |
| 38 | 1 | 0 | -1.869970 | -3.937887 | -1.248433 |
| 39 | 1 | 0 | -3.831575 | -1.515954 | -1.181114 |
| 40 | 8 | 0 | -4.464323 | -2.010375 | -0.624051 |
| 41 | 1 | 0 | -4.860708 | -1.346189 | -0.014687 |
| 42 | 1 | 0 | -0.847662 | -1.064812 | 1.165701 |
| 43 | 8 | 0 | -0.733012 | -1.960657 | 1.595774 |

| 44 | 1 | 0 | 0.223355 | -2.144736 | 1.488287 |
|----|---|---|----------|-----------|----------|
| 45 | 1 | 0 | -1.656867 | -1.836059 | 3.101483 |
| 46 | 8 | 0 | -2.343048 | -1.621517 | 3.782176 |
| 47 | 1 | 0 | -3.046979 | -2.270386 | 3.628954 |
| 48 | 1 | 0 | -1.944807 | -3.214478 | 0.852215 |
| 49 | 8 | 0 | -2.601781 | -3.826397 | 0.454936 |
| 50 | 1 | 0 | -3.353363 | -3.247451 | 0.179614 |
| 51 | 1 | 0 | 2.816465 | 1.024139 | -0.349095 |
| 52 | 8 | 0 | 3.769296 | 1.284433 | -0.214281 |
| 53 | 1 | 0 | 4.141875 | 0.590024 | 0.364135 |
| 54 | 1 | 0 | 3.527289 | 2.751943 | 0.736901 |
| 55 | 8 | 0 | 3.220396 | 3.527803 | 1.273584 |
| 56 | 1 | 0 | 3.423512 | 4.310456 | 0.741796 |
| 57 | 1 | 0 | -2.912549 | -0.008539 | 2.964230 |
| 58 | 8 | 0 | -3.161896 | 0.718587 | 2.350330 |
| 59 | 1 | 0 | -2.434337 | 0.745699 | 1.680167 |
| 60 | 1 | 0 | -4.616935 | 0.249836 | 1.616685 |
| 61 | 8 | 0 | -5.448266 | -0.072571 | 1.162537 |
| 62 | 1 | 0 | -5.847773 | 0.712152 | 0.760954 |
| 63 | 6 | 0 | 0.227862 | 4.115941 | -2.418266 |
| 64 | 6 | 0 | -1.101764 | 4.343406 | -2.779777 |
| 65 | 1 | 0 | -2.583159 | 2.052290 | -0.741269 |
| 66 | 1 | 0 | -3.152852 | 3.764280 | -2.447800 |
| 67 | 1 | 0 | 1.577652 | 2.972046 | -1.194422 |
| 68 | 1 | 0 | 1.026415 | 4.686340 | -2.887611 |
| 69 | 1 | 0 | -1.345600 | 5.092438 | -3.529757 |
| 70 | 1 | 0 | 1.720521 | 2.865998 | 3.576164 |
| 71 | 1 | 0 | -0.009187 | 2.785962 | 3.980437 |
| 72 | 1 | 0 | 1.125183 | 1.611812 | 4.686197 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1778.52641035     A.U. after    1 cycles

Convg  =    0.4358D-08          -V/T =  2.0093

S**2  =  0.0000

Zero-point correction=                     0.608558 (a.u.)

Thermal correction to Energy=               0.659034

Thermal correction to Enthalpy=             0.659978

Thermal correction to Gibbs Free Energy=        0.521684

Sum of electronic and zero-point Energies=        -1777.917853

Sum of electronic and thermal Energies=           -1777.867376

Sum of electronic and thermal Enthalpies=         -1777.866432

Sum of electronic and thermal Free Energies=       -1778.004727


 n=24 TS

N-ethyl benzamide and HO-(H2O)24 TS1(am)

tuka02hh.chk    Stoichiometry C9H60NO26(1-)

Standard orientation:
--------------------------------------------------------------------

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) | | |
| --- | --- | --- | --- | --- | --- |
| | | | X | Y | Z |
| 1 | 6 | 0 | 0.738258 | -2.509405 | -1.715082 |
| 2 | 6 | 0 | 0.594643 | -1.699462 | -0.426315 |
| 3 | 8 | 0 | 1.570108 | -0.877410 | -0.130417 |
| 4 | 7 | 0 | 0.103841 | -2.494532 | 0.616265 |
| 5 | 6 | 0 | -0.143069 | -1.947900 | 1.950257 |
| 6 | 6 | 0 | 2.007121 | -2.660926 | -2.284112 |
| 7 | 6 | 0 | 2.181726 | -3.427656 | -3.437988 |
| 8 | 6 | 0 | -0.355031 | -3.144732 | -2.321755 |
| 9 | 1 | 0 | -0.613125 | -3.145510 | 0.314979 |
| 10 | 6 | 0 | -0.407308 | -3.072920 | 2.947823 |
| 11 | 1 | 0 | 0.742337 | -1.388943 | 2.258055 |
| 12 | 1 | 0 | -0.988243 | -1.240491 | 1.943996 |
| 13 | 8 | 0 | -0.781220 | -0.650915 | -0.859048 |
| 14 | 1 | 0 | -0.576717 | -0.264679 | -1.736238 |
| 15 | 1 | 0 | -1.087316 | 0.620945 | 0.074125 |
| 16 | 8 | 0 | -1.361981 | 1.442795 | 0.614372 |
| 17 | 1 | 0 | -2.066870 | 1.135496 | 1.216455 |
| 18 | 1 | 0 | -2.149021 | 2.399507 | -0.557720 |
| 19 | 8 | 0 | -2.659783 | 2.965456 | -1.205951 |
| 20 | 1 | 0 | -2.955561 | 2.351807 | -1.898076 |
| 21 | 1 | 0 | -4.163798 | 3.237811 | -0.208607 |
| 22 | 8 | 0 | -4.914690 | 3.072197 | 0.412580 |
| 23 | 1 | 0 | -4.716337 | 3.565598 | 1.235706 |
| 24 | 1 | 0 | -1.097528 | 3.562183 | -2.261258 |
| 25 | 8 | 0 | -0.400074 | 3.461938 | -2.939667 |
| 26 | 1 | 0 | 0.458973 | 3.691662 | -2.506759 |
| 27 | 1 | 0 | -0.266921 | 1.801460 | -3.296016 |
| 28 | 8 | 0 | -0.130682 | 0.813414 | -3.391166 |
| 29 | 1 | 0 | -0.400437 | 0.576619 | -4.290773 |
| 30 | 1 | 0 | -4.392196 | 1.508496 | 1.126124 |
| 31 | 8 | 0 | -3.984127 | 0.812970 | 1.701040 |
| 32 | 1 | 0 | -4.741238 | 0.247948 | 1.987873 |
| 33 | 1 | 0 | 2.090146 | 0.178309 | -1.396954 |
| 34 | 8 | 0 | 2.385434 | 0.777147 | -2.138122 |
| 35 | 1 | 0 | 1.692183 | 0.665341 | -2.822586 |
| 36 | 1 | 0 | 2.235303 | 2.578685 | -1.938139 |
| 37 | 8 | 0 | 2.155527 | 3.562507 | -1.883697 |
| 38 | 1 | 0 | 2.468600 | 3.754987 | -0.974071 |
| 39 | 1 | 0 | 4.159941 | 1.175235 | -1.693977 |
| 40 | 8 | 0 | 4.890883 | 1.571106 | -1.172531 |
| 41 | 1 | 0 | 5.365097 | 0.810758 | -0.759734 |

| 42 | 1 | 0 | 1.360421 | 0.502979 | 0.857924 |
|----|---|---|----------|----------|----------|
| 43 | 8 | 0 | 1.316054 | 1.328690 | 1.417338 |
| 44 | 1 | 0 | 0.380592 | 1.612765 | 1.327253 |
| 45 | 1 | 0 | 2.290103 | 0.859139 | 2.906188 |
| 46 | 8 | 0 | 3.059008 | 0.511615 | 3.413806 |
| 47 | 1 | 0 | 3.677692 | 1.278609 | 3.469776 |
| 48 | 1 | 0 | 2.636211 | 2.436175 | 0.869083 |
| 49 | 8 | 0 | 3.383472 | 3.044130 | 0.647894 |
| 50 | 1 | 0 | 3.992890 | 2.522253 | 0.063980 |
| 51 | 1 | 0 | -2.457100 | -1.037366 | -0.736288 |
| 52 | 8 | 0 | -3.432660 | -1.081385 | -0.520621 |
| 53 | 1 | 0 | -3.543076 | -0.463984 | 0.230614 |
| 54 | 1 | 0 | -4.803207 | -2.429323 | 0.022137 |
| 55 | 8 | 0 | -5.772283 | -2.544561 | 0.117012 |
| 56 | 1 | 0 | -6.093812 | -2.079037 | -0.695677 |
| 57 | 1 | 0 | 3.567158 | -0.719878 | 2.218929 |
| 58 | 8 | 0 | 3.697086 | -1.436974 | 1.544002 |
| 59 | 1 | 0 | 2.924033 | -1.350156 | 0.926139 |
| 60 | 1 | 0 | 5.140353 | -1.008059 | 0.634627 |
| 61 | 8 | 0 | 5.909995 | -0.701307 | 0.086764 |
| 62 | 1 | 0 | 6.170616 | -1.458297 | -0.457241 |
| 63 | 6 | 0 | -0.180496 | -3.915172 | -3.471377 |
| 64 | 6 | 0 | 1.089731 | -4.058341 | -4.034605 |
| 65 | 1 | 0 | 2.853572 | -2.168139 | -1.818501 |
| 66 | 1 | 0 | 3.174166 | -3.530627 | -3.869460 |
| 67 | 1 | 0 | -1.351327 | -3.014993 | -1.908966 |
| 68 | 1 | 0 | -1.040118 | -4.395826 | -3.931614 |
| 69 | 1 | 0 | 1.225097 | -4.654483 | -4.933617 |
| 70 | 1 | 0 | -1.299388 | -3.651537 | 2.670855 |
| 71 | 1 | 0 | 0.449876 | -3.751639 | 2.993534 |
| 72 | 1 | 0 | -0.566608 | -2.658265 | 3.948104 |
| 73 | 1 | 0 | -6.474175 | 1.996705 | -0.051040 |
| 74 | 8 | 0 | -7.047551 | 1.220321 | -0.209643 |
| 75 | 1 | 0 | -6.994931 | 0.684482 | 0.606675 |
| 76 | 1 | 0 | -3.876564 | 2.363983 | 2.951024 |
| 77 | 8 | 0 | -4.075970 | 3.311804 | 3.103375 |
| 78 | 1 | 0 | -3.289205 | 3.692816 | 3.520553 |
| 79 | 1 | 0 | 3.962371 | 3.980391 | -2.799560 |
| 80 | 8 | 0 | 4.914729 | 3.914056 | -3.004513 |
| 81 | 1 | 0 | 5.213318 | 3.181548 | -2.433777 |
| 82 | 1 | 0 | 2.527482 | -0.761728 | 4.831879 |
| 83 | 8 | 0 | 2.251030 | -1.556837 | 5.327895 |
| 84 | 1 | 0 | 2.546784 | -2.299258 | 4.763522 |
| 85 | 1 | 0 | 4.207175 | 3.049694 | 2.212505 |
| 86 | 8 | 0 | 4.551482 | 2.853297 | 3.123880 |
| 87 | 1 | 0 | 4.356822 | 3.635756 | 3.659389 |

| | | | | | |
|---|---|---|---|---|---|
| 88 | 1 | 0 | -6.168502 | -1.448665 | 1.307970 |
| 89 | 8 | 0 | -6.320697 | -0.660580 | 1.919117 |
| 90 | 1 | 0 | -6.798493 | -0.989496 | 2.695009 |
| 91 | 1 | 0 | -4.989381 | -0.663008 | -1.728971 |
| 92 | 8 | 0 | -5.941282 | -0.718363 | -1.951647 |
| 93 | 1 | 0 | -6.361277 | 0.040341 | -1.484060 |
| 94 | 1 | 0 | 3.469268 | -2.857466 | 2.661140 |
| 95 | 8 | 0 | 3.346017 | -3.495274 | 3.405449 |
| 96 | 1 | 0 | 4.240946 | -3.707518 | 3.708641 |

-----------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -2390.06356594    A.U. after    1 cycles

Convg  =    0.5806D-08          -V/T =  2.0093

S**2  =  0.0000

Zero-point correction=                       0.816166 (a.u.)

Thermal correction to Energy=                0.885905

Thermal correction to Enthalpy=              0.886849

Thermal correction to Gibbs Free Energy=     0.706041

Sum of electronic and zero-point Energies=       -2389.247400

Sum of electronic and thermal Energies=          -2389.177661

Sum of electronic and thermal Enthalpies=        -2389.176717

Sum of electronic and thermal Free Energies=     -2389.357525

n=32 TS

N-ethyl benzamide and HO-(H2O)32  TS1(am)

tuka02ww.chk    Stoichiometry: C9H76NO34(1-)

Standard orientation:

-----------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| Number | Number | Type | X | Y | Z |

-----------------------------------------------------------------------

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.833024 | -0.878535 | 2.940360 |
| 2 | 6 | 0 | -0.976524 | -1.087997 | 1.431556 |
| 3 | 8 | 0 | -1.844492 | -0.320763 | 0.810826 |
| 4 | 7 | 0 | -1.027926 | -2.458438 | 1.128574 |
| 5 | 6 | 0 | -1.234583 | -2.946187 | -0.233602 |
| 6 | 6 | 0 | -1.888653 | -0.288664 | 3.643804 |
| 7 | 6 | 0 | -1.816955 | -0.127597 | 5.028610 |
| 8 | 6 | 0 | 0.293802 | -1.314104 | 3.651610 |
| 9 | 1 | 0 | -0.360418 | -3.007762 | 1.658779 |
| 10 | 6 | 0 | -1.432565 | -4.460543 | -0.229213 |
| 11 | 1 | 0 | -2.128723 | -2.462462 | -0.632956 |
| 12 | 1 | 0 | -0.395952 | -2.678488 | -0.898026 |
| 13 | 8 | 0 | 0.585530 | -0.560251 | 0.857661 |
| 14 | 1 | 0 | 0.687228 | 0.366715 | 1.177956 |
| 15 | 1 | 0 | 0.781550 | -0.396100 | -0.716540 |

| 16 | 8 | 0 | 1.012333 | -0.188019 | -1.690256 |
| 17 | 1 | 0 | 1.488497 | -0.962872 | -2.031600 |
| 18 | 1 | 0 | 2.173747 | 1.076515 | -1.357837 |
| 19 | 8 | 0 | 2.879813 | 1.757760 | -1.215869 |
| 20 | 1 | 0 | 3.155433 | 1.711500 | -0.261194 |
| 21 | 1 | 0 | 4.181737 | 1.274257 | -2.085151 |
| 22 | 8 | 0 | 5.001999 | 0.856213 | -2.491266 |
| 23 | 1 | 0 | 4.796508 | 0.643921 | -3.427166 |
| 24 | 1 | 0 | 1.889755 | 3.353952 | -0.937201 |
| 25 | 8 | 0 | 1.559155 | 4.060430 | -0.343432 |
| 26 | 1 | 0 | 0.642448 | 4.275653 | -0.637028 |
| 27 | 1 | 0 | 1.130128 | 2.895389 | 1.049311 |
| 28 | 8 | 0 | 1.010941 | 2.212414 | 1.752955 |
| 29 | 1 | 0 | 1.929729 | 2.085480 | 2.066869 |
| 30 | 1 | 0 | 4.237327 | -0.868759 | -2.032396 |
| 31 | 8 | 0 | 3.808102 | -1.752528 | -2.073510 |
| 32 | 1 | 0 | 4.544060 | -2.379892 | -1.882180 |
| 33 | 1 | 0 | -1.791160 | 1.387047 | 1.166166 |
| 34 | 8 | 0 | -1.763594 | 2.361171 | 1.378762 |
| 35 | 1 | 0 | -0.962447 | 2.452428 | 1.932596 |
| 36 | 1 | 0 | -1.380459 | 3.553434 | 0.024200 |
| 37 | 8 | 0 | -1.201508 | 4.218928 | -0.683957 |
| 38 | 1 | 0 | -1.767892 | 3.916208 | -1.422358 |
| 39 | 1 | 0 | -3.511901 | 2.979703 | 1.123112 |
| 40 | 8 | 0 | -4.274695 | 3.239775 | 0.561274 |
| 41 | 1 | 0 | -5.031646 | 2.671021 | 0.829120 |
| 42 | 1 | 0 | -1.739802 | 0.024083 | -0.834330 |
| 43 | 8 | 0 | -1.755243 | 0.297295 | -1.799503 |
| 44 | 1 | 0 | -0.818586 | 0.216757 | -2.077436 |
| 45 | 1 | 0 | -3.120965 | -0.633193 | -2.546260 |
| 46 | 8 | 0 | -4.056248 | -0.935281 | -2.637458 |
| 47 | 1 | 0 | -4.525561 | -0.186380 | -3.066451 |
| 48 | 1 | 0 | -2.707263 | 1.852631 | -1.853296 |
| 49 | 8 | 0 | -3.288370 | 2.644615 | -1.958950 |
| 50 | 1 | 0 | -3.691915 | 2.824536 | -1.068359 |
| 51 | 1 | 0 | 2.081331 | -1.351721 | 0.897169 |
| 52 | 8 | 0 | 2.985675 | -1.762596 | 0.736632 |
| 53 | 1 | 0 | 3.086982 | -1.805028 | -0.237245 |
| 54 | 1 | 0 | 4.229409 | -3.008362 | 1.475174 |
| 55 | 8 | 0 | 5.183298 | -3.193659 | 1.631927 |
| 56 | 1 | 0 | 5.508055 | -2.328094 | 1.968573 |
| 57 | 1 | 0 | -4.330662 | -0.803808 | -0.823854 |
| 58 | 8 | 0 | -4.454849 | -0.814606 | 0.155151 |
| 59 | 1 | 0 | -3.538833 | -0.761502 | 0.534096 |
| 60 | 1 | 0 | -5.485750 | 0.501971 | 0.706425 |
| 61 | 8 | 0 | -6.149928 | 1.213549 | 0.897622 |

| 62 | 1 | 0 | -6.850617 | 0.767090 | 1.424156 |
|---|---|---|---|---|---|
| 63 | 6 | 0 | 0.364285 | -1.157093 | 5.035979 |
| 64 | 6 | 0 | -0.691085 | -0.561002 | 5.729209 |
| 65 | 1 | 0 | -2.765088 | 0.044819 | 3.099111 |
| 66 | 1 | 0 | -2.644493 | 0.337546 | 5.557798 |
| 67 | 1 | 0 | 1.130467 | -1.755920 | 3.118141 |
| 68 | 1 | 0 | 1.250126 | -1.490841 | 5.570496 |
| 69 | 1 | 0 | -0.633398 | -0.431941 | 6.807043 |
| 70 | 1 | 0 | -0.529197 | -4.979778 | 0.119586 |
| 71 | 1 | 0 | -2.261733 | -4.734769 | 0.430912 |
| 72 | 1 | 0 | -1.672556 | -4.825538 | -1.232502 |
| 73 | 1 | 0 | 6.255670 | 0.130455 | -1.424705 |
| 74 | 8 | 0 | 6.840452 | -0.264038 | -0.735530 |
| 75 | 1 | 0 | 6.862922 | -1.228007 | -0.922534 |
| 76 | 1 | 0 | 3.816914 | -1.304763 | -4.024203 |
| 77 | 8 | 0 | 4.106392 | -0.656216 | -4.699529 |
| 78 | 1 | 0 | 3.355493 | -0.522909 | -5.296640 |
| 79 | 1 | 0 | -2.539030 | 5.680379 | -0.060437 |
| 80 | 8 | 0 | -3.396398 | 6.052913 | 0.219823 |
| 81 | 1 | 0 | -3.934537 | 5.257925 | 0.392915 |
| 82 | 1 | 0 | -4.997285 | -2.585313 | -2.735552 |
| 83 | 8 | 0 | -5.603348 | -3.347395 | -2.624337 |
| 84 | 1 | 0 | -6.198690 | -3.079335 | -1.893847 |
| 85 | 1 | 0 | -4.561407 | 2.038449 | -2.909071 |
| 86 | 8 | 0 | -5.251271 | 1.495495 | -3.394293 |
| 87 | 1 | 0 | -5.386335 | 1.916259 | -4.256019 |
| 88 | 1 | 0 | 5.756673 | -3.047089 | -0.065667 |
| 89 | 8 | 0 | 6.087658 | -2.981643 | -0.997819 |
| 90 | 1 | 0 | 6.549369 | -3.832248 | -1.113752 |
| 91 | 1 | 0 | 4.407829 | -0.689625 | 1.293108 |
| 92 | 8 | 0 | 5.274157 | -0.379941 | 1.649285 |
| 93 | 1 | 0 | 5.852303 | -0.253742 | 0.862897 |
| 94 | 1 | 0 | -6.077827 | -1.790753 | -0.053728 |
| 95 | 8 | 0 | -6.972609 | -1.922988 | -0.434951 |
| 96 | 1 | 0 | -7.114508 | -1.115153 | -0.992178 |
| 97 | 1 | 0 | 6.168764 | -4.784550 | 1.190766 |
| 98 | 8 | 0 | 6.701957 | -5.308309 | 0.557642 |
| 99 | 1 | 0 | 6.882344 | -6.160174 | 0.979228 |
| 100 | 1 | 0 | 4.477517 | 1.386155 | 1.687708 |
| 101 | 8 | 0 | 3.759602 | 1.987918 | 1.399755 |
| 102 | 1 | 0 | 4.134264 | 2.897303 | 1.234680 |
| 103 | 1 | 0 | -6.984504 | 1.030619 | -0.769107 |
| 104 | 8 | 0 | -7.316293 | 0.593695 | -1.586738 |
| 105 | 1 | 0 | -6.728247 | 0.919735 | -2.298257 |
| 106 | 1 | 0 | 5.841696 | 2.781386 | -2.011199 |
| 107 | 8 | 0 | 6.198535 | 3.523438 | -1.490234 |

| 108 | 1 | 0 | 6.993535 | 3.147901 | -1.051096 |
|-----|---|---|----------|----------|-----------|
| 109 | 1 | 0 | 3.507718 | 4.654927 | 0.148984 |
| 110 | 8 | 0 | 4.395095 | 4.446738 | 0.501990 |
| 111 | 1 | 0 | 4.978543 | 4.250048 | -0.267001 |
| 112 | 1 | 0 | 8.022422 | 1.126947 | -0.462587 |
| 113 | 8 | 0 | 8.382562 | 2.039939 | -0.406176 |
| 114 | 1 | 0 | 9.186833 | 2.045694 | -0.945147 |
| 115 | 1 | 0 | -4.617525 | -4.863445 | -2.487079 |
| 116 | 8 | 0 | -4.080019 | -5.689465 | -2.547463 |
| 117 | 1 | 0 | -4.458454 | -6.163991 | -3.301517 |
| 118 | 1 | 0 | -7.867566 | -1.223989 | 1.032024 |
| 119 | 8 | 0 | -8.153797 | -0.610321 | 1.753285 |
| 120 | 1 | 0 | -9.059864 | -0.353283 | 1.527145 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -3001.59879182    A.U. after    1 cycles

     Convg  =    0.4028D-08          -V/T =  2.0093

     S**2  =   0.0000

Zero-point correction=                          1.023828 (a.u.)

Thermal correction to Energy=                   1.112687

Thermal correction to Enthalpy=                 1.113631

Thermal correction to Gibbs Free Energy=        0.891095

Sum of electronic and zero-point Energies=          -3000.574964

Sum of electronic and thermal Energies=             -3000.486105

Sum of electronic and thermal Enthalpies=           -3000.485160

Sum of electronic and thermal Free Energies=        -3000.707697


=======================================================================

[3]  Geometries of the n=16 ester hydrolysis in Figure 3

(3-1) reactant-like complex (precursor)
  zuka02aa.for.g09.chk    Stoichiometry C9H43O19(1-)
              Standard orientation:
---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|-------|-------|-------|
| Number | Number | Type | X | Y | Z |

---------------------------------------------------------------------

| 1 | 6 | 0 | -3.459320 | -1.804560 | 0.269734 |
| 2 | 6 | 0 | -2.283186 | -1.463164 | -0.575967 |
| 3 | 8 | 0 | -1.787277 | -0.333465 | -0.624450 |
| 4 | 8 | 0 | -1.825966 | -2.489807 | -1.284015 |
| 5 | 6 | 0 | -0.640002 | -2.277620 | -2.118665 |
| 6 | 6 | 0 | -3.927062 | -0.854667 | 1.189895 |
| 7 | 6 | 0 | -5.027542 | -1.147187 | 1.992776 |
| 8 | 6 | 0 | -4.101807 | -3.047369 | 0.162822 |
| 9 | 6 | 0 | -0.415874 | -3.552816 | -2.904888 |
| 10 | 1 | 0 | -0.833317 | -1.419907 | -2.768374 |
| 11 | 1 | 0 | 0.202810 | -2.057319 | -1.456905 |
| 12 | 8 | 0 | 2.076165 | -1.796150 | -0.184243 |
| 13 | 1 | 0 | 1.681141 | -1.360514 | 0.602432 |
| 14 | 1 | 0 | 2.268714 | -1.038424 | -0.827995 |
| 15 | 8 | 0 | 2.614487 | 0.294854 | -1.742392 |
| 16 | 1 | 0 | 2.896190 | 0.073593 | -2.642200 |
| 17 | 1 | 0 | 3.836438 | 0.681503 | -0.817596 |
| 18 | 8 | 0 | 4.588474 | 0.797383 | -0.126145 |
| 19 | 1 | 0 | 4.608672 | -0.074901 | 0.335457 |
| 20 | 1 | 0 | 6.065693 | 0.619315 | -0.936853 |
| 21 | 8 | 0 | 6.912396 | 0.304427 | -1.377402 |
| 22 | 1 | 0 | 6.773283 | 0.435874 | -2.326643 |
| 23 | 1 | 0 | 3.665902 | 1.567905 | 1.251537 |
| 24 | 8 | 0 | 3.135639 | 1.647849 | 2.081604 |
| 25 | 1 | 0 | 2.541874 | 2.433663 | 1.985131 |
| 26 | 1 | 0 | 1.921115 | 0.395666 | 2.055002 |
| 27 | 8 | 0 | 1.303490 | -0.370551 | 2.218764 |
| 28 | 1 | 0 | 1.812276 | -0.865812 | 2.895851 |
| 29 | 1 | 0 | 6.976068 | -1.388456 | -0.864211 |
| 30 | 8 | 0 | 6.918778 | -2.303198 | -0.482413 |
| 31 | 1 | 0 | 7.660959 | -2.367700 | 0.136419 |
| 32 | 1 | 0 | -1.130036 | 0.805365 | 1.006731 |
| 33 | 8 | 0 | -0.979457 | 1.136625 | 1.910816 |
| 34 | 1 | 0 | -0.273683 | 0.535819 | 2.254802 |
| 35 | 1 | 0 | 0.344328 | 2.767015 | 2.031655 |
| 36 | 8 | 0 | 1.044765 | 3.436797 | 1.905043 |
| 37 | 1 | 0 | 0.801114 | 3.838531 | 1.040065 |

| 38 | 1 | 0 | -2.118464 | 2.779205 | 1.681139 |
| 39 | 8 | 0 | -2.431985 | 3.559127 | 1.186870 |
| 40 | 1 | 0 | -3.300531 | 3.322741 | 0.792255 |
| 41 | 1 | 0 | -0.240093 | 0.748692 | -1.446701 |
| 42 | 8 | 0 | 0.328011 | 1.461773 | -1.785521 |
| 43 | 1 | 0 | 1.284443 | 1.055652 | -1.798075 |
| 44 | 1 | 0 | -0.618570 | 2.515831 | -2.988439 |
| 45 | 8 | 0 | -1.304715 | 3.191459 | -3.202563 |
| 46 | 1 | 0 | -1.131196 | 3.863182 | -2.512426 |
| 47 | 1 | 0 | -0.003139 | 3.038724 | -0.849627 |
| 48 | 8 | 0 | -0.260908 | 3.945570 | -0.559642 |
| 49 | 1 | 0 | -1.086414 | 3.845516 | -0.027336 |
| 50 | 1 | 0 | 3.704684 | -2.012179 | 0.503529 |
| 51 | 8 | 0 | 4.550041 | -1.808395 | 0.987915 |
| 52 | 1 | 0 | 5.303203 | -2.182728 | 0.478896 |
| 53 | 1 | 0 | 4.149656 | -1.327511 | 2.777341 |
| 54 | 8 | 0 | 3.744257 | -0.904473 | 3.565611 |
| 55 | 1 | 0 | 3.803764 | 0.051118 | 3.374802 |
| 56 | 1 | 0 | -2.725928 | 2.260990 | -2.665366 |
| 57 | 8 | 0 | -3.381013 | 1.641465 | -2.244724 |
| 58 | 1 | 0 | -2.831540 | 1.019213 | -1.734709 |
| 59 | 1 | 0 | -4.312069 | 2.461639 | -1.044899 |
| 60 | 8 | 0 | -4.747661 | 2.891569 | -0.258847 |
| 61 | 1 | 0 | -5.491484 | 2.321255 | -0.019267 |
| 62 | 6 | 0 | -5.206572 | -3.330135 | 0.962581 |
| 63 | 6 | 0 | -5.670450 | -2.381788 | 1.877857 |
| 64 | 1 | 0 | -3.412622 | 0.094633 | 1.286780 |
| 65 | 1 | 0 | -5.376935 | -0.412724 | 2.712802 |
| 66 | 1 | 0 | -3.733656 | -3.779869 | -0.546490 |
| 67 | 1 | 0 | -5.704504 | -4.291852 | 0.873961 |
| 68 | 1 | 0 | -6.529595 | -2.607112 | 2.504558 |
| 69 | 1 | 0 | -0.243025 | -4.399383 | -2.232937 |
| 70 | 1 | 0 | -1.268672 | -3.782271 | -3.553311 |
| 71 | 1 | 0 | 0.473850 | -3.431009 | -3.531782 |

---------------------------------------------------------------------

SCF Done:  E(RB3LYP) =  -1798.42467109     A.U. after    1 cycles

          Convg  =    0.2884D-08          -V/T =  2.0093

Zero-point correction=                           0.596344 (a.u.)

Thermal correction to Energy=                    0.647470

Thermal correction to Enthalpy=                  0.648414

Thermal correction to Gibbs Free Energy=         0.506284

Sum of electronic and zero-point Energies=          -1797.828327

Sum of electronic and thermal Energies=             -1797.777202

Sum of electronic and thermal Enthalpies=           -1797.776257

Sum of electronic and thermal Free Energies=        -1797.918387

(3-2) TS1(es) which is also shown in n=16 of Figure 1
      ethyl benzoate + HO-(H2O)16 TS1(es)
   zuka02aa.chk    Stoichiometry C9H43O19(1-)
                Standard orientation:
---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.029063 | 2.670394 | -0.007977 |
| 2 | 6 | 0 | -0.333003 | 1.442850 | 0.812460 |
| 3 | 8 | 0 | -1.376670 | 0.754484 | 0.605280 |
| 4 | 8 | 0 | 0.171988 | 1.585091 | 2.066932 |
| 5 | 6 | 0 | -0.139275 | 0.572461 | 3.039007 |
| 6 | 6 | 0 | -1.002168 | 3.171408 | -0.877904 |
| 7 | 6 | 0 | -0.749097 | 4.321731 | -1.629854 |
| 8 | 6 | 0 | 1.198353 | 3.337491 | 0.111139 |
| 9 | 6 | 0 | 0.566257 | 0.950146 | 4.329589 |
| 10 | 1 | 0 | -1.223399 | 0.524903 | 3.180571 |
| 11 | 1 | 0 | 0.203927 | -0.397340 | 2.667420 |
| 12 | 8 | 0 | 1.112393 | 0.292708 | 0.071213 |
| 13 | 1 | 0 | 0.932669 | 0.320348 | -0.890057 |
| 14 | 1 | 0 | 1.114067 | -1.184518 | 0.519889 |
| 15 | 8 | 0 | 1.192987 | -2.180322 | 0.801716 |
| 16 | 1 | 0 | 1.845657 | -2.191722 | 1.527157 |
| 17 | 1 | 0 | 2.282543 | -2.529205 | -0.575781 |
| 18 | 8 | 0 | 3.048589 | -2.485507 | -1.207847 |
| 19 | 1 | 0 | 3.408064 | -1.583854 | -1.018809 |
| 20 | 1 | 0 | 4.170642 | -3.491734 | -0.329493 |
| 21 | 8 | 0 | 4.696286 | -3.933476 | 0.394713 |
| 22 | 1 | 0 | 4.341013 | -4.832240 | 0.461187 |
| 23 | 1 | 0 | 2.010705 | -2.321772 | -2.810826 |
| 24 | 8 | 0 | 1.402411 | -2.060926 | -3.535093 |
| 25 | 1 | 0 | 0.524611 | -2.466652 | -3.319601 |
| 26 | 1 | 0 | 1.016843 | -0.447951 | -3.233872 |
| 27 | 8 | 0 | 0.682451 | 0.445165 | -2.919219 |
| 28 | 1 | 0 | 1.211674 | 1.125550 | -3.359063 |
| 29 | 1 | 0 | 4.222380 | -2.794697 | 1.660728 |
| 30 | 8 | 0 | 3.807768 | -2.051158 | 2.172094 |
| 31 | 1 | 0 | 4.304338 | -1.966378 | 2.999044 |
| 32 | 1 | 0 | -1.780425 | 0.266555 | -1.176166 |
| 33 | 8 | 0 | -1.957116 | 0.073115 | -2.124303 |
| 34 | 1 | 0 | -1.149027 | 0.394229 | -2.581711 |
| 35 | 1 | 0 | -1.491720 | -1.730337 | -2.649809 |
| 36 | 8 | 0 | -1.210496 | -2.637471 | -2.894836 |
| 37 | 1 | 0 | -1.749771 | -3.194595 | -2.285945 |
| 38 | 1 | 0 | -3.752133 | -0.711160 | -2.126512 |

| 39 | 8 | 0 | -4.520913 | -1.258597 | -1.870622 |
|----|---|---|-----------|-----------|-----------|
| 40 | 1 | 0 | -5.010333 | -0.733016 | -1.199075 |
| 41 | 1 | 0 | -1.479635 | -1.082881 | 0.892639 |
| 42 | 8 | 0 | -1.537605 | -2.041667 | 1.114426 |
| 43 | 1 | 0 | -0.594979 | -2.336076 | 1.095771 |
| 44 | 1 | 0 | -2.722830 | -2.085136 | 2.424479 |
| 45 | 8 | 0 | -3.492898 | -1.889416 | 3.015905 |
| 46 | 1 | 0 | -4.215209 | -2.436026 | 2.670742 |
| 47 | 1 | 0 | -2.530443 | -3.008100 | -0.197370 |
| 48 | 8 | 0 | -3.023201 | -3.456601 | -0.916608 |
| 49 | 1 | 0 | -3.672187 | -2.781392 | -1.227886 |
| 50 | 1 | 0 | 2.757130 | 0.240645 | 0.083527 |
| 51 | 8 | 0 | 3.733753 | -0.035893 | 0.041959 |
| 52 | 1 | 0 | 3.882110 | -0.538171 | 0.868944 |
| 53 | 1 | 0 | 4.855338 | 1.390809 | -0.064081 |
| 54 | 8 | 0 | 5.487433 | 2.140200 | -0.180177 |
| 55 | 1 | 0 | 5.722263 | 2.112831 | -1.118899 |
| 56 | 1 | 0 | -3.796555 | -0.141584 | 2.455045 |
| 57 | 8 | 0 | -3.878579 | 0.723874 | 1.990145 |
| 58 | 1 | 0 | -3.022635 | 0.840248 | 1.523462 |
| 59 | 1 | 0 | -5.125077 | 0.487778 | 0.813224 |
| 60 | 8 | 0 | -5.812308 | 0.299351 | 0.117364 |
| 61 | 1 | 0 | -6.118306 | 1.164679 | -0.190050 |
| 62 | 6 | 0 | 1.449119 | 4.483124 | -0.640012 |
| 63 | 6 | 0 | 0.475828 | 4.978745 | -1.514168 |
| 64 | 1 | 0 | -1.953836 | 2.658323 | -0.964538 |
| 65 | 1 | 0 | -1.512870 | 4.701300 | -2.304012 |
| 66 | 1 | 0 | 1.955900 | 2.940920 | 0.777266 |
| 67 | 1 | 0 | 2.408934 | 4.984545 | -0.546915 |
| 68 | 1 | 0 | 0.674130 | 5.872185 | -2.101826 |
| 69 | 1 | 0 | 1.650787 | 0.994343 | 4.183860 |
| 70 | 1 | 0 | 0.226743 | 1.928073 | 4.686954 |
| 71 | 1 | 0 | 0.347041 | 0.204541 | 5.102382 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) = -1798.39889531    A.U. after   1 cycles

      Convg  =   0.2155D-08         -V/T = 2.0093

      S**2  =  0.0000

Zero-point correction=                    0.595360 (a.u.)

Thermal correction to Energy=             0.646200

Thermal correction to Enthalpy=           0.647145

Thermal correction to Gibbs Free Energy=    0.506737

Sum of electronic and zero-point Energies=      -1797.803536

Sum of electronic and thermal Energies=         -1797.752695

Sum of electronic and thermal Enthalpies=       -1797.751751

Sum of electronic and thermal Free Energies=      -1797.892158

(3-3) Anionic tetrahedral intermediate, Ph-C(-O-)(OH)OEt and
   (H2O)16, Int1(es)

zukaphxx.rev.chk   Stoichiometry  C9H43O19(1-)

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.111915 | -0.725212 | -0.378531 |
| 2 | 6 | 0 | -1.576014 | -0.782626 | -0.487489 |
| 3 | 8 | 0 | -0.945002 | 0.206886 | 0.156154 |
| 4 | 8 | 0 | -1.221740 | -0.830325 | -1.885831 |
| 5 | 1 | 0 | -0.732841 | -0.010069 | -2.113484 |
| 6 | 6 | 0 | -3.730511 | 0.009293 | 0.637318 |
| 7 | 6 | 0 | -5.123175 | 0.034248 | 0.753237 |
| 8 | 6 | 0 | -3.913865 | -1.443990 | -1.275576 |
| 9 | 8 | 0 | -1.137670 | -2.111359 | -0.052893 |
| 10 | 6 | 0 | -1.322683 | -2.409897 | 1.328027 |
| 11 | 1 | 0 | -2.391551 | -2.375426 | 1.583352 |
| 12 | 6 | 0 | -0.757158 | -3.797001 | 1.594879 |
| 13 | 1 | 0 | -0.805651 | -1.665519 | 1.946612 |
| 14 | 1 | 0 | 0.675680 | 0.029075 | 0.058930 |
| 15 | 8 | 0 | 1.683714 | -0.060530 | 0.020282 |
| 16 | 1 | 0 | 2.021972 | 0.654192 | -0.572520 |
| 17 | 1 | 0 | 2.132218 | -1.496278 | -0.871309 |
| 18 | 8 | 0 | 2.558599 | -2.267743 | -1.332570 |
| 19 | 1 | 0 | 1.812192 | -2.685543 | -1.835752 |
| 20 | 1 | 0 | 3.998168 | -1.181151 | -1.971487 |
| 21 | 8 | 0 | 4.619630 | -0.422791 | -2.039773 |
| 22 | 1 | 0 | 5.035071 | -0.356754 | -1.150688 |
| 23 | 1 | 0 | 3.343172 | -1.835876 | 1.807950 |
| 24 | 8 | 0 | 3.279182 | -0.871825 | 2.023269 |
| 25 | 1 | 0 | 2.650025 | -0.513596 | 1.335196 |
| 26 | 1 | 0 | 2.248112 | -0.578918 | 3.432133 |
| 27 | 8 | 0 | 1.566646 | -0.327865 | 4.108210 |
| 28 | 1 | 0 | 2.018655 | 0.267892 | 4.723496 |
| 29 | 1 | 0 | 3.490891 | 0.963351 | -2.091341 |
| 30 | 8 | 0 | 2.752764 | 1.602867 | -1.910900 |
| 31 | 1 | 0 | 2.032721 | 1.412043 | -2.554532 |
| 32 | 1 | 0 | -0.600645 | 0.678743 | 1.837811 |
| 33 | 8 | 0 | -0.319804 | 1.179633 | 2.646924 |
| 34 | 1 | 0 | 0.265901 | 0.588558 | 3.174339 |
| 35 | 1 | 0 | 0.582157 | 2.629089 | 1.997402 |
| 36 | 8 | 0 | 0.718231 | 3.538923 | 1.630082 |
| 37 | 1 | 0 | 0.070180 | 4.065969 | 2.135594 |
| 38 | 1 | 0 | -1.632247 | 2.653029 | 2.992915 |

| 39 | 8 | 0 | -2.034693 | 3.511422 | 2.750960 |
|----|---|---|-----------|----------|----------|
| 40 | 1 | 0 | -2.241088 | 3.392711 | 1.801807 |
| 41 | 1 | 0 | -1.437233 | 1.885258 | -0.094453 |
| 42 | 8 | 0 | -1.513928 | 2.878780 | -0.079418 |
| 43 | 1 | 0 | -0.674611 | 3.154111 | 0.347674 |
| 44 | 1 | 0 | -1.011030 | 3.495581 | -1.734358 |
| 45 | 8 | 0 | -0.415272 | 3.715019 | -2.491448 |
| 46 | 1 | 0 | 0.410889 | 4.024272 | -2.044068 |
| 47 | 1 | 0 | 4.797175 | -0.320928 | 1.218549 |
| 48 | 8 | 0 | 5.569548 | -0.081045 | 0.646423 |
| 49 | 1 | 0 | 5.705553 | 0.868634 | 0.781461 |
| 50 | 1 | 0 | -0.166470 | -3.576720 | -1.595083 |
| 51 | 8 | 0 | 0.183463 | -3.184297 | -2.413004 |
| 52 | 1 | 0 | -0.286059 | -2.314198 | -2.390678 |
| 53 | 1 | 0 | 3.144510 | -3.142376 | 0.051664 |
| 54 | 8 | 0 | 3.491605 | -3.433606 | 0.939375 |
| 55 | 1 | 0 | 4.421265 | -3.661299 | 0.789917 |
| 56 | 1 | 0 | 0.109798 | 1.089196 | -4.134283 |
| 57 | 8 | 0 | 0.296835 | 1.258880 | -3.199005 |
| 58 | 1 | 0 | -0.019940 | 2.199291 | -3.010603 |
| 59 | 1 | 0 | 2.392829 | 3.327855 | -1.243030 |
| 60 | 8 | 0 | 1.919347 | 4.143427 | -0.971531 |
| 61 | 1 | 0 | 1.639781 | 3.991614 | -0.045836 |
| 62 | 6 | 0 | -5.303071 | -1.421313 | -1.161580 |
| 63 | 6 | 0 | -5.914145 | -0.680477 | -0.145641 |
| 64 | 1 | 0 | -3.116298 | 0.568798 | 1.334651 |
| 65 | 1 | 0 | -5.585249 | 0.617008 | 1.546450 |
| 66 | 1 | 0 | -3.438299 | -2.010193 | -2.069832 |
| 67 | 1 | 0 | -5.911614 | -1.978884 | -1.870326 |
| 68 | 1 | 0 | -6.998208 | -0.659450 | -0.059163 |
| 69 | 1 | 0 | -0.887902 | -4.059991 | 2.651217 |
| 70 | 1 | 0 | -1.271941 | -4.551369 | 0.987883 |
| 71 | 1 | 0 | 0.313544 | -3.835493 | 1.365509 |

-------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) = -1798.42108073    A.U. after   1 cycles

Convg  =   0.1330D-08         -V/T = 2.0093

S**2  =   0.0000

Zero-point correction=                    0.600051 (a.u.)

Thermal correction to Energy=             0.649207

Thermal correction to Enthalpy=           0.650151

Thermal correction to Gibbs Free Energy=       0.515271

Sum of electronic and zero-point Energies=        -1797.821030

Sum of electronic and thermal Energies=           -1797.771874

Sum of electronic and thermal Enthalpies=         -1797.770929

Sum of electronic and thermal Free Energies=      -1797.905810

(3-4) TS2'(es),
formation of the neutral tetrahedral intermediate Int2'(es)

zuka07.g09.chk   Stoichiometry  C9H43O19(1-)

Standard orientation:

----------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.555055 | -0.970578 | 0.235205 |
| 2 | 6 | 0 | 1.227882 | -0.783265 | -0.515696 |
| 3 | 8 | 0 | 0.413977 | 0.062830 | 0.228759 |
| 4 | 8 | 0 | 0.533823 | -2.024998 | -0.638932 |
| 5 | 6 | 0 | 1.178608 | -3.053926 | -1.418704 |
| 6 | 6 | 0 | 2.533033 | -1.351652 | 1.584195 |
| 7 | 6 | 0 | 3.722602 | -1.547373 | 2.283201 |
| 8 | 6 | 0 | 3.787924 | -0.805534 | -0.401950 |
| 9 | 6 | 0 | 0.246492 | -4.251973 | -1.486423 |
| 10 | 1 | 0 | 1.386978 | -2.665482 | -2.419955 |
| 11 | 1 | 0 | 2.131314 | -3.320039 | -0.942933 |
| 12 | 8 | 0 | 1.411337 | -0.316771 | -1.829095 |
| 13 | 1 | 0 | 1.761716 | 0.612026 | -1.835068 |
| 14 | 1 | 0 | -1.777450 | 1.599943 | -2.223302 |
| 15 | 8 | 0 | -1.598654 | 1.834067 | -3.161625 |
| 16 | 1 | 0 | -1.308499 | 0.977582 | -3.553117 |
| 17 | 1 | 0 | -0.298336 | 3.020613 | -3.147124 |
| 18 | 8 | 0 | 0.456511 | 3.648370 | -2.987828 |
| 19 | 1 | 0 | 0.171581 | 4.188643 | -2.205685 |
| 20 | 1 | 0 | 1.651193 | 2.803048 | -2.421183 |
| 21 | 8 | 0 | 2.395890 | 2.249507 | -1.979159 |
| 22 | 1 | 0 | 3.185936 | 2.370010 | -2.526220 |
| 23 | 1 | 0 | 1.103317 | 1.807659 | 0.598097 |
| 24 | 8 | 0 | 1.542555 | 2.682886 | 0.681264 |
| 25 | 1 | 0 | 2.139342 | 2.694342 | -0.095367 |
| 26 | 1 | 0 | 0.469941 | 4.204054 | -0.052908 |
| 27 | 8 | 0 | -0.126532 | 4.797058 | -0.554367 |
| 28 | 1 | 0 | -1.014932 | 4.514212 | -0.232836 |
| 29 | 1 | 0 | 0.481260 | 3.298046 | 2.254706 |
| 30 | 8 | 0 | -0.345120 | 3.408928 | 2.761229 |
| 31 | 1 | 0 | -0.321438 | 2.736296 | 3.478812 |
| 32 | 1 | 0 | -0.531131 | 0.223854 | -0.215418 |
| 33 | 8 | 0 | -1.945989 | 0.603759 | -0.564615 |
| 34 | 1 | 0 | -2.301052 | -0.123247 | -1.121016 |
| 35 | 1 | 0 | -2.613063 | 0.518277 | 0.451015 |
| 36 | 8 | 0 | -3.206903 | 0.419887 | 1.513819 |
| 37 | 1 | 0 | -3.491425 | 1.319428 | 1.743899 |
| 38 | 1 | 0 | -2.121959 | 2.568589 | 0.187768 |

| 39 | 8 | 0 | -2.224944 | 3.403341 | 0.682048 |
|----|---|---|-----------|-----------|-----------|
| 40 | 1 | 0 | -1.653992 | 3.322876 | 1.484156 |
| 41 | 1 | 0 | 0.020459 | -0.700075 | -3.102361 |
| 42 | 8 | 0 | -0.721635 | -0.789960 | -3.734211 |
| 43 | 1 | 0 | -1.427407 | -1.245495 | -3.228501 |
| 44 | 1 | 0 | -1.907334 | -0.118995 | 2.365362 |
| 45 | 8 | 0 | -1.023220 | -0.485633 | 2.694796 |
| 46 | 1 | 0 | -0.410858 | -0.269494 | 1.959577 |
| 47 | 1 | 0 | -0.577764 | 0.579331 | 3.999679 |
| 48 | 8 | 0 | -0.315440 | 1.298216 | 4.635315 |
| 49 | 1 | 0 | 0.551586 | 1.042681 | 4.981867 |
| 50 | 6 | 0 | 4.981095 | -0.997827 | 0.300207 |
| 51 | 6 | 0 | 4.952093 | -1.366669 | 1.644127 |
| 52 | 1 | 0 | 1.582287 | -1.504318 | 2.084773 |
| 53 | 1 | 0 | 3.688965 | -1.842870 | 3.328709 |
| 54 | 1 | 0 | 3.812189 | -0.530975 | -1.451080 |
| 55 | 1 | 0 | 5.932242 | -0.860503 | -0.208200 |
| 56 | 1 | 0 | 5.879714 | -1.516168 | 2.191067 |
| 57 | 1 | 0 | 0.044213 | -4.660405 | -0.491034 |
| 58 | 1 | 0 | -0.707030 | -3.976438 | -1.947911 |
| 59 | 1 | 0 | 0.708655 | -5.039093 | -2.093735 |
| 60 | 1 | 0 | -1.235267 | -2.283844 | 2.078360 |
| 61 | 8 | 0 | -1.161430 | -3.052670 | 1.470295 |
| 62 | 1 | 0 | -0.569271 | -2.719985 | 0.765066 |
| 63 | 1 | 0 | -4.453370 | -0.680269 | 1.440930 |
| 64 | 8 | 0 | -5.125998 | -1.426798 | 1.378582 |
| 65 | 1 | 0 | -5.304238 | -1.689564 | 2.293195 |
| 66 | 1 | 0 | -3.778062 | -1.408312 | -2.532918 |
| 67 | 8 | 0 | -2.927316 | -1.637004 | -2.129822 |
| 68 | 1 | 0 | -3.140646 | -2.276763 | -1.382669 |
| 69 | 1 | 0 | -4.172381 | -2.662534 | 0.468176 |
| 70 | 8 | 0 | -3.527711 | -3.211886 | -0.041134 |
| 71 | 1 | 0 | -2.720278 | -3.238879 | 0.527796 |

---------------------------------------------------------------------

SCF Done:  E(RB3LYP) =  -1798.41015057    A.U. after   1 cycles

Convg  =   0.2134D-08          -V/T =  2.0092

Zero-point correction=                   0.594718 (a.u.)

Thermal correction to Energy=                 0.642635

Thermal correction to Enthalpy=               0.643579

Thermal correction to Gibbs Free Energy=        0.512714

Sum of electronic and zero-point Energies=       -1797.815432

Sum of electronic and thermal Energies=          -1797.767516

Sum of electronic and thermal Enthalpies=        -1797.766572

Sum of electronic and thermal Free Energies=      -1797.897436


(3-5) The neutral tetrahedral intermediate Int2'(es)

zuka07.for.chk    Stoichiometry  C9H43O19(1-)

Standard orientation:

-----------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|--------|--------|--------|
| Number | Number | Type | X | Y | Z |

-----------------------------------------------------------------------

| Center | Atomic | Atomic | X | Y | Z |
|--------|--------|--------|--------|--------|--------|
| 1 | 6 | 0 | -2.443018 | -1.094886 | -0.243629 |
| 2 | 6 | 0 | -1.077415 | -1.053117 | 0.453195 |
| 3 | 8 | 0 | -0.374982 | 0.057453 | -0.027965 |
| 4 | 8 | 0 | -0.294947 | -2.195187 | 0.122159 |
| 5 | 6 | 0 | -0.788351 | -3.474836 | 0.571680 |
| 6 | 6 | 0 | -2.502676 | -1.020639 | -1.642185 |
| 7 | 6 | 0 | -3.730119 | -1.077252 | -2.299410 |
| 8 | 6 | 0 | -3.628291 | -1.243256 | 0.481205 |
| 9 | 6 | 0 | 0.219723 | -4.535372 | 0.163350 |
| 10 | 1 | 0 | -0.910111 | -3.447450 | 1.658583 |
| 11 | 1 | 0 | -1.768642 | -3.661814 | 0.114503 |
| 12 | 8 | 0 | -1.175880 | -1.032465 | 1.851313 |
| 13 | 1 | 0 | -1.563196 | -0.170638 | 2.165214 |
| 14 | 1 | 0 | 2.088190 | 0.934990 | 2.689447 |
| 15 | 8 | 0 | 1.924718 | 0.886810 | 3.658185 |
| 16 | 1 | 0 | 1.673226 | -0.055781 | 3.783440 |
| 17 | 1 | 0 | 0.567238 | 2.004791 | 3.846448 |
| 18 | 8 | 0 | -0.218085 | 2.611911 | 3.805177 |
| 19 | 1 | 0 | -0.000717 | 3.282082 | 3.104701 |
| 20 | 1 | 0 | -1.433279 | 1.822811 | 3.220924 |
| 21 | 8 | 0 | -2.216884 | 1.319495 | 2.781246 |
| 22 | 1 | 0 | -2.904359 | 1.248449 | 3.459913 |
| 23 | 1 | 0 | -1.303083 | 1.752489 | 0.054376 |
| 24 | 8 | 0 | -1.866034 | 2.535807 | 0.229681 |
| 25 | 1 | 0 | -2.338759 | 2.276565 | 1.046745 |
| 26 | 1 | 0 | -0.693388 | 3.803740 | 1.117817 |
| 27 | 8 | 0 | 0.012013 | 4.259796 | 1.622315 |
| 28 | 1 | 0 | 0.762828 | 4.242742 | 0.981708 |
| 29 | 1 | 0 | -1.435197 | 3.662797 | -1.387160 |
| 30 | 8 | 0 | -0.874720 | 4.114505 | -2.046001 |
| 31 | 1 | 0 | -0.833619 | 3.524913 | -2.831650 |
| 32 | 1 | 0 | 0.540583 | 0.122936 | 0.410667 |
| 33 | 8 | 0 | 2.094153 | 0.427400 | 0.879975 |
| 34 | 1 | 0 | 2.555845 | -0.437213 | 0.975757 |
| 35 | 1 | 0 | 2.551339 | 0.914862 | 0.113337 |
| 36 | 8 | 0 | 3.047408 | 1.481682 | -1.318678 |
| 37 | 1 | 0 | 3.590021 | 2.275409 | -1.441314 |
| 38 | 1 | 0 | 1.922479 | 3.096545 | -0.831240 |
| 39 | 8 | 0 | 1.585802 | 4.001423 | -0.664399 |
| 40 | 1 | 0 | 0.794391 | 4.105553 | -1.244504 |

| 41 | 1 | 0 | 0.363452 | -1.631537 | 2.856697 |
|----|---|---|----------|-----------|----------|
| 42 | 8 | 0 | 1.167324 | -1.853199 | 3.368910 |
| 43 | 1 | 0 | 1.832207 | -2.097720 | 2.692766 |
| 44 | 1 | 0 | 1.828232 | 1.007480 | -2.229356 |
| 45 | 8 | 0 | 0.979224 | 0.574039 | -2.601012 |
| 46 | 1 | 0 | 0.405316 | 0.494441 | -1.813556 |
| 47 | 1 | 0 | 0.132583 | 1.656696 | -3.668588 |
| 48 | 8 | 0 | -0.428422 | 2.310570 | -4.166534 |
| 49 | 1 | 0 | -1.129596 | 1.792259 | -4.586250 |
| 50 | 6 | 0 | -4.859199 | -1.297287 | -0.178448 |
| 51 | 6 | 0 | -4.913585 | -1.211683 | -1.568752 |
| 52 | 1 | 0 | -1.585616 | -0.927932 | -2.215206 |
| 53 | 1 | 0 | -3.762501 | -1.017839 | -3.384188 |
| 54 | 1 | 0 | -3.585400 | -1.319346 | 1.562426 |
| 55 | 1 | 0 | -5.774029 | -1.407396 | 0.398338 |
| 56 | 1 | 0 | -5.870792 | -1.252024 | -2.082454 |
| 57 | 1 | 0 | 0.334516 | -4.580280 | -0.924572 |
| 58 | 1 | 0 | 1.198873 | -4.329585 | 0.606885 |
| 59 | 1 | 0 | -0.119934 | -5.516752 | 0.514405 |
| 60 | 1 | 0 | 1.252712 | -1.293925 | -2.630020 |
| 61 | 8 | 0 | 1.202038 | -2.244142 | -2.374988 |
| 62 | 1 | 0 | 0.665204 | -2.233473 | -1.557205 |
| 63 | 1 | 0 | 4.151669 | 0.346578 | -1.692363 |
| 64 | 8 | 0 | 4.843114 | -0.355436 | -1.951272 |
| 65 | 1 | 0 | 4.937175 | -0.277504 | -2.911882 |
| 66 | 1 | 0 | 4.112443 | -2.017726 | 1.751151 |
| 67 | 8 | 0 | 3.234208 | -2.113016 | 1.352534 |
| 68 | 1 | 0 | 3.397224 | -2.431135 | 0.407017 |
| 69 | 1 | 0 | 4.190635 | -1.933715 | -1.490003 |
| 70 | 8 | 0 | 3.693743 | -2.738408 | -1.191266 |
| 71 | 1 | 0 | 2.831088 | -2.670670 | -1.668841 |

-----------------------------------------------------------------

SCF Done: E(RB3LYP) = -1798.41464479    A.U. after    1 cycles

Convg  =    0.2877D-08          -V/T =  2.0093

Zero-point correction=                     0.598737 (a.u.)

Thermal correction to Energy=              0.647229

Thermal correction to Enthalpy=            0.648173

Thermal correction to Gibbs Free Energy=      0.516669

Sum of electronic and zero-point Energies=        -1797.815908

Sum of electronic and thermal Energies=           -1797.767416

Sum of electronic and thermal Enthalpies=         -1797.766471

Sum of electronic and thermal Free Energies=      -1797.897975


 (3-6)  TS2(es),  MeO- dissociation along with ethanol formation

zukaphxx.chk    Stoichiometry C9H43O19(1-)

Standard orientation:

```
----------------------------------------------------------------------
Center     Atomic     Atomic          Coordinates (Angstroms)
Number     Number      Type        X          Y          Z
----------------------------------------------------------------------
   1          6          0       -3.277696   -0.456962   -0.444548
   2          6          0       -1.848302   -0.009070   -0.660236
   3          8          0       -1.387972    0.974205    0.000929
   4          8          0       -1.486841   -0.143223   -1.981988
   5          1          0       -0.754402    0.480849   -2.192822
   6          6          0       -4.008673    0.092464    0.613114
   7          6          0       -5.335165   -0.287535    0.830182
   8          6          0       -3.895718   -1.386162   -1.292627
   9          8          0       -0.944167   -1.494976   -0.022935
  10          6          0       -1.235077   -1.921964    1.298982
  11          1          0       -1.881845   -1.182393    1.795255
  12          6          0       -1.905215   -3.295308    1.336169
  13          1          0       -0.301261   -1.957481    1.883135
  14          1          0        0.562466   -0.889020    0.011992
  15          8          0        1.563775   -0.733516    0.063702
  16          1          0        1.818213    0.049217   -0.480187
  17          1          0        2.110630   -2.109538   -0.800231
  18          8          0        2.411976   -2.935418   -1.268746
  19          1          0        1.571741   -3.233119   -1.697125
  20          1          0        3.874878   -1.826116   -1.950778
  21          8          0        4.488666   -1.061373   -1.979431
  22          1          0        4.909436   -1.039451   -1.089883
  23          1          0        3.194218   -2.402841    1.945885
  24          8          0        3.145209   -1.427665    2.099746
  25          1          0        2.527333   -1.110310    1.382316
  26          1          0        2.054275   -0.825147    3.393721
  27          8          0        1.376263   -0.374730    3.956937
  28          1          0        1.878058    0.172097    4.578984
  29          1          0        3.417345    0.378658   -1.912391
  30          8          0        2.742970    1.066350   -1.673193
  31          1          0        2.081139    1.104272   -2.399718
  32          1          0       -0.586647    1.081181    1.617636
  33          8          0       -0.156936    1.457469    2.425237
  34          1          0        0.298786    0.728274    2.904816
  35          1          0        0.916212    2.749155    1.848870
  36          8          0        1.217557    3.642171    1.536486
  37          1          0        0.739591    4.248458    2.132822
  38          1          0       -1.198731    3.105038    2.922617
  39          8          0       -1.427675    4.050077    2.810305
  40          1          0       -1.696582    4.106884    1.872728
  41          1          0       -1.344826    2.752728   -0.224953
  42          8          0       -1.113869    3.712331   -0.165725
```

| 43 | 1 | 0 | -0.247516 | 3.708440 | 0.297319 |
|----|---|---|-----------|----------|-----------|
| 44 | 1 | 0 | -0.299646 | 4.043655 | -1.804467 |
| 45 | 8 | 0 | 0.379674 | 4.024431 | -2.520625 |
| 46 | 1 | 0 | 1.239200 | 4.089830 | -2.030638 |
| 47 | 1 | 0 | 4.679456 | -0.968643 | 1.274360 |
| 48 | 8 | 0 | 5.464098 | -0.793102 | 0.694886 |
| 49 | 1 | 0 | 5.668074 | 0.146563 | 0.814193 |
| 50 | 1 | 0 | -0.584199 | -2.622944 | -1.275531 |
| 51 | 8 | 0 | -0.256189 | -3.148906 | -2.061928 |
| 52 | 1 | 0 | -0.451527 | -2.556211 | -2.804143 |
| 53 | 1 | 0 | 2.990066 | -3.789738 | 0.176305 |
| 54 | 8 | 0 | 3.366068 | -4.028144 | 1.065103 |
| 55 | 1 | 0 | 4.301268 | -4.220406 | 0.900862 |
| 56 | 1 | 0 | 0.312211 | 1.384131 | -4.170561 |
| 57 | 8 | 0 | 0.477949 | 1.478332 | -3.220982 |
| 58 | 1 | 0 | 0.390251 | 2.465698 | -3.012666 |
| 59 | 1 | 0 | 2.871819 | 2.853758 | -1.141019 |
| 60 | 8 | 0 | 2.675882 | 3.796967 | -0.945535 |
| 61 | 1 | 0 | 2.315408 | 3.803385 | -0.035005 |
| 62 | 6 | 0 | -5.220692 | -1.761675 | -1.078647 |
| 63 | 6 | 0 | -5.944635 | -1.215573 | -0.014152 |
| 64 | 1 | 0 | -3.529179 | 0.828341 | 1.250552 |
| 65 | 1 | 0 | -5.891806 | 0.147444 | 1.656793 |
| 66 | 1 | 0 | -3.330976 | -1.810104 | -2.115645 |
| 67 | 1 | 0 | -5.690449 | -2.482996 | -1.743314 |
| 68 | 1 | 0 | -6.978192 | -1.510722 | 0.151940 |
| 69 | 1 | 0 | -2.097479 | -3.601033 | 2.373192 |
| 70 | 1 | 0 | -2.857712 | -3.276769 | 0.796687 |
| 71 | 1 | 0 | -1.263548 | -4.052613 | 0.870738 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1798.40938611    A.U. after    1 cycles

      Convg  =    0.2706D-08            -V/T =  2.0093

      S**2  =   0.0000

Zero-point correction=                       0.597771 (a.u.)

Thermal correction to Energy=                0.646983

Thermal correction to Enthalpy=              0.647927

Thermal correction to Gibbs Free Energy=        0.512972

Sum of electronic and zero-point Energies=        -1797.811615

Sum of electronic and thermal Energies=           -1797.762403

Sum of electronic and thermal Enthalpies=         -1797.761459

Sum of electronic and thermal Free Energies=      -1797.896414


(3-7) Ph-COOH + Et-OH + OH-(H2O)15,  Int2(es)

zukaphxx.for.chk    Stoichiometry  C9H43O19(1-)

           Standard orientation:

---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| Number | Number | Type | X | Y | Z |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.193976 | 0.341137 | -0.306271 |
| 2 | 6 | 0 | -3.073311 | 1.316272 | -0.427954 |
| 3 | 8 | 0 | -2.367550 | 1.660314 | 0.519539 |
| 4 | 8 | 0 | -2.913768 | 1.789396 | -1.663375 |
| 5 | 1 | 0 | -2.087408 | 2.349659 | -1.754490 |
| 6 | 6 | 0 | -4.400550 | -0.316598 | 0.915160 |
| 7 | 6 | 0 | -5.442877 | -1.233326 | 1.041538 |
| 8 | 6 | 0 | -5.037490 | 0.070674 | -1.394749 |
| 9 | 8 | 0 | -0.355133 | -2.736659 | -0.195011 |
| 10 | 6 | 0 | -0.786356 | -3.295921 | 1.046540 |
| 11 | 1 | 0 | -1.027749 | -2.486302 | 1.747335 |
| 12 | 6 | 0 | -2.012649 | -4.163785 | 0.806592 |
| 13 | 1 | 0 | 0.021667 | -3.897180 | 1.491356 |
| 14 | 1 | 0 | 0.384132 | -2.067892 | -0.020314 |
| 15 | 8 | 0 | 1.670034 | -1.049276 | 0.159293 |
| 16 | 1 | 0 | 1.421906 | -0.272406 | -0.379055 |
| 17 | 1 | 0 | 2.387987 | -1.929564 | -1.069778 |
| 18 | 8 | 0 | 2.859456 | -2.393765 | -1.835464 |
| 19 | 1 | 0 | 2.212385 | -3.067452 | -2.149344 |
| 20 | 1 | 0 | 3.287948 | -0.805725 | -2.751490 |
| 21 | 8 | 0 | 3.443353 | 0.131511 | -3.009112 |
| 22 | 1 | 0 | 4.070772 | 0.488171 | -2.332972 |
| 23 | 1 | 0 | 4.661120 | -1.624809 | 0.547541 |
| 24 | 8 | 0 | 4.205786 | -0.856350 | 0.965702 |
| 25 | 1 | 0 | 3.244123 | -0.914400 | 0.644553 |
| 26 | 1 | 0 | 3.992912 | -0.985124 | 2.675642 |
| 27 | 8 | 0 | 3.674409 | -0.969244 | 3.621144 |
| 28 | 1 | 0 | 4.210040 | -0.292597 | 4.059560 |
| 29 | 1 | 0 | 2.008931 | 0.881112 | -2.363909 |
| 30 | 8 | 0 | 1.341290 | 1.239841 | -1.716759 |
| 31 | 1 | 0 | 0.645582 | 1.729680 | -2.196823 |
| 32 | 1 | 0 | 1.312665 | -0.519892 | 1.647904 |
| 33 | 8 | 0 | 1.169882 | -0.135529 | 2.584532 |
| 34 | 1 | 0 | 1.918069 | -0.490860 | 3.116732 |
| 35 | 1 | 0 | 1.426486 | 1.490519 | 2.468576 |
| 36 | 8 | 0 | 1.575440 | 2.487937 | 2.392446 |
| 37 | 1 | 0 | 1.955144 | 2.765645 | 3.239004 |
| 38 | 1 | 0 | -0.683609 | -0.087319 | 2.981430 |
| 39 | 8 | 0 | -1.646155 | 0.101389 | 3.003684 |
| 40 | 1 | 0 | -1.798969 | 0.663503 | 2.223831 |
| 41 | 1 | 0 | -1.342745 | 3.180209 | 1.191539 |
| 42 | 8 | 0 | -0.739964 | 3.870313 | 1.531790 |
| 43 | 1 | 0 | 0.001537 | 3.373345 | 1.944740 |

| 44 | 1 | 0 | 0.048753 | 4.593871 | 0.119716 |
|----|---|---|----------|----------|----------|
| 45 | 8 | 0 | 0.542171 | 4.770171 | -0.724381 |
| 46 | 1 | 0 | 1.419163 | 4.339843 | -0.576553 |
| 47 | 1 | 0 | 4.732834 | 0.543463 | -0.136967 |
| 48 | 8 | 0 | 4.897046 | 1.223386 | -0.832146 |
| 49 | 1 | 0 | 4.319835 | 1.976186 | -0.581746 |
| 50 | 1 | 0 | 0.211973 | -3.674764 | -1.512276 |
| 51 | 8 | 0 | 0.642931 | -4.064269 | -2.325603 |
| 52 | 1 | 0 | 0.115597 | -3.731893 | -3.066903 |
| 53 | 1 | 0 | 4.390763 | -2.879496 | -1.162742 |
| 54 | 8 | 0 | 5.248233 | -2.915453 | -0.658388 |
| 55 | 1 | 0 | 5.899645 | -2.499937 | -1.242951 |
| 56 | 1 | 0 | -0.843289 | 3.597790 | -3.210556 |
| 57 | 8 | 0 | -0.702742 | 3.146102 | -2.365120 |
| 58 | 1 | 0 | -0.232912 | 3.814705 | -1.756225 |
| 59 | 1 | 0 | 2.201448 | 2.355504 | -0.708156 |
| 60 | 8 | 0 | 2.699354 | 3.030587 | -0.174541 |
| 61 | 1 | 0 | 2.452978 | 2.841712 | 0.757515 |
| 62 | 6 | 0 | -6.082383 | -0.840299 | -1.258633 |
| 63 | 6 | 0 | -6.286355 | -1.493750 | -0.040722 |
| 64 | 1 | 0 | -3.735679 | -0.129278 | 1.751059 |
| 65 | 1 | 0 | -5.591293 | -1.746676 | 1.987341 |
| 66 | 1 | 0 | -4.865744 | 0.574816 | -2.338959 |
| 67 | 1 | 0 | -6.734249 | -1.044843 | -2.103960 |
| 68 | 1 | 0 | -7.098603 | -2.209251 | 0.062506 |
| 69 | 1 | 0 | -2.349600 | -4.616812 | 1.747128 |
| 70 | 1 | 0 | -2.833651 | -3.564577 | 0.397947 |
| 71 | 1 | 0 | -1.787806 | -4.970313 | 0.098374 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1798.44248409    A.U. after    1 cycles

Convg  =    0.3169D-08         -V/T =  2.0093

S**2  =   0.0000

Zero-point correction=                       0.598206 (a.u.)

Thermal correction to Energy=                0.648012

Thermal correction to Enthalpy=              0.648956

Thermal correction to Gibbs Free Energy=     0.509867

Sum of electronic and zero-point Energies=        -1797.844278

Sum of electronic and thermal Energies=           -1797.794472

Sum of electronic and thermal Enthalpies=         -1797.793528

Sum of electronic and thermal Free Energies=      -1797.932617


 (3-8)  TS3(es) toward the product, PhCOO-, EtOH and (H2O)16,
carboxylate formation TS, TS3(es),
zukaphqd.g09.chk    Stoichiometry  C9H43O19(1-)

Standard orientation:

---------------------------------------------------------------------

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| | | | X | Y | Z |
| 1 | 6 | 0 | 2.036322 | 2.500396 | 0.716031 |
| 2 | 6 | 0 | 1.909812 | 1.150472 | 1.353015 |
| 3 | 8 | 0 | 2.914070 | 0.447730 | 1.555548 |
| 4 | 8 | 0 | 0.318486 | -2.944046 | -1.562960 |
| 5 | 6 | 0 | -0.110992 | -4.151317 | -2.210893 |
| 6 | 6 | 0 | 3.198964 | 3.253240 | 0.944045 |
| 7 | 6 | 0 | 3.353802 | 4.501892 | 0.343613 |
| 8 | 6 | 0 | 1.036135 | 3.009249 | -0.122835 |
| 9 | 1 | 0 | -0.721390 | -3.896559 | -3.087719 |
| 10 | 1 | 0 | -0.735378 | -4.732893 | -1.519061 |
| 11 | 6 | 0 | 1.112609 | -4.950554 | -2.627568 |
| 12 | 8 | 0 | 0.688578 | 0.806480 | 1.666504 |
| 13 | 1 | 0 | -2.260745 | -0.022289 | 1.454031 |
| 14 | 1 | 0 | 0.527563 | -0.197389 | 2.081489 |
| 15 | 8 | 0 | 0.043161 | -1.413979 | 2.541757 |
| 16 | 1 | 0 | 0.423671 | -1.659501 | 3.419380 |
| 17 | 1 | 0 | 1.057858 | -1.668522 | -2.753803 |
| 18 | 8 | 0 | 1.223272 | -0.956092 | -3.407913 |
| 19 | 1 | 0 | 2.145784 | -0.657610 | -3.257490 |
| 20 | 8 | 0 | -2.054632 | 0.699559 | 0.725116 |
| 21 | 1 | 0 | -1.815200 | -0.703556 | -0.565800 |
| 22 | 1 | 0 | -1.204383 | 1.074424 | 1.020041 |
| 23 | 8 | 0 | -2.430225 | -1.202052 | 2.380535 |
| 24 | 1 | 0 | -1.040192 | -1.385072 | 2.569535 |
| 25 | 1 | 0 | -2.861512 | -0.949293 | 3.210338 |
| 26 | 1 | 0 | 0.732609 | -2.784371 | 1.521053 |
| 27 | 8 | 0 | 1.334862 | -3.405062 | 1.049727 |
| 28 | 1 | 0 | 1.116148 | -3.278938 | 0.100279 |
| 29 | 8 | 0 | -1.902783 | -1.421712 | -1.233307 |
| 30 | 1 | 0 | -0.492596 | -2.406098 | -1.341850 |
| 31 | 1 | 0 | -1.843496 | -0.945461 | -2.110788 |
| 32 | 1 | 0 | 3.296770 | -1.329875 | 2.230344 |
| 33 | 8 | 0 | 3.372939 | -2.259713 | 2.524447 |
| 34 | 1 | 0 | 2.807964 | -2.756651 | 1.881462 |
| 35 | 8 | 0 | -2.158405 | 2.214390 | -1.788640 |
| 36 | 1 | 0 | -2.186583 | 1.718756 | -0.945485 |
| 37 | 1 | 0 | -3.108880 | 2.360930 | -1.999252 |
| 38 | 8 | 0 | -4.985421 | 2.262719 | -1.940182 |
| 39 | 1 | 0 | -5.077312 | 1.631593 | -1.181975 |
| 40 | 1 | 0 | -5.482973 | 3.049967 | -1.674478 |
| 41 | 1 | 0 | 4.226611 | 0.536469 | 0.222657 |
| 42 | 8 | 0 | 4.811194 | 0.733534 | -0.544868 |
| 43 | 1 | 0 | 4.719752 | 1.690848 | -0.669896 |

| 44 | 1 | 0 | 4.256618 | -0.019601 | -2.071558 |
|----|---|---|----------|-----------|-----------|
| 45 | 8 | 0 | 3.980121 | -0.366981 | -2.954242 |
| 46 | 1 | 0 | 4.479339 | -1.187297 | -3.077858 |
| 47 | 1 | 0 | -3.623462 | -1.823936 | 1.217544 |
| 48 | 8 | 0 | -4.226169 | -1.901614 | 0.427352 |
| 49 | 1 | 0 | -3.602728 | -1.971836 | -0.324860 |
| 50 | 1 | 0 | -3.992744 | 1.020436 | 0.628488 |
| 51 | 8 | 0 | -4.890001 | 0.735260 | 0.356843 |
| 52 | 1 | 0 | -4.792561 | -0.260778 | 0.316529 |
| 53 | 8 | 0 | -1.400483 | 0.049349 | -3.454810 |
| 54 | 1 | 0 | -0.428894 | -0.095184 | -3.523973 |
| 55 | 1 | 0 | -1.544350 | 0.923306 | -3.026704 |
| 56 | 8 | 0 | 1.661088 | -2.251286 | 4.642235 |
| 57 | 1 | 0 | 1.505813 | -3.170858 | 4.903652 |
| 58 | 1 | 0 | 2.389517 | -2.289075 | 3.960020 |
| 59 | 8 | 0 | -6.977170 | 1.580539 | 2.059644 |
| 60 | 1 | 0 | -6.229476 | 1.301961 | 1.481970 |
| 61 | 1 | 0 | -7.336579 | 0.751392 | 2.407048 |
| 62 | 6 | 0 | 1.203692 | 4.250024 | -0.737908 |
| 63 | 6 | 0 | 2.358162 | 4.998642 | -0.503059 |
| 64 | 1 | 0 | 3.962992 | 2.859267 | 1.608241 |
| 65 | 1 | 0 | 4.248349 | 5.088032 | 0.537806 |
| 66 | 1 | 0 | 0.140447 | 2.433601 | -0.324746 |
| 67 | 1 | 0 | 0.427907 | 4.620485 | -1.401192 |
| 68 | 1 | 0 | 2.484082 | 5.967915 | -0.978714 |
| 69 | 1 | 0 | 1.729616 | -4.375932 | -3.327050 |
| 70 | 1 | 0 | 1.723879 | -5.208388 | -1.755604 |
| 71 | 1 | 0 | 0.807267 | -5.880872 | -3.120978 |

---

SCF Done:  E(RB3LYP) =  -1798.42252801    A.U. after  15 cycles

Convg  =    0.2447D-08        -V/T =  2.0093

Zero-point correction=                         0.590177 (a.u.)

Thermal correction to Energy=                  0.641587

Thermal correction to Enthalpy=                0.642531

Thermal correction to Gibbs Free Energy=       0.497017

Sum of electronic and zero-point Energies=        -1797.832351

Sum of electronic and thermal Energies=           -1797.780941

Sum of electronic and thermal Enthalpies=         -1797.779997

Sum of electronic and thermal Free Energies=      -1797.925511


 (3-9)  Product,  Ph-COO-, EtOH and OH-(H2O)16

zukaphqd.g09for.chk       Stoichiometry C9H43O19(1-)

Standard orientation:

---------------------------------------------------------------------

Center    Atomic    Atomic             Coordinates (Angstroms)

Number    Number    Type          X         Y         Z

```
-----------------------------------------------------------------------
  1        6        0      2.219578    2.139236    0.842410
  2        6        0      1.923938    0.731695    1.320712
  3        8        0      2.918525   -0.024143    1.524212
  4        8        0     -0.185925   -2.827564   -1.798361
  5        6        0     -0.627622   -3.958382   -2.564240
  6        6        0      3.368116    2.801805    1.301942
  7        6        0      3.658344    4.097017    0.870804
  8        6        0      1.376885    2.792605   -0.064693
  9        1        0     -1.058588   -3.610937   -3.513216
 10        1        0     -1.411547   -4.491939   -2.008992
 11        6        0      0.559777   -4.871739   -2.819788
 12        8        0      0.709770    0.407138    1.494778
 13        1        0     -2.188560    0.162170    1.149848
 14        1        0      0.053178   -1.008404    2.352242
 15        8        0     -0.478975   -1.760878    2.723587
 16        1        0      0.048229   -2.114184    3.481699
 17        1        0      0.812747   -1.570209   -2.854656
 18        8        0      1.080835   -0.868694   -3.484645
 19        1        0      2.010309   -0.639534   -3.259418
 20        8        0     -1.761933    0.809997    0.528895
 21        1        0     -1.907845   -0.377443   -0.904654
 22        1        0     -0.819097    0.855268    0.850324
 23        8        0     -3.019880   -1.014296    2.174836
 24        1        0     -2.191889   -1.375066    2.586868
 25        1        0     -3.511393   -0.476141    2.832208
 26        1        0      0.036492   -3.046286    1.431097
 27        8        0      0.559913   -3.643216    0.850841
 28        1        0      0.376440   -3.344465   -0.066150
 29        8        0     -2.207248   -0.994241   -1.613231
 30        1        0     -0.956380   -2.212033   -1.670144
 31        1        0     -2.013562   -0.493549   -2.460441
 32        1        0      2.889542   -1.785661    1.996860
 33        8        0      2.840777   -2.744130    2.229916
 34        1        0      2.176308   -3.119339    1.604682
 35        8        0     -1.763474    2.641465   -1.871371
 36        1        0     -1.772815    2.103032   -1.057856
 37        1        0     -2.670333    3.017230   -1.921219
 38        8        0     -4.460081    3.524067   -1.508504
 39        1        0     -4.636050    2.886434   -0.773889
 40        1        0     -4.523428    4.404544   -1.110315
 41        1        0      4.189568    0.109361    0.298625
 42        8        0      4.813458    0.304885   -0.450137
 43        1        0      4.860064    1.273260   -0.463463
 44        1        0      4.138867   -0.206654   -1.997860
 45        8        0      3.824867   -0.478742   -2.898705
```

| 46 | 1 | 0 | 4.278548 | -1.314039 | -3.082664 |
|----|---|---|----------|-----------|-----------|
| 47 | 1 | 0 | -4.182598 | -1.280129 | 0.627216 |
| 48 | 8 | 0 | -4.630780 | -0.959268 | -0.183552 |
| 49 | 1 | 0 | -3.944749 | -1.065859 | -0.883124 |
| 50 | 1 | 0 | -3.490773 | 1.669166 | 0.622887 |
| 51 | 8 | 0 | -4.470788 | 1.664031 | 0.558759 |
| 52 | 1 | 0 | -4.654144 | 0.754274 | 0.185961 |
| 53 | 8 | 0 | -1.349041 | 0.491579 | -3.690083 |
| 54 | 1 | 0 | -0.408952 | 0.189933 | -3.700295 |
| 55 | 1 | 0 | -1.375254 | 1.355328 | -3.222302 |
| 56 | 8 | 0 | 1.366157 | -2.869816 | 4.479592 |
| 57 | 1 | 0 | 1.223322 | -3.812856 | 4.647460 |
| 58 | 1 | 0 | 2.021849 | -2.835555 | 3.720585 |
| 59 | 8 | 0 | -4.834060 | 0.862922 | 3.230160 |
| 60 | 1 | 0 | -4.825465 | 1.269647 | 2.329815 |
| 61 | 1 | 0 | -5.724283 | 0.498637 | 3.342652 |
| 62 | 6 | 0 | 1.678089 | 4.078641 | -0.514149 |
| 63 | 6 | 0 | 2.816014 | 4.736362 | -0.043056 |
| 64 | 1 | 0 | 4.019357 | 2.294013 | 2.007588 |
| 65 | 1 | 0 | 4.541929 | 4.607041 | 1.247672 |
| 66 | 1 | 0 | 0.494086 | 2.290927 | -0.442657 |
| 67 | 1 | 0 | 1.019382 | 4.557697 | -1.233086 |
| 68 | 1 | 0 | 3.047650 | 5.741529 | -0.387324 |
| 69 | 1 | 0 | 1.336266 | -4.345479 | -3.385478 |
| 70 | 1 | 0 | 0.992363 | -5.217080 | -1.874665 |
| 71 | 1 | 0 | 0.245581 | -5.748867 | -3.397969 |

---------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) = -1798.45216901    A.U. after   1 cycles

Convg  =   0.1812D-08        -V/T =  2.0093

S**2  =  0.0000

Zero-point correction=                    0.598603 (a.u.)

Thermal correction to Energy=             0.649832

Thermal correction to Enthalpy=           0.650776

Thermal correction to Gibbs Free Energy=      0.506339

Sum of electronic and zero-point Energies=      -1797.853566

Sum of electronic and thermal Energies=         -1797.802337

Sum of electronic and thermal Enthalpies=       -1797.801393

Sum of electronic and thermal Free Energies=      -1797.945830

===========================================================================

[4] Geometries of the n=16 amide hydrolysis in Figure 4

(4-1) N-ethyl benzamide(C6H5-C(=O)-NH-C2H5) + HO-(H2O)16,
    Reactant-like complex (precursor)
tuka02aa.for.chk    Stoichiometry  C9H44NO18(1-)
                Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| | | | X | Y | Z |
| 1 | 6 | 0 | -0.861514 | 2.709843 | -0.501915 |
| 2 | 6 | 0 | -0.690971 | 1.733148 | 0.623989 |
| 3 | 8 | 0 | -1.420190 | 0.704973 | 0.673568 |
| 4 | 7 | 0 | 0.198295 | 2.031833 | 1.579504 |
| 5 | 6 | 0 | 0.502385 | 1.152724 | 2.711487 |
| 6 | 6 | 0 | -2.117233 | 2.786377 | -1.120274 |
| 7 | 6 | 0 | -2.336311 | 3.684164 | -2.163839 |
| 8 | 6 | 0 | 0.179791 | 3.532840 | -0.955945 |
| 9 | 1 | 0 | 0.867083 | 2.785764 | 1.420775 |
| 10 | 6 | 0 | 0.927105 | 1.965886 | 3.932425 |
| 11 | 1 | 0 | -0.391108 | 0.566469 | 2.930386 |
| 12 | 1 | 0 | 1.292101 | 0.450170 | 2.418390 |
| 13 | 8 | 0 | 1.800161 | 0.573021 | -1.007530 |
| 14 | 1 | 0 | 1.415834 | 0.314744 | -1.868968 |
| 15 | 1 | 0 | 1.820346 | -0.262685 | -0.444009 |
| 16 | 8 | 0 | 2.048665 | -1.644330 | 0.456905 |
| 17 | 1 | 0 | 2.685518 | -1.419381 | 1.154218 |
| 18 | 1 | 0 | 2.740073 | -2.246120 | -0.557112 |
| 19 | 8 | 0 | 3.320823 | -2.682721 | -1.389643 |
| 20 | 1 | 0 | 3.607329 | -1.919098 | -1.917349 |
| 21 | 1 | 0 | 4.675702 | -3.026385 | -0.452523 |
| 22 | 8 | 0 | 5.414589 | -3.075584 | 0.228531 |
| 23 | 1 | 0 | 5.157318 | -3.799741 | 0.818625 |
| 24 | 1 | 0 | 1.885758 | -3.106436 | -2.481622 |
| 25 | 8 | 0 | 1.152818 | -3.050877 | -3.140570 |
| 26 | 1 | 0 | 0.342078 | -3.426739 | -2.713636 |
| 27 | 1 | 0 | 0.735115 | -1.473943 | -3.304279 |
| 28 | 8 | 0 | 0.431496 | -0.507791 | -3.325079 |
| 29 | 1 | 0 | 0.483269 | -0.224639 | -4.249477 |
| 30 | 1 | 0 | 5.233637 | -1.506476 | 1.020961 |
| 31 | 8 | 0 | 5.054676 | -0.638899 | 1.472446 |
| 32 | 1 | 0 | 5.843688 | -0.450428 | 2.001146 |
| 33 | 1 | 0 | -1.765896 | -0.256752 | -1.013946 |
| 34 | 8 | 0 | -1.976963 | -0.715244 | -1.854467 |
| 35 | 1 | 0 | -1.221079 | -0.513885 | -2.451679 |
| 36 | 1 | 0 | -1.625342 | -2.651273 | -2.056358 |

| | | | | | |
|---|---|---|---|---|---|
| 37 | 8 | 0 | -1.355092 | -3.588200 | -2.154826 |
| 38 | 1 | 0 | -1.640726 | -3.984455 | -1.303000 |
| 39 | 1 | 0 | -3.710527 | -1.546114 | -1.314937 |
| 40 | 8 | 0 | -4.306091 | -2.108197 | -0.783809 |
| 41 | 1 | 0 | -4.814834 | -1.506730 | -0.194797 |
| 42 | 1 | 0 | -0.703828 | -1.041623 | 1.125764 |
| 43 | 8 | 0 | -0.396350 | -1.938459 | 1.363296 |
| 44 | 1 | 0 | 0.568963 | -1.949541 | 1.047982 |
| 45 | 1 | 0 | -1.444357 | -2.417297 | 2.850279 |
| 46 | 8 | 0 | -2.328893 | -2.616090 | 3.233185 |
| 47 | 1 | 0 | -2.693022 | -3.228655 | 2.562453 |
| 48 | 1 | 0 | -1.655209 | -3.102923 | 0.673297 |
| 49 | 8 | 0 | -2.397843 | -3.728163 | 0.500124 |
| 50 | 1 | 0 | -3.129147 | -3.183637 | 0.119158 |
| 51 | 1 | 0 | 3.332473 | 1.267120 | -0.539690 |
| 52 | 8 | 0 | 4.107862 | 1.629142 | -0.036233 |
| 53 | 1 | 0 | 4.461253 | 0.863013 | 0.466471 |
| 54 | 1 | 0 | 3.328200 | 2.800314 | 0.916351 |
| 55 | 8 | 0 | 2.779249 | 3.491708 | 1.391457 |
| 56 | 1 | 0 | 3.215407 | 4.337144 | 1.213258 |
| 57 | 1 | 0 | -3.091092 | -0.994891 | 2.938067 |
| 58 | 8 | 0 | -3.401774 | -0.099038 | 2.648308 |
| 59 | 1 | 0 | -2.727902 | 0.209064 | 2.008869 |
| 60 | 1 | 0 | -4.840916 | -0.315391 | 1.729737 |
| 61 | 8 | 0 | -5.603076 | -0.466255 | 1.103993 |
| 62 | 1 | 0 | -5.944689 | 0.412480 | 0.886411 |
| 63 | 6 | 0 | -0.041641 | 4.422326 | -2.006988 |
| 64 | 6 | 0 | -1.298655 | 4.505151 | -2.609470 |
| 65 | 1 | 0 | -2.912840 | 2.133405 | -0.777830 |
| 66 | 1 | 0 | -3.315344 | 3.736255 | -2.632579 |
| 67 | 1 | 0 | 1.168678 | 3.455182 | -0.517107 |
| 68 | 1 | 0 | 0.775669 | 5.044505 | -2.362531 |
| 69 | 1 | 0 | -1.465934 | 5.199529 | -3.429295 |
| 70 | 1 | 0 | 1.807594 | 2.577053 | 3.709358 |
| 71 | 1 | 0 | 0.116881 | 2.625437 | 4.263823 |
| 72 | 1 | 0 | 1.175471 | 1.288048 | 4.756365 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1778.55871751     A.U. after    1 cycles
          Convg  =    0.3275D-08             -V/T =  2.0093
          S**2   =   0.0000

Zero-point correction=                         0.606387 (a.u.)
Thermal correction to Energy=                  0.657935
Thermal correction to Enthalpy=                0.658880
Thermal correction to Gibbs Free Energy=       0.516969
Sum of electronic and zero-point Energies=          -1777.952330
Sum of electronic and thermal Energies=             -1777.900782

Sum of electronic and thermal Enthalpies=      -1777.899838
Sum of electronic and thermal Free Energies=      -1778.041748


 (4-2)  N-ethyl benzamide + HO-(H2O)16 TS1(am)
tuka02aa.chk    Stoichiometry C9H44NO18(1-)
                Standard orientation:

---------------------------------------------------------------------
Center   Atomic   Atomic         Coordinates (Angstroms)
Number   Number   Type        X        Y        Z
---------------------------------------------------------------------
  1        6       0     -0.470652   2.399800  -0.844394
  2        6       0     -0.180315   1.366931   0.254620
  3        8       0     -1.118661   0.470879   0.459457
  4        7       0      0.342700   2.010664   1.397317
  5        6       0      0.645579   1.245170   2.603188
  6        6       0     -1.799864   2.635945  -1.211927
  7        6       0     -2.113841   3.598584  -2.173143
  8        6       0      0.540684   3.151935  -1.458527
  9        1       0      1.076941   2.683243   1.182820
 10        6       0      0.885925   2.186439   3.783055
 11        1       0     -0.202787   0.591747   2.814586
 12        1       0      1.528264   0.597069   2.466522
 13        8       0      1.157664   0.509965  -0.411976
 14        1       0      0.896889   0.227086  -1.314410
 15        1       0      1.587771  -0.852260   0.345443
 16        8       0      1.952299  -1.713037   0.748674
 17        1       0      2.700652  -1.434461   1.313807
 18        1       0      2.706877  -2.407177  -0.567744
 19        8       0      3.249789  -2.785737  -1.325315
 20        1       0      3.390337  -2.037032  -1.927494
 21        1       0      4.767183  -3.037333  -0.478314
 22        8       0      5.544084  -3.023980   0.142972
 23        1       0      5.564892  -3.901335   0.552826
 24        1       0      1.612379  -3.375996  -2.394466
 25        8       0      0.918694  -3.204272  -3.058986
 26        1       0      0.050873  -3.504101  -2.664685
 27        1       0      0.661174  -1.532679  -3.126138
 28        8       0      0.461399  -0.551175  -3.066459
 29        1       0      0.752093  -0.153017  -3.899660
 30        1       0      5.065508  -1.649753   1.162312
 31        8       0      4.574746  -0.895313   1.578999
 32        1       0      5.059210  -0.636911   2.376590
 33        1       0     -1.776876  -0.345121  -0.967672
 34        8       0     -2.108694  -0.773240  -1.803528
 35        1       0     -1.432968  -0.526168  -2.465828
 36        1       0     -1.815175  -2.628230  -2.039072

| 37 | 8 | 0 | -1.576407 | -3.579154 | -2.121011 |
| 38 | 1 | 0 | -1.869970 | -3.937887 | -1.248433 |
| 39 | 1 | 0 | -3.831575 | -1.515954 | -1.181114 |
| 40 | 8 | 0 | -4.464323 | -2.010375 | -0.624051 |
| 41 | 1 | 0 | -4.860708 | -1.346189 | -0.014687 |
| 42 | 1 | 0 | -0.847662 | -1.064812 | 1.165701 |
| 43 | 8 | 0 | -0.733012 | -1.960657 | 1.595774 |
| 44 | 1 | 0 | 0.223355 | -2.144736 | 1.488287 |
| 45 | 1 | 0 | -1.656867 | -1.836059 | 3.101483 |
| 46 | 8 | 0 | -2.343048 | -1.621517 | 3.782176 |
| 47 | 1 | 0 | -3.046979 | -2.270386 | 3.628954 |
| 48 | 1 | 0 | -1.944807 | -3.214478 | 0.852215 |
| 49 | 8 | 0 | -2.601781 | -3.826397 | 0.454936 |
| 50 | 1 | 0 | -3.353363 | -3.247451 | 0.179614 |
| 51 | 1 | 0 | 2.816465 | 1.024139 | -0.349095 |
| 52 | 8 | 0 | 3.769296 | 1.284433 | -0.214281 |
| 53 | 1 | 0 | 4.141875 | 0.590024 | 0.364135 |
| 54 | 1 | 0 | 3.527289 | 2.751943 | 0.736901 |
| 55 | 8 | 0 | 3.220396 | 3.527803 | 1.273584 |
| 56 | 1 | 0 | 3.423512 | 4.310456 | 0.741796 |
| 57 | 1 | 0 | -2.912549 | -0.008539 | 2.964230 |
| 58 | 8 | 0 | -3.161896 | 0.718587 | 2.350330 |
| 59 | 1 | 0 | -2.434337 | 0.745699 | 1.680167 |
| 60 | 1 | 0 | -4.616935 | 0.249836 | 1.616685 |
| 61 | 8 | 0 | -5.448266 | -0.072571 | 1.162537 |
| 62 | 1 | 0 | -5.847773 | 0.712152 | 0.760954 |
| 63 | 6 | 0 | 0.227862 | 4.115941 | -2.418266 |
| 64 | 6 | 0 | -1.101764 | 4.343406 | -2.779777 |
| 65 | 1 | 0 | -2.583159 | 2.052290 | -0.741269 |
| 66 | 1 | 0 | -3.152852 | 3.764280 | -2.447800 |
| 67 | 1 | 0 | 1.577652 | 2.972046 | -1.194422 |
| 68 | 1 | 0 | 1.026415 | 4.686340 | -2.887611 |
| 69 | 1 | 0 | -1.345600 | 5.092438 | -3.529757 |
| 70 | 1 | 0 | 1.720521 | 2.865998 | 3.576164 |
| 71 | 1 | 0 | -0.009187 | 2.785962 | 3.980437 |
| 72 | 1 | 0 | 1.125183 | 1.611812 | 4.686197 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1778.52641035     A.U. after    1 cycles
          Convg  =    0.4358D-08          -V/T =  2.0093
          S**2  =   0.0000

Zero-point correction=                    0.608558 (a.u.)
Thermal correction to Energy=                  0.659034
Thermal correction to Enthalpy=               0.659978
Thermal correction to Gibbs Free Energy=       0.521684
Sum of electronic and zero-point Energies=        -1777.917853
Sum of electronic and thermal Energies=           -1777.867376

Sum of electronic and thermal Enthalpies=      -1777.866432
Sum of electronic and thermal Free Energies=     -1778.004727


 (4-3) Anionic tetrahedral intermediate, Ph-C(-O-)(OH)-NHEt.
    and (H2O)16, Int1(am)
tuka02bz.for.chk     Stoichiometry C9H44NO18(1-)
                 Standard orientation:

---------------------------------------------------------------------
Center    Atomic    Atomic          Coordinates (Angstroms)
Number    Number     Type        X         Y         Z
---------------------------------------------------------------------
   1        6         0      -2.067584   1.034754  -1.070918
   2        6         0      -2.457612  -0.414114  -0.686843
   3        8         0      -2.751103  -0.572288   0.617198
   4        7         0      -1.339821  -1.302903  -1.096324
   5        6         0      -1.564909  -2.744696  -0.866782
   6        6         0      -1.958955   2.030089  -0.094613
   7        6         0      -1.587899   3.333692  -0.443703
   8        6         0      -1.313346   3.657355  -1.774834
   9        1         0      -1.158577  -1.155697  -2.089346
  10        1         0      -1.673067  -2.894227   0.210747
  11        1         0      -2.496669  -3.084170  -1.339183
  12        6         0      -0.386642  -3.560354  -1.395960
  13        8         0      -3.599778  -0.782632  -1.536658
  14        1         0      -4.335859  -0.183612  -1.296683
  15        1         0      -5.378808  -2.690503   0.302076
  16        8         0      -5.720654  -2.549036  -0.617186
  17        1         0      -4.911031  -2.289241  -1.103936
  18        1         0       0.107994  -0.783608  -0.169393
  19        8         0       0.835107  -0.456274   0.447240
  20        1         0       0.371427  -0.359323   1.313565
  21        1         0       2.526871  -1.109194   0.402407
  22        8         0       3.497338  -1.101165   0.233204
  23        1         0       3.952325  -1.864076   0.668396
  24        1         0      -6.279761  -0.891325  -0.528003
  25        8         0      -6.273330   0.106477  -0.530482
  26        1         0      -7.025452   0.389068  -1.070454
  27        1         0      -4.077507   0.236117   1.399659
  28        8         0      -4.837317   0.505058   1.982080
  29        1         0      -5.560743   0.655204   1.345331
  30        1         0       4.178602  -0.957740  -1.530744
  31        8         0       4.768583  -0.704682  -2.272788
  32        1         0       4.684572   0.275613  -2.284350
  33        1         0       4.310649   0.350994   0.782877
  34        8         0       4.874743   1.136011   1.013423
  35        1         0       4.292906   1.732146   1.540572

| 36 | 1 | 0 | -3.673658 | -1.917405 | 1.315724 |
| 37 | 8 | 0 | -4.372549 | -2.428948 | 1.802795 |
| 38 | 1 | 0 | -4.831264 | -1.710639 | 2.278351 |
| 39 | 1 | 0 | 6.335458 | 0.311650 | 1.476782 |
| 40 | 8 | 0 | 7.073155 | -0.345797 | 1.586263 |
| 41 | 1 | 0 | 7.803916 | 0.129573 | 2.006959 |
| 42 | 1 | 0 | 6.287328 | -1.409699 | -1.522286 |
| 43 | 8 | 0 | 6.943310 | -1.857370 | -0.932353 |
| 44 | 1 | 0 | 7.203696 | -1.183599 | -0.274887 |
| 45 | 1 | 0 | -1.087765 | -1.005513 | 3.122527 |
| 46 | 8 | 0 | -1.003326 | -0.241127 | 2.532190 |
| 47 | 1 | 0 | -1.675592 | -0.395624 | 1.783945 |
| 48 | 1 | 0 | -2.136801 | 1.222803 | 3.368597 |
| 49 | 8 | 0 | -2.813242 | 1.884631 | 3.610345 |
| 50 | 1 | 0 | -3.634275 | 1.560642 | 3.188606 |
| 51 | 1 | 0 | 4.674528 | 1.896816 | -0.759697 |
| 52 | 8 | 0 | 4.278766 | 2.033619 | -1.647049 |
| 53 | 1 | 0 | 3.321465 | 2.081946 | -1.451292 |
| 54 | 1 | 0 | 0.815768 | 2.517386 | -0.649988 |
| 55 | 8 | 0 | 1.618305 | 2.050728 | -0.358979 |
| 56 | 1 | 0 | 1.313988 | 1.132913 | -0.118258 |
| 57 | 6 | 0 | -1.819063 | 1.377674 | -2.409636 |
| 58 | 6 | 0 | -1.435777 | 2.672038 | -2.760064 |
| 59 | 1 | 0 | -2.169131 | 1.795320 | 0.942208 |
| 60 | 1 | 0 | -1.517779 | 4.092297 | 0.331583 |
| 61 | 1 | 0 | -1.020490 | 4.668824 | -2.045106 |
| 62 | 1 | 0 | -1.944369 | 0.629505 | -3.188135 |
| 63 | 1 | 0 | -1.238319 | 2.914074 | -3.801278 |
| 64 | 1 | 0 | -0.262775 | -3.428882 | -2.478911 |
| 65 | 1 | 0 | 0.551677 | -3.267257 | -0.912802 |
| 66 | 1 | 0 | -0.549644 | -4.627742 | -1.209502 |
| 67 | 1 | 0 | 2.344756 | 2.656711 | 1.166887 |
| 68 | 8 | 0 | 2.873671 | 2.809113 | 1.989543 |
| 69 | 1 | 0 | 2.291095 | 2.561152 | 2.722928 |
| 70 | 1 | 0 | 5.887994 | -2.246807 | 1.778406 |
| 71 | 8 | 0 | 5.406533 | -2.838816 | 1.172905 |
| 72 | 1 | 0 | 5.926085 | -2.733198 | 0.335964 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1778.53261788     A.U. after    1 cycles

      Convg  =    0.3824D-08          -V/T =  2.0093

      S**2   =   0.0000

Zero-point correction=                         0.609918 (a.u.)

Thermal correction to Energy=               0.660861

Thermal correction to Enthalpy=             0.661805

Thermal correction to Gibbs Free Energy=       0.520198

Sum of electronic and zero-point Energies=        -1777.922699

Sum of electronic and thermal Energies=         -1777.871757
Sum of electronic and thermal Enthalpies=       -1777.870813
Sum of electronic and thermal Free Energies=     -1778.012420

 (4-4)  TS2(am) toward the zwitterion
tuka02bz.chk   Stoichiometry C9H44NO18(1-)
                Standard orientation:

---------------------------------------------------------------------
Center     Atomic    Atomic          Coordinates (Angstroms)
Number     Number     Type        X        Y        Z
---------------------------------------------------------------------
   1         6         0      -1.426006   0.980577  -0.999213
   2         6         0      -1.786729  -0.421078  -0.455536
   3         8         0      -2.578588  -0.402326   0.624639
   4         7         0      -0.478914  -1.140013  -0.117061
   5         6         0      -0.683466  -2.536538   0.362438
   6         6         0      -1.793698   2.134399  -0.299002
   7         6         0      -1.486990   3.401563  -0.806915
   8         6         0      -0.800916   3.527668  -2.017650
   9         1         0       0.146908  -1.152380  -0.931889
  10         1         0      -1.229858  -2.469040   1.305768
  11         1         0      -1.318884  -3.057636  -0.358032
  12         6         0       0.638982  -3.273683   0.554122
  13         8         0      -2.330426  -1.200880  -1.535684
  14         1         0      -3.236708  -0.863874  -1.702930
  15         1         0      -5.100238  -2.891886  -0.082925
  16         8         0      -5.417161  -3.143475  -0.999782
  17         1         0      -4.687202  -3.655178  -1.380562
  18         1         0       0.104738  -0.493688   0.726444
  19         8         0       0.785877   0.223401   1.602588
  20         1         0       0.183983   0.404241   2.348025
  21         1         0       2.305833  -0.405076   1.595610
  22         8         0       3.196585  -0.637142   1.184077
  23         1         0       3.591935  -1.460900   1.547352
  24         1         0      -5.366391  -1.536602  -1.685492
  25         8         0      -5.151141  -0.597555  -1.936673
  26         1         0      -5.473203  -0.469080  -2.840633
  27         1         0      -4.132038   0.364554   0.633142
  28         8         0      -5.085576   0.608137   0.784389
  29         1         0      -5.468738   0.543553  -0.108618
  30         1         0       2.633217  -1.020960  -0.508125
  31         8         0       2.440339  -1.152233  -1.467662
  32         1         0       2.620638  -0.252755  -1.835051
  33         1         0       4.336556   0.538531   0.680169
  34         8         0       5.009973   1.148281   0.273406
  35         1         0       4.880657   2.000778   0.750307

| 36 | 1 | 0 | -3.658976 | -1.720010 | 1.057869 |
|----|---|---|-----------|-----------|----------|
| 37 | 8 | 0 | -4.488674 | -2.189139 | 1.350947 |
| 38 | 1 | 0 | -5.084270 | -1.427532 | 1.496466 |
| 39 | 1 | 0 | 6.254229 | -0.054466 | 0.013515 |
| 40 | 8 | 0 | 6.733955 | -0.909165 | -0.145561 |
| 41 | 1 | 0 | 7.609123 | -0.669561 | -0.482678 |
| 42 | 1 | 0 | 3.978844 | -2.230211 | -1.588311 |
| 43 | 8 | 0 | 4.800639 | -2.731836 | -1.372881 |
| 44 | 1 | 0 | 5.492576 | -2.053099 | -1.241742 |
| 45 | 1 | 0 | -2.145580 | -0.140940 | 3.660184 |
| 46 | 8 | 0 | -1.856804 | 0.530201 | 3.023786 |
| 47 | 1 | 0 | -2.086228 | 0.156068 | 2.120884 |
| 48 | 1 | 0 | -3.310854 | 1.904746 | 3.021787 |
| 49 | 8 | 0 | -4.097240 | 2.466401 | 2.867742 |
| 50 | 1 | 0 | -4.612551 | 1.983963 | 2.192251 |
| 51 | 1 | 0 | 3.929226 | 1.470476 | -1.318630 |
| 52 | 8 | 0 | 3.104753 | 1.538949 | -1.845956 |
| 53 | 1 | 0 | 2.466792 | 1.898178 | -1.189394 |
| 54 | 1 | 0 | 0.805915 | 2.919446 | 0.168080 |
| 55 | 8 | 0 | 1.600155 | 2.429492 | 0.438460 |
| 56 | 1 | 0 | 1.252221 | 1.590785 | 0.911587 |
| 57 | 6 | 0 | -0.751043 | 1.117312 | -2.220945 |
| 58 | 6 | 0 | -0.432870 | 2.379110 | -2.724060 |
| 59 | 1 | 0 | -2.325836 | 2.048201 | 0.641008 |
| 60 | 1 | 0 | -1.793901 | 4.285767 | -0.253776 |
| 61 | 1 | 0 | -0.558021 | 4.512018 | -2.410395 |
| 62 | 1 | 0 | -0.481563 | 0.230058 | -2.786635 |
| 63 | 1 | 0 | 0.104183 | 2.464446 | -3.664766 |
| 64 | 1 | 0 | 1.202412 | -3.341508 | -0.382170 |
| 65 | 1 | 0 | 1.271665 | -2.778389 | 1.296602 |
| 66 | 1 | 0 | 0.438730 | -4.292206 | 0.905971 |
| 67 | 1 | 0 | 3.026573 | 3.148059 | 1.171342 |
| 68 | 8 | 0 | 3.914585 | 3.386642 | 1.547680 |
| 69 | 1 | 0 | 3.812637 | 3.296255 | 2.506525 |
| 70 | 1 | 0 | 5.704698 | -2.335997 | 1.422046 |
| 71 | 8 | 0 | 4.876556 | -2.846946 | 1.428272 |
| 72 | 1 | 0 | 4.743094 | -3.029493 | 0.465511 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1778.52293385     A.U. after    1 cycles

Convg  =    0.7811D-09          -V/T =  2.0093

S**2  =   0.0000

Zero-point correction=                      0.605542 (a.u.)

Thermal correction to Energy=               0.655730

Thermal correction to Enthalpy=             0.656674

Thermal correction to Gibbs Free Energy=       0.517388

Sum of electronic and zero-point Energies=        -1777.917392

Sum of electronic and thermal Energies=        -1777.867204
Sum of electronic and thermal Enthalpies=       -1777.866260
Sum of electronic and thermal Free Energies=     -1778.005546


 (4-5) Zwitterion(Mulliken CT complex), Ph-C(-O-)(OH)NH2(+)Et,
     and OH-(H2O)15. Int2(am)
tukats3a.rev.chk    Stoichiometry  C9H44NO18(1-)
             Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number    Type        X        Y         Z
-----------------------------------------------------------------------
   1       6      0     -2.439399   1.804122  -0.099189
   2       6      0     -1.805413   0.408481  -0.212268
   3       8      0     -2.610018  -0.607732  -0.040179
   4       7      0     -0.630464   0.343444   0.957058
   5       6      0     -1.098495   0.232628   2.371488
   6       6      0     -3.644497   1.958688   0.595504
   7       6      0     -4.234641   3.217784   0.725993
   8       6      0     -3.630560   4.339123   0.156600
   9       1      0     -0.072267  -0.501527   0.734281
  10       6      0     -1.047097   1.555605   3.130421
  11       1      0     -2.112525  -0.173727   2.334463
  12       1      0     -0.464471  -0.511673   2.862654
  13       8      0     -1.006667   0.357775  -1.382329
  14       1      0     -1.031312  -0.562879  -1.744583
  15       1      0     -0.983017  -3.888192  -0.249569
  16       8      0     -0.150609  -3.838334  -0.782471
  17       1      0      0.437292  -3.257086  -0.243265
  18       1      0      0.019543   1.143325   0.841618
  19       8      0      1.394248   2.432852   0.601870
  20       1      0      1.347030   3.349900   0.908154
  21       1      0      2.361464   2.077250   0.814268
  22       8      0      3.698809   1.471961   0.917096
  23       1      0      3.957164   1.217365   1.815208
  24       1      0     -0.629643  -2.839024  -2.015457
  25       8      0     -0.965143  -2.143753  -2.666242
  26       1      0     -0.343526  -2.142034  -3.409337
  27       1      0     -3.493702  -1.155630  -1.601154
  28       8      0     -3.803842  -1.702491  -2.360126
  29       1      0     -2.960709  -2.029990  -2.730495
  30       1      0      3.437160   0.068180   0.046822
  31       8      0      3.341487  -0.741925  -0.546401
  32       1      0      3.469619  -0.379954  -1.458860
  33       1      0      4.868659   1.772490   0.020420
  34       8      0      5.632218   1.843832  -0.687297

| 35 | 1 | 0 | 5.981229 | 2.745193 | -0.629437 |
|----|---|---|----------|----------|-----------|
| 36 | 1 | 0 | -2.370908 | -2.404604 | 0.390872 |
| 37 | 8 | 0 | -2.465558 | -3.354095 | 0.637227 |
| 38 | 1 | 0 | -3.299123 | -3.628403 | 0.184618 |
| 39 | 1 | 0 | 6.706300 | 0.558896 | -0.047308 |
| 40 | 8 | 0 | 7.236388 | -0.196509 | 0.314579 |
| 41 | 1 | 0 | 7.598542 | -0.640839 | -0.466479 |
| 42 | 1 | 0 | 4.595053 | -1.755855 | 0.207658 |
| 43 | 8 | 0 | 5.202075 | -2.170996 | 0.870406 |
| 44 | 1 | 0 | 5.946586 | -1.533775 | 0.923446 |
| 45 | 1 | 0 | 1.926312 | -1.499256 | 0.084800 |
| 46 | 8 | 0 | 1.236974 | -1.905278 | 0.676218 |
| 47 | 1 | 0 | 1.769251 | -2.214986 | 1.447224 |
| 48 | 1 | 0 | 3.169771 | -3.684279 | 2.687454 |
| 49 | 8 | 0 | 3.155179 | -2.719537 | 2.602125 |
| 50 | 1 | 0 | 3.978807 | -2.495571 | 2.089696 |
| 51 | 1 | 0 | -4.270579 | -2.144786 | 1.977319 |
| 52 | 8 | 0 | -4.768049 | -1.448459 | 1.517138 |
| 53 | 1 | 0 | -4.074084 | -1.011088 | 0.967491 |
| 54 | 1 | 0 | -5.299009 | -2.826525 | 0.046972 |
| 55 | 8 | 0 | -5.004541 | -3.503190 | -0.595078 |
| 56 | 1 | 0 | -4.696887 | -2.972163 | -1.369433 |
| 57 | 1 | 0 | 4.472357 | 1.337700 | -2.231239 |
| 58 | 8 | 0 | 3.803508 | 0.847094 | -2.752654 |
| 59 | 1 | 0 | 2.957713 | 1.346755 | -2.656605 |
| 60 | 1 | 0 | 0.593392 | 1.406064 | -2.162363 |
| 61 | 8 | 0 | 1.319685 | 2.059209 | -2.171783 |
| 62 | 1 | 0 | 1.415886 | 2.280865 | -1.215600 |
| 63 | 6 | 0 | -1.843370 | 2.932940 | -0.678640 |
| 64 | 6 | 0 | -2.435384 | 4.190426 | -0.549770 |
| 65 | 1 | 0 | -4.128990 | 1.090792 | 1.027902 |
| 66 | 1 | 0 | -5.172899 | 3.315855 | 1.266443 |
| 67 | 1 | 0 | -4.091689 | 5.319233 | 0.253703 |
| 68 | 1 | 0 | -0.924492 | 2.830670 | -1.243650 |
| 69 | 1 | 0 | -1.963338 | 5.053211 | -1.013537 |
| 70 | 1 | 0 | -0.021877 | 1.936282 | 3.188837 |
| 71 | 1 | 0 | -1.674326 | 2.316054 | 2.657079 |
| 72 | 1 | 0 | -1.412527 | 1.401489 | 4.151947 |

-------------------------------------------------------------------

SCF Done:  E(RB3LYP) = -1778.53687506    A.U. after    1 cycles

Convg  =   0.1842D-08          -V/T = 2.0093

Zero-point correction=                        0.610433 (a.u.)

Thermal correction to Energy=                0.660107

Thermal correction to Enthalpy=              0.661051

Thermal correction to Gibbs Free Energy=        0.525179

Sum of electronic and zero-point Energies=         -1777.926443

Sum of electronic and thermal Energies=        -1777.876768
Sum of electronic and thermal Enthalpies=       -1777.875824
Sum of electronic and thermal Free Energies=      -1778.011696

(4-6) TS3(am) separation TS to Ph-COOH, Et-NH2 and OH-
tukats3a.chk   Stoichiometry C9H44NO18(1-)

                Standard orientation:
---------------------------------------------------------------------
Center   Atomic   Atomic       Coordinates (Angstroms)
Number   Number   Type       X        Y        Z
---------------------------------------------------------------------
   1       6       0     -2.513671   1.819091  -0.178684
   2       6       0     -1.966925   0.418312  -0.360133
   3       8       0     -2.720371  -0.582303  -0.123813
   4       7       0     -0.629241   0.383448   1.084708
   5       6       0     -1.153917   0.268281   2.461286
   6       6       0     -3.683180   2.001384   0.570112
   7       6       0     -4.215926   3.278310   0.752941
   8       6       0     -3.590474   4.387951   0.182828
   9       1       0     -0.074423  -0.453199   0.863533
  10       6       0     -1.149938   1.598687   3.211385
  11       1       0     -2.172414  -0.134145   2.389371
  12       1       0     -0.558551  -0.471381   3.009646
  13       8       0     -1.088145   0.339309  -1.415207
  14       1       0     -1.002760  -0.606027  -1.713894
  15       1       0     -0.969490  -3.864083  -0.055178
  16       8       0     -0.123257  -3.832883  -0.565790
  17       1       0      0.473401  -3.263800  -0.017171
  18       1       0      0.004259   1.187539   0.979171
  19       8       0      1.439013   2.546970   0.605852
  20       1       0      1.436917   3.473525   0.885975
  21       1       0      2.389355   2.169022   0.809865
  22       8       0      3.741225   1.523162   0.907582
  23       1       0      4.015212   1.287882   1.806255
  24       1       0     -0.515298  -2.863368  -1.811753
  25       8       0     -0.815801  -2.187074  -2.506587
  26       1       0     -0.144656  -2.196333  -3.205691
  27       1       0     -3.486853  -1.335607  -1.757061
  28       8       0     -3.680806  -1.960538  -2.487041
  29       1       0     -2.783286  -2.247979  -2.749569
  30       1       0      3.434517   0.106323   0.085399
  31       8       0      3.321311  -0.711812  -0.495623
  32       1       0      3.429723  -0.361084  -1.414174
  33       1       0      4.879883   1.796021  -0.009280
  34       8       0      5.627796   1.860010  -0.742812
  35       1       0      5.975612   2.762952  -0.707332

| 36 | 1 | 0 | -2.443574 | -2.395990 | 0.459412 |
| 37 | 8 | 0 | -2.514216 | -3.334071 | 0.736616 |
| 38 | 1 | 0 | -3.315480 | -3.658759 | 0.258736 |
| 39 | 1 | 0 | 6.733878 | 0.586757 | -0.160375 |
| 40 | 8 | 0 | 7.289343 | -0.169217 | 0.161965 |
| 41 | 1 | 0 | 7.610919 | -0.599727 | -0.644183 |
| 42 | 1 | 0 | 4.626476 | -1.715883 | 0.172523 |
| 43 | 8 | 0 | 5.283023 | -2.153942 | 0.770787 |
| 44 | 1 | 0 | 6.028244 | -1.515833 | 0.797256 |
| 45 | 1 | 0 | 1.967282 | -1.526632 | 0.226403 |
| 46 | 8 | 0 | 1.325827 | -1.962898 | 0.845983 |
| 47 | 1 | 0 | 1.907124 | -2.278322 | 1.576964 |
| 48 | 1 | 0 | 3.413686 | -3.788784 | 2.644919 |
| 49 | 8 | 0 | 3.382971 | -2.820986 | 2.622363 |
| 50 | 1 | 0 | 4.161546 | -2.554759 | 2.062438 |
| 51 | 1 | 0 | -4.586548 | -2.005617 | 1.883658 |
| 52 | 8 | 0 | -5.032543 | -1.422184 | 1.248503 |
| 53 | 1 | 0 | -4.286237 | -0.990628 | 0.773155 |
| 54 | 1 | 0 | -5.314818 | -2.937894 | -0.099118 |
| 55 | 8 | 0 | -4.948318 | -3.661463 | -0.646953 |
| 56 | 1 | 0 | -4.609827 | -3.201788 | -1.451038 |
| 57 | 1 | 0 | 4.438776 | 1.336036 | -2.232233 |
| 58 | 8 | 0 | 3.751484 | 0.852229 | -2.737070 |
| 59 | 1 | 0 | 2.917252 | 1.367254 | -2.627638 |
| 60 | 1 | 0 | 0.574392 | 1.426560 | -2.122290 |
| 61 | 8 | 0 | 1.283371 | 2.095564 | -2.134774 |
| 62 | 1 | 0 | 1.385132 | 2.327703 | -1.179144 |
| 63 | 6 | 0 | -1.895039 | 2.935561 | -0.758150 |
| 64 | 6 | 0 | -2.431779 | 4.210483 | -0.576008 |
| 65 | 1 | 0 | -4.181768 | 1.142086 | 1.004018 |
| 66 | 1 | 0 | -5.125847 | 3.400936 | 1.334943 |
| 67 | 1 | 0 | -4.006903 | 5.382810 | 0.321817 |
| 68 | 1 | 0 | -0.998598 | 2.812402 | -1.353724 |
| 69 | 1 | 0 | -1.943522 | 5.065690 | -1.036497 |
| 70 | 1 | 0 | -0.128430 | 1.978296 | 3.326563 |
| 71 | 1 | 0 | -1.740279 | 2.355491 | 2.685784 |
| 72 | 1 | 0 | -1.579493 | 1.466835 | 4.211249 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) = -1778.53528511    A.U. after    1 cycles

Convg  =    0.3375D-08          -V/T =  2.0093

S**2  =  0.0000

Zero-point correction=                    0.608607 (a.u.)

Thermal correction to Energy=             0.658437

Thermal correction to Enthalpy=           0.659381

Thermal correction to Gibbs Free Energy=       0.522666

Sum of electronic and zero-point Energies=        -1777.926678

Sum of electronic and thermal Energies=        -1777.876848
Sum of electronic and thermal Enthalpies=       -1777.875904
Sum of electronic and thermal Free Energies=      -1778.012620


 (4-7)  Ph-COOH, H2N-Et and OH-(H2O)15
 after the separation TS,  Int3(am)
tukats3a.for.chk   Stoichiometry  C9H44NO18(1-)
                 Standard orientation:

---------------------------------------------------------------------
Center   Atomic   Atomic            Coordinates (Angstroms)
Number   Number    Type         X         Y         Z
---------------------------------------------------------------------
   1        6        0       3.924412  -1.742043  -0.374241
   2        6        0       3.267864  -0.455164  -0.734334
   3        8        0       3.688204   0.632796  -0.343246
   4        7        0      -0.336771   1.284013   2.085206
   5        6        0      -0.860941   1.672280   3.406744
   6        6        0       5.037708  -1.694749   0.478207
   7        6        0       5.696233  -2.868347   0.833525
   8        6        0       5.248095  -4.096867   0.339740
   9        1        0      -0.981298   1.612875   1.359543
  10        6        0       0.060939   1.195532   4.527877
  11        1        0      -0.931714   2.766911   3.429201
  12        1        0      -1.878618   1.284969   3.576594
  13        8        0       2.194494  -0.576538  -1.521526
  14        1        0       1.840929   0.326904  -1.806814
  15        1        0      -0.451264   4.032268  -1.542706
  16        8        0      -0.737261   3.180852  -1.959029
  17        1        0      -1.386547   2.773701  -1.327342
  18        1        0      -0.330828   0.261600   2.013912
  19        8        0      -0.626344  -1.891677   1.820171
  20        1        0      -0.358941  -2.536210   2.491310
  21        1        0      -1.658275  -1.937858   1.771885
  22        8        0      -3.170471  -1.998656   1.510605
  23        1        0      -3.719446  -1.582639   2.191129
  24        1        0       0.487836   2.254846  -2.269917
  25        8        0       1.293145   1.702913  -2.589924
  26        1        0       1.116367   1.526786  -3.526950
  27        1        0       3.931374   2.407320  -1.303127
  28        8        0       3.646788   3.162338  -1.850509
  29        1        0       2.819417   2.821185  -2.250833
  30        1        0      -3.173111  -1.014196   0.165878
  31        8        0      -3.181790  -0.538837  -0.724611
  32        1        0      -2.889147  -1.234570  -1.363434
  33        1        0      -3.877423  -3.043325   0.742392
  34        8        0      -4.330733  -3.710513   0.064125

| 35 | 1 | 0 | -4.353351 | -4.574994 | 0.499400 |
| 36 | 1 | 0 | -0.436796 | 5.700328 | 0.068011 |
| 37 | 8 | 0 | 0.118500 | 5.507836 | -0.701655 |
| 38 | 1 | 0 | 1.015048 | 5.261702 | -0.328107 |
| 39 | 1 | 0 | -5.908713 | -2.970262 | -0.295293 |
| 40 | 8 | 0 | -6.755150 | -2.517785 | -0.547271 |
| 41 | 1 | 0 | -6.847236 | -2.687712 | -1.496715 |
| 42 | 1 | 0 | -4.873340 | -0.113651 | -0.955290 |
| 43 | 8 | 0 | -5.818435 | 0.186358 | -0.926336 |
| 44 | 1 | 0 | -6.306797 | -0.612659 | -0.634519 |
| 45 | 1 | 0 | -2.585227 | 1.080088 | -0.426619 |
| 46 | 8 | 0 | -2.430988 | 2.018764 | -0.147858 |
| 47 | 1 | 0 | -3.341432 | 2.376718 | -0.032485 |
| 48 | 1 | 0 | -5.447152 | 3.229324 | -0.750018 |
| 49 | 8 | 0 | -5.208695 | 2.674353 | 0.007093 |
| 50 | 1 | 0 | -5.559768 | 1.773120 | -0.224159 |
| 51 | 1 | 0 | 1.299818 | 1.971300 | 1.806679 |
| 52 | 8 | 0 | 2.221753 | 2.361958 | 1.699313 |
| 53 | 1 | 0 | 2.702483 | 1.745805 | 1.119329 |
| 54 | 1 | 0 | 2.366062 | 3.945167 | 0.850669 |
| 55 | 8 | 0 | 2.514017 | 4.722933 | 0.254414 |
| 56 | 1 | 0 | 2.988207 | 4.335883 | -0.516138 |
| 57 | 1 | 0 | -3.038211 | -3.373838 | -1.369577 |
| 58 | 8 | 0 | -2.444360 | -2.899044 | -1.989104 |
| 59 | 1 | 0 | -1.544228 | -2.937416 | -1.588858 |
| 60 | 1 | 0 | 0.568295 | -1.930691 | -1.087328 |
| 61 | 8 | 0 | 0.070827 | -2.685752 | -0.729967 |
| 62 | 1 | 0 | -0.150789 | -2.420098 | 0.200004 |
| 63 | 6 | 0 | 3.476049 | -2.975949 | -0.867362 |
| 64 | 6 | 0 | 4.139910 | -4.148202 | -0.507924 |
| 65 | 1 | 0 | 5.368407 | -0.731039 | 0.850625 |
| 66 | 1 | 0 | 6.556953 | -2.826550 | 1.495544 |
| 67 | 1 | 0 | 5.761319 | -5.013963 | 0.618562 |
| 68 | 1 | 0 | 2.606984 | -3.021359 | -1.511683 |
| 69 | 1 | 0 | 3.784737 | -5.102204 | -0.887095 |
| 70 | 1 | 0 | 0.143660 | 0.101354 | 4.523471 |
| 71 | 1 | 0 | 1.067065 | 1.610497 | 4.405693 |
| 72 | 1 | 0 | -0.327535 | 1.499169 | 5.507872 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1778.56315896     A.U. after    1 cycles
        Convg  =    0.7820D-08           -V/T =  2.0094
        S**2  =   0.0000

Zero-point correction=                      0.606326 (a.u.)
Thermal correction to Energy=                0.657939
Thermal correction to Enthalpy=              0.658883
Thermal correction to Gibbs Free Energy=     0.513262

Sum of electronic and zero-point Energies=      -1777.956833
Sum of electronic and thermal Energies=      -1777.905220
Sum of electronic and thermal Enthalpies=      -1777.904276
Sum of electronic and thermal Free Energies=      -1778.049897


 (4-8)  TS4(am), the last TS leading to the benzoate ion
   by the proton transfer from HO-
tukats4a.chk    Stoichiometry  C9H44NO18(1-)
                Standard orientation:
---------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type       X        Y        Z
---------------------------------------------------------------------
   1       6       0     2.345740   2.904003   0.073873
   2       6       0     2.784754   1.571736   0.601881
   3       8       0     3.427534   0.783201  -0.104275
   4       7       0     0.205785  -2.618635  -1.359206
   5       6       0    -0.272325  -3.851730  -2.012484
   6       6       0     2.756199   3.293149  -1.210105
   7       6       0     2.366539   4.529724  -1.723926
   8       6       0     1.564620   5.382876  -0.959816
   9       1       0    -0.174608  -2.553899  -0.397622
  10       1       0     0.192092  -3.912038  -3.005745
  11       1       0     0.111631  -4.705034  -1.440991
  12       6       0    -1.795301  -3.970319  -2.144287
  13       8       0     2.436005   1.347340   1.845363
  14       1       0     2.696402   0.383167   2.206178
  15       1       0     1.899067  -3.327056   1.756263
  16       8       0     1.495008  -2.739260   2.448460
  17       1       0     0.518276  -2.481606   2.055607
  18       1       0    -0.184710  -1.812573  -1.855398
  19       8       0    -1.444181  -0.126959  -2.736057
  20       1       0    -1.658975  -0.169579  -3.678969
  21       1       0    -2.293162  -0.288394  -2.244397
  22       8       0    -3.625144  -0.312013  -1.122452
  23       1       0    -4.344974  -0.988387  -1.069378
  24       1       0     2.252092  -1.787777   2.629016
  25       8       0     3.039462  -0.903327   2.810337
  26       1       0     3.151201  -0.809447   3.768373
  27       1       0     4.889341  -0.396560   0.613178
  28       8       0     5.284294  -1.102119   1.160738
  29       1       0     4.601874  -1.199663   1.865453
  30       1       0    -3.112463  -0.427073  -0.250000
  31       8       0    -2.452380  -0.432184   1.225911
  32       1       0    -2.073417   0.471233   1.303596
  33       1       0    -4.303867   1.193909  -0.785750

| 34 | 8 | 0 | -4.625308 | 2.083444 | -0.447026 |
|---|---|---|---|---|---|
| 35 | 1 | 0 | -4.748410 | 2.651686 | -1.221215 |
| 36 | 1 | 0 | 1.822566 | -3.653953 | -0.345315 |
| 37 | 8 | 0 | 2.383167 | -4.168254 | 0.267959 |
| 38 | 1 | 0 | 3.307788 | -3.934955 | -0.006651 |
| 39 | 1 | 0 | -5.676489 | 1.869844 | 1.011186 |
| 40 | 8 | 0 | -6.119757 | 1.634215 | 1.859031 |
| 41 | 1 | 0 | -5.689791 | 2.182797 | 2.532116 |
| 42 | 1 | 0 | -4.080023 | -0.823164 | 1.931829 |
| 43 | 8 | 0 | -5.042944 | -1.017553 | 2.059081 |
| 44 | 1 | 0 | -5.474733 | -0.136579 | 2.092485 |
| 45 | 1 | 0 | -1.693782 | -1.154835 | 1.352146 |
| 46 | 8 | 0 | -0.746187 | -2.298362 | 1.440836 |
| 47 | 1 | 0 | -1.282795 | -3.032793 | 1.777153 |
| 48 | 1 | 0 | -6.580926 | -1.839322 | -0.562470 |
| 49 | 8 | 0 | -5.654036 | -2.045594 | -0.374326 |
| 50 | 1 | 0 | -5.501242 | -1.756825 | 0.572048 |
| 51 | 1 | 0 | 1.983701 | -1.870298 | -1.728145 |
| 52 | 8 | 0 | 2.845070 | -1.447474 | -1.971965 |
| 53 | 1 | 0 | 2.940545 | -0.680823 | -1.375710 |
| 54 | 1 | 0 | 4.216656 | -2.577344 | -1.313203 |
| 55 | 8 | 0 | 4.756021 | -3.149743 | -0.720271 |
| 56 | 1 | 0 | 5.070716 | -2.528859 | -0.021780 |
| 57 | 1 | 0 | -2.912495 | 2.453905 | 0.487681 |
| 58 | 8 | 0 | -1.996414 | 2.368716 | 0.815051 |
| 59 | 1 | 0 | -1.456345 | 2.416088 | -0.006435 |
| 60 | 1 | 0 | 0.213377 | 2.523123 | -1.693226 |
| 61 | 8 | 0 | -0.747348 | 2.395341 | -1.743774 |
| 62 | 1 | 0 | -0.889808 | 1.496536 | -2.123216 |
| 63 | 6 | 0 | 1.538199 | 3.760647 | 0.835114 |
| 64 | 6 | 0 | 1.150502 | 4.995987 | 0.316779 |
| 65 | 1 | 0 | 3.381584 | 2.617072 | -1.784277 |
| 66 | 1 | 0 | 2.686903 | 4.827438 | -2.718860 |
| 67 | 1 | 0 | 1.256595 | 6.344205 | -1.363279 |
| 68 | 1 | 0 | 1.208734 | 3.443843 | 1.817828 |
| 69 | 1 | 0 | 0.513884 | 5.649983 | 0.905870 |
| 70 | 1 | 0 | -2.278487 | -3.929950 | -1.161617 |
| 71 | 1 | 0 | -2.203817 | -3.150430 | -2.747944 |
| 72 | 1 | 0 | -2.076651 | -4.916923 | -2.625116 |

---------------------------------------------------------------------

SCF Done:  E(RB3LYP) =  -1778.54304325    A.U. after    1 cycles
          Convg  =    0.3577D-08          -V/T =  2.0093
Zero-point correction=                          0.600546 (a.u.)
Thermal correction to Energy=                   0.651295
Thermal correction to Enthalpy=                 0.652239
Thermal correction to Gibbs Free Energy=        0.509907

Sum of electronic and zero-point Energies=       -1777.942497
Sum of electronic and thermal Energies=           -1777.891748
Sum of electronic and thermal Enthalpies=         -1777.890804
Sum of electronic and thermal Free Energies=      -1778.033136


 (4-9) The product, Ph-COO-, H2N-Et and (H2O)16
tukats4a.for.chk       Stoichiometry C9H44NO18(1-)
                  Standard orientation:

---------------------------------------------------------------------
Center    Atomic    Atomic         Coordinates (Angstroms)
Number    Number    Type       X         Y         Z
---------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.039785 | 2.600811 | -0.048224 |
| 2 | 6 | 0 | 3.292980 | 1.256315 | 0.619339 |
| 3 | 8 | 0 | 3.808549 | 0.345323 | -0.094641 |
| 4 | 7 | 0 | -0.030889 | -2.413096 | -1.375682 |
| 5 | 6 | 0 | -0.486541 | -3.347048 | -2.421459 |
| 6 | 6 | 0 | 3.337127 | 2.789305 | -1.404370 |
| 7 | 6 | 0 | 3.108304 | 4.024142 | -2.013126 |
| 8 | 6 | 0 | 2.581920 | 5.085979 | -1.272902 |
| 9 | 1 | 0 | -0.551716 | -2.571170 | -0.507088 |
| 10 | 1 | 0 | 0.109491 | -3.150926 | -3.321311 |
| 11 | 1 | 0 | -0.228450 | -4.361565 | -2.095571 |
| 12 | 6 | 0 | -1.980146 | -3.276084 | -2.759445 |
| 13 | 8 | 0 | 2.969910 | 1.160790 | 1.837406 |
| 14 | 1 | 0 | 2.992197 | -0.298820 | 2.584297 |
| 15 | 1 | 0 | 1.452475 | -3.579406 | 1.749444 |
| 16 | 8 | 0 | 1.055716 | -3.099051 | 2.523420 |
| 17 | 1 | 0 | -0.427122 | -2.676877 | 1.961371 |
| 18 | 1 | 0 | -0.253489 | -1.452022 | -1.649885 |
| 19 | 8 | 0 | -1.048658 | 0.550988 | -2.083741 |
| 20 | 1 | 0 | -0.926074 | 0.816128 | -3.006989 |
| 21 | 1 | 0 | -2.020433 | 0.429581 | -1.942534 |
| 22 | 8 | 0 | -3.633209 | 0.311149 | -1.184368 |
| 23 | 1 | 0 | -4.399832 | -0.249096 | -1.466216 |
| 24 | 1 | 0 | 1.692468 | -2.379502 | 2.741662 |
| 25 | 8 | 0 | 3.034854 | -1.181315 | 3.078477 |
| 26 | 1 | 0 | 3.181432 | -0.951287 | 4.007417 |
| 27 | 1 | 0 | 4.795384 | -0.961940 | 0.728679 |
| 28 | 8 | 0 | 5.166378 | -1.743819 | 1.205558 |
| 29 | 1 | 0 | 4.576214 | -1.804156 | 1.982940 |
| 30 | 1 | 0 | -3.359739 | -0.077420 | -0.302724 |
| 31 | 8 | 0 | -3.082064 | -0.495851 | 1.334816 |
| 32 | 1 | 0 | -2.735981 | 0.371847 | 1.673955 |
| 33 | 1 | 0 | -4.240241 | 1.810403 | -0.616862 |
| 34 | 8 | 0 | -4.566335 | 2.618891 | -0.125600 |

| 35 | 1 | 0 | -4.393819 | 3.382776 | -0.695420 |
|----|---|---|-----------|----------|-----------|
| 36 | 1 | 0 | 1.384181 | -3.598572 | -0.406353 |
| 37 | 8 | 0 | 1.840148 | -4.254594 | 0.159489 |
| 38 | 1 | 0 | 2.797859 | -4.153276 | -0.088034 |
| 39 | 1 | 0 | -5.993053 | 2.192160 | 0.917233 |
| 40 | 8 | 0 | -6.653320 | 1.797257 | 1.532079 |
| 41 | 1 | 0 | -6.433943 | 2.150925 | 2.407078 |
| 42 | 1 | 0 | -4.906876 | -0.859399 | 1.487967 |
| 43 | 8 | 0 | -5.873707 | -0.932137 | 1.313158 |
| 44 | 1 | 0 | -6.226428 | -0.027634 | 1.467803 |
| 45 | 1 | 0 | -2.390618 | -1.191821 | 1.483797 |
| 46 | 8 | 0 | -1.342263 | -2.596849 | 1.536871 |
| 47 | 1 | 0 | -1.819752 | -3.385504 | 1.834462 |
| 48 | 1 | 0 | -6.712244 | -0.980182 | -1.749236 |
| 49 | 8 | 0 | -5.870592 | -1.282477 | -1.378782 |
| 50 | 1 | 0 | -5.975098 | -1.237598 | -0.385735 |
| 51 | 1 | 0 | 1.944658 | -1.794996 | -1.682031 |
| 52 | 8 | 0 | 2.831492 | -1.512699 | -1.990128 |
| 53 | 1 | 0 | 3.113582 | -0.802864 | -1.369762 |
| 54 | 1 | 0 | 3.961612 | -2.915458 | -1.341485 |
| 55 | 8 | 0 | 4.355517 | -3.589462 | -0.741862 |
| 56 | 1 | 0 | 4.747573 | -3.045511 | -0.015275 |
| 57 | 1 | 0 | -3.176240 | 2.480261 | 1.282226 |
| 58 | 8 | 0 | -2.421681 | 2.120631 | 1.788026 |
| 59 | 1 | 0 | -1.648760 | 2.300093 | 1.198935 |
| 60 | 1 | 0 | 0.347210 | 2.816504 | -0.051249 |
| 61 | 8 | 0 | -0.591056 | 2.639604 | -0.237756 |
| 62 | 1 | 0 | -0.610730 | 1.892070 | -0.876970 |
| 63 | 6 | 0 | 2.512027 | 3.670985 | 0.689912 |
| 64 | 6 | 0 | 2.284767 | 4.907542 | 0.080847 |
| 65 | 1 | 0 | 3.751584 | 1.955937 | -1.962043 |
| 66 | 1 | 0 | 3.341952 | 4.159074 | -3.066758 |
| 67 | 1 | 0 | 2.403284 | 6.047757 | -1.748228 |
| 68 | 1 | 0 | 2.294492 | 3.512125 | 1.741369 |
| 69 | 1 | 0 | 1.876039 | 5.730541 | 0.662325 |
| 70 | 1 | 0 | -2.595884 | -3.490483 | -1.877715 |
| 71 | 1 | 0 | -2.257447 | -2.278430 | -3.121302 |
| 72 | 1 | 0 | -2.242279 | -4.003308 | -3.539213 |

-------------------------------------------------------------------

SCF Done:  E(RB3LYP) =  -1778.57194124     A.U. after    1 cycles

Convg  =    0.5257D-08              -V/T =  2.0094

Zero-point correction=                        0.608726 (a.u.)

Thermal correction to Energy=                 0.660999

Thermal correction to Enthalpy=               0.661943

Thermal correction to Gibbs Free Energy=      0.515024

Sum of electronic and zero-point Energies=        -1777.963215

Sum of electronic and thermal Energies=        -1777.910942
Sum of electronic and thermal Enthalpies=       -1777.909998
Sum of electronic and thermal Free Energies=      -1778.056918

=======================================================================

[5] The result of ADMP dynamical calculations starting from the n = 16 TS1(es) in Figures 1 and 3. The geometry after 800 femtoseconds shown in Figure S3.

TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ

----------------------------------------------------------------------

INPUT DATA FOR L121

----------------------------------------------------------------------

General parameters:
Maximum Steps          =   8000
Random Number Generator Seed =  398465
Time Step              =  0.10000 femtosec
Ficticious electronic mass   =  0.10000 amu
MW individual basis funct.   = True
Initial nuclear kin. energy  =  0.10000 hartree
Initial electr. kin. energy  =  0.00000 hartree
 Initial electr. KE scheme  =  0
Multitime step - NDtrC     =     1
Multitime step - NDtrP     =     1
No Thermostats chosen to control nuclear temperature
Integration parameters:
Follow Rxn Path (DVV)      = False
Constraint Scheme      =     10
Projection of angular mom.   = True
Rotate density with nuclei   = True

----------------------------------------------------------------------

TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ-TRJ
Symmetry turned off by external request.
Stoichiometry   C9H43O19(1-)
{the geometry after 800 femtoseconds (1 femtosecond = 10**-15 seconds)}
              Z-Matrix orientation:

----------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.155426 | 3.218905 | 0.002278 |
| 2 | 6 | 0 | -0.646047 | 2.589342 | 1.101693 |
| 3 | 8 | 0 | -1.871292 | 2.518345 | 1.088164 |
| 4 | 8 | 0 | 0.075124 | 2.073706 | 2.088168 |
| 5 | 6 | 0 | -0.595911 | 1.507661 | 3.252822 |
| 6 | 6 | 0 | -0.416272 | 3.291273 | -1.276570 |
| 7 | 6 | 0 | 0.296954 | 3.903214 | -2.307088 |
| 8 | 6 | 0 | 1.409210 | 3.766710 | 0.267399 |
| 9 | 6 | 0 | 0.406709 | 1.663979 | 4.391734 |
| 10 | 1 | 0 | -1.563735 | 2.059907 | 3.379593 |
| 11 | 1 | 0 | -0.762703 | 0.498800 | 3.004392 |
| 12 | 8 | 0 | 2.816336 | -0.173554 | 1.683389 |

| 13 | 1 | 0 | 2.209735 | 0.559851 | 1.484686 |
|---|---|---|---|---|---|
| 14 | 1 | 0 | 2.167136 | -1.027442 | 1.661518 |
| 15 | 8 | 0 | 1.313067 | -2.213730 | 1.261694 |
| 16 | 1 | 0 | 1.507436 | -2.869930 | 1.937406 |
| 17 | 1 | 0 | 1.920583 | -2.650400 | -0.098705 |
| 18 | 8 | 0 | 2.439874 | -2.905666 | -0.967106 |
| 19 | 1 | 0 | 3.013158 | -2.124998 | -1.078767 |
| 20 | 1 | 0 | 3.727949 | -3.304084 | 0.343191 |
| 21 | 8 | 0 | 4.309682 | -3.064242 | 1.097955 |
| 22 | 1 | 0 | 3.913903 | -2.251324 | 1.388929 |
| 23 | 1 | 0 | 1.312373 | -2.568487 | -2.210448 |
| 24 | 8 | 0 | 0.632085 | -2.143044 | -2.803458 |
| 25 | 1 | 0 | -0.173855 | -2.705488 | -2.761394 |
| 26 | 1 | 0 | 0.109565 | -0.874167 | -1.940661 |
| 27 | 8 | 0 | -0.210573 | -0.036392 | -1.430478 |
| 28 | 1 | 0 | 0.470751 | 0.657633 | -1.384100 |
| 29 | 1 | 0 | 5.691134 | -2.451894 | 0.228626 |
| 30 | 8 | 0 | 6.357180 | -1.975578 | -0.341479 |
| 31 | 1 | 0 | 6.497649 | -2.609818 | -1.066708 |
| 32 | 1 | 0 | -3.039242 | -0.008823 | -1.052541 |
| 33 | 8 | 0 | -2.815206 | 0.019488 | -1.983876 |
| 34 | 1 | 0 | -1.832790 | 0.103786 | -1.960300 |
| 35 | 1 | 0 | -2.281365 | -1.871016 | -2.637962 |
| 36 | 8 | 0 | -2.020125 | -2.793245 | -2.738273 |
| 37 | 1 | 0 | -2.413503 | -3.154669 | -1.939234 |
| 38 | 1 | 0 | -4.747538 | -0.696026 | -2.192923 |
| 39 | 8 | 0 | -5.479214 | -1.087296 | -1.653605 |
| 40 | 1 | 0 | -5.400819 | -0.661292 | -0.783208 |
| 41 | 1 | 0 | -0.998480 | -1.167647 | 0.054654 |
| 42 | 8 | 0 | -1.175027 | -1.864633 | 0.691197 |
| 43 | 1 | 0 | -0.247486 | -2.147829 | 0.916200 |
| 44 | 1 | 0 | -4.068531 | -4.443679 | 2.165563 |
| 45 | 8 | 0 | -4.775902 | -3.791957 | 1.920986 |
| 46 | 1 | 0 | -4.475020 | -3.579291 | 0.950969 |
| 47 | 1 | 0 | -2.883988 | -2.484765 | -0.003515 |
| 48 | 8 | 0 | -3.634781 | -2.971167 | -0.386722 |
| 49 | 1 | 0 | -4.236954 | -2.286467 | -0.756061 |
| 50 | 1 | 0 | 3.641435 | -0.270137 | 0.024448 |
| 51 | 8 | 0 | 3.972294 | -0.498072 | -0.845719 |
| 52 | 1 | 0 | 4.949851 | -0.703501 | -0.755248 |
| 53 | 1 | 0 | 3.890378 | 1.131399 | -1.687917 |
| 54 | 8 | 0 | 3.778614 | 1.999372 | -2.050654 |
| 55 | 1 | 0 | 3.104196 | 1.854822 | -2.686036 |
| 56 | 1 | 0 | -3.577743 | -2.350941 | 2.442126 |
| 57 | 8 | 0 | -3.066596 | -1.514112 | 2.539212 |
| 58 | 1 | 0 | -2.252961 | -1.618986 | 1.943870 |

| 59 | 1 | 0 | -3.594694 | -0.510124 | 1.263144 |
|----|---|---|-----------|-----------|-----------|
| 60 | 8 | 0 | -4.033255 | 0.024472 | 0.527858 |
| 61 | 1 | 0 | -3.800716 | 0.961021 | 0.653188 |
| 62 | 6 | 0 | 2.108074 | 4.428121 | -0.721073 |
| 63 | 6 | 0 | 1.520000 | 4.509117 | -1.990104 |
| 64 | 1 | 0 | -1.397772 | 2.856362 | -1.356030 |
| 65 | 1 | 0 | -0.113251 | 3.985188 | -3.340080 |
| 66 | 1 | 0 | 1.833899 | 3.759543 | 1.257922 |
| 67 | 1 | 0 | 3.075326 | 4.821603 | -0.543185 |
| 68 | 1 | 0 | 2.137321 | 4.975422 | -2.711986 |
| 69 | 1 | 0 | 1.385433 | 1.240245 | 4.061821 |
| 70 | 1 | 0 | 0.531687 | 2.707257 | 4.694864 |
| 71 | 1 | 0 | 0.074879 | 1.091183 | 5.236612 |

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[6] Figure S2. The geometry of the Mulliken CT complex composed of benzoic acid, ethylamine and $(H_2O)_5$.

Stoichiometry    C9H23NO7

(6-1) B3LYP/6-31(+)G(d) SCRF=(PCM, solvent=water)

Standard orientation:

---------------------------------------------------------------------

| Center | Atomic | Atomic |        | Coordinates (Angstroms) |        |
|--------|--------|--------|--------|--------|--------|
| Number | Number | Type   | X      | Y      | Z      |

---------------------------------------------------------------------

| 1  | 6 | 0 | 1.378914  | 0.023134  | -0.547205 |
| 2  | 6 | 0 | -0.145270 | -0.023195 | -0.400133 |
| 3  | 8 | 0 | -0.787734 | 1.100493  | -0.555506 |
| 4  | 7 | 0 | -0.439871 | -0.573994 | 1.147628  |
| 5  | 6 | 0 | 0.080117  | 0.269889  | 2.272742  |
| 6  | 6 | 0 | 2.045308  | 1.251447  | -0.474904 |
| 7  | 6 | 0 | 3.435485  | 1.312912  | -0.597999 |
| 8  | 6 | 0 | 4.175513  | 0.146236  | -0.797221 |
| 9  | 1 | 0 | -1.473870 | -0.616798 | 1.216332  |
| 10 | 6 | 0 | 1.351675  | -0.291678 | 2.898318  |
| 11 | 1 | 0 | 0.236945  | 1.273218  | 1.869617  |
| 12 | 1 | 0 | -0.715836 | 0.336486  | 3.018729  |
| 13 | 8 | 0 | -0.643004 | -1.120753 | -1.164171 |
| 14 | 1 | 0 | -1.514256 | -0.880986 | -1.571619 |
| 15 | 1 | 0 | -0.114161 | -1.545282 | 1.225145  |
| 16 | 6 | 0 | 2.128244  | -1.144734 | -0.752334 |
| 17 | 6 | 0 | 3.516920  | -1.083710 | -0.875761 |
| 18 | 1 | 0 | 1.474530  | 2.161402  | -0.328416 |
| 19 | 1 | 0 | 3.937852  | 2.274701  | -0.541068 |
| 20 | 1 | 0 | 5.256616  | 0.194044  | -0.894080 |
| 21 | 1 | 0 | 1.628406  | -2.104661 | -0.825676 |
| 22 | 1 | 0 | 4.082944  | -1.996822 | -1.037927 |
| 23 | 1 | 0 | 1.176803  | -1.286889 | 3.323072  |
| 24 | 1 | 0 | 2.165715  | -0.360204 | 2.171661  |
| 25 | 1 | 0 | 1.674517  | 0.366978  | 3.710757  |
| 26 | 8 | 0 | -0.639103 | -3.472836 | 0.355528  |
| 27 | 1 | 0 | -0.693621 | -2.839077 | -0.392720 |
| 28 | 1 | 0 | -0.109820 | -4.220585 | 0.036973  |
| 29 | 8 | 0 | -3.317812 | -0.469181 | 1.641665  |
| 30 | 1 | 0 | -3.586124 | 0.140010  | 0.913339  |
| 31 | 1 | 0 | -3.813604 | -1.290534 | 1.496896  |
| 32 | 8 | 0 | -3.113129 | -0.755855 | -2.397756 |
| 33 | 1 | 0 | -3.019803 | -0.467445 | -3.319746 |
| 34 | 1 | 0 | -3.466816 | 0.021561  | -1.905037 |
| 35 | 1 | 0 | -2.433125 | 1.258785  | -0.531835 |
| 36 | 8 | 0 | -3.440495 | 1.210291  | -0.536000 |
| 37 | 1 | 0 | -3.778883 | 2.119564  | -0.548447 |
| 38 | 1 | 0 | -0.615256 | 2.777225  | -0.008805 |

| 39 | 8 | 0 | -0.624720 | 3.720150 | 0.288050 |
|---|---|---|---|---|---|
| 40 | 1 | 0 | -0.493506 | 4.242986 | -0.518044 |

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(6-2) B3PW91/ 6-311+G(d,p) SCRF=(PCM, solvent=water)

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| | | | X | Y | Z |

---

| 1 | 6 | 0 | -1.338509 | 0.306952 | 0.190768 |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 0.183042 | 0.158319 | 0.113469 |
| 3 | 8 | 0 | 0.784193 | 1.018905 | -0.657224 |
| 4 | 7 | 0 | 0.474155 | -1.334316 | -0.465400 |
| 5 | 6 | 0 | -0.084800 | -1.656097 | -1.809858 |
| 6 | 6 | 0 | -2.000907 | 0.989736 | -0.829173 |
| 7 | 6 | 0 | -3.384981 | 1.140032 | -0.798325 |
| 8 | 6 | 0 | -4.121122 | 0.609987 | 0.257722 |
| 9 | 1 | 0 | 1.507998 | -1.403054 | -0.517435 |
| 10 | 6 | 0 | -1.338660 | -2.507845 | -1.740585 |
| 11 | 1 | 0 | -0.264616 | -0.704249 | -2.312586 |
| 12 | 1 | 0 | 0.698456 | -2.174652 | -2.365584 |
| 13 | 8 | 0 | 0.697632 | 0.046286 | 1.431667 |
| 14 | 1 | 0 | 1.566339 | 0.509760 | 1.480366 |
| 15 | 1 | 0 | 0.184038 | -2.022740 | 0.238246 |
| 16 | 6 | 0 | -2.081588 | -0.218367 | 1.249885 |
| 17 | 6 | 0 | -3.464937 | -0.067080 | 1.283369 |
| 18 | 1 | 0 | -1.419957 | 1.409998 | -1.642249 |
| 19 | 1 | 0 | -3.887355 | 1.674795 | -1.597983 |
| 20 | 1 | 0 | -5.199488 | 0.728127 | 0.285319 |
| 21 | 1 | 0 | -1.580689 | -0.736316 | 2.058857 |
| 22 | 1 | 0 | -4.030688 | -0.475016 | 2.114792 |
| 23 | 1 | 0 | -1.135127 | -3.469867 | -1.261576 |
| 24 | 1 | 0 | -2.138949 | -2.006726 | -1.192693 |
| 25 | 1 | 0 | -1.695168 | -2.708484 | -2.753563 |
| 26 | 8 | 0 | 0.635159 | -2.639725 | 2.200611 |
| 27 | 1 | 0 | 0.711661 | -1.670230 | 2.251357 |
| 28 | 1 | 0 | 0.064927 | -2.896984 | 2.930625 |
| 29 | 8 | 0 | 3.296670 | -1.625392 | -0.973289 |
| 30 | 1 | 0 | 3.555047 | -0.681992 | -1.031224 |
| 31 | 1 | 0 | 3.862874 | -2.011523 | -0.298444 |
| 32 | 8 | 0 | 3.179348 | 1.209358 | 1.766342 |
| 33 | 1 | 0 | 3.171878 | 2.085538 | 2.163430 |
| 34 | 1 | 0 | 3.473627 | 1.339285 | 0.841859 |
| 35 | 1 | 0 | 2.358614 | 1.104036 | -0.921567 |
| 36 | 8 | 0 | 3.365910 | 1.098059 | -0.952616 |

| 37 | 1 | 0 | 3.644562 | 1.718944 | -1.631720 |
| 38 | 1 | 0 | 0.491739 | 2.735312 | -0.442923 |
| 39 | 8 | 0 | 0.423128 | 3.713549 | -0.351394 |
| 40 | 1 | 0 | -0.520355 | 3.894112 | -0.353902 |

------------------------------------------------------------------

[7] The Na$^+$-containing ester hydrolysis shown in Figure S3.

(7-1) Reactant-like complex (precursor) composed of
     ethyl benzoate and NaOH(H2O)16
zuka02aana.rev.chk    Stoichiometry    C9H43NaO19
                 Standard orientation:

---------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.388983 | 1.084531 | -0.238450 |
| 2 | 6 | 0 | -2.311023 | 0.885381 | 0.765159 |
| 3 | 8 | 0 | -1.851612 | -0.221371 | 1.075184 |
| 4 | 8 | 0 | -1.892283 | 2.025436 | 1.294757 |
| 5 | 6 | 0 | -0.750531 | 2.022834 | 2.198127 |
| 6 | 6 | 0 | -3.490066 | 2.300178 | -0.935378 |
| 7 | 6 | 0 | -4.286689 | 0.038594 | -0.507493 |
| 8 | 6 | 0 | -5.282757 | 0.206205 | -1.466944 |
| 9 | 6 | 0 | -0.630785 | 3.423268 | 2.764910 |
| 10 | 1 | 0 | -0.922276 | 1.271010 | 2.974200 |
| 11 | 1 | 0 | 0.132814 | 1.745474 | 1.615759 |
| 12 | 8 | 0 | 1.894450 | 0.641843 | -1.302515 |
| 13 | 1 | 0 | 2.652481 | 0.617919 | -1.923905 |
| 14 | 1 | 0 | 2.261343 | 0.465369 | -0.356275 |
| 15 | 8 | 0 | 2.717642 | 0.205981 | 1.118014 |
| 16 | 1 | 0 | 2.735848 | 1.085475 | 1.536479 |
| 17 | 1 | 0 | 4.136370 | -0.155804 | 0.923675 |
| 18 | 8 | 0 | 5.155663 | -0.301630 | 0.690940 |
| 19 | 1 | 0 | 5.555201 | -0.773370 | 1.437455 |
| 20 | 1 | 0 | 5.622590 | 1.376874 | 0.639269 |
| 21 | 8 | 0 | 5.711780 | 2.367914 | 0.649429 |
| 22 | 1 | 0 | 6.012940 | 2.620669 | -0.235738 |
| 23 | 1 | 0 | 5.220295 | -1.250663 | -0.855889 |
| 24 | 8 | 0 | 5.164896 | -1.736680 | -1.713131 |
| 25 | 1 | 0 | 4.617928 | -2.531860 | -1.532928 |
| 26 | 1 | 0 | 4.227152 | -0.874556 | -2.810240 |
| 27 | 8 | 0 | 3.545948 | -0.381622 | -3.359519 |
| 28 | 1 | 0 | 4.018766 | -0.020852 | -4.124023 |
| 29 | 1 | 0 | 4.149565 | 2.967704 | 1.142789 |
| 30 | 8 | 0 | 3.231127 | 3.183582 | 1.456394 |
| 31 | 1 | 0 | 3.333079 | 3.883093 | 2.118603 |
| 32 | 1 | 0 | 1.305247 | -0.787126 | -1.902009 |
| 33 | 8 | 0 | 1.094471 | -1.636323 | -2.405239 |
| 34 | 1 | 0 | 1.638389 | -1.524606 | -3.209234 |
| 35 | 1 | 0 | 2.429778 | -3.020543 | -1.830332 |
| 36 | 8 | 0 | 3.109382 | -3.652396 | -1.521197 |

| 37 | 1 | 0 | 2.704866 | -4.083840 | -0.751471 |
|----|---|---|----------|-----------|-----------|
| 38 | 1 | 0 | -0.747735 | -1.596664 | -2.440227 |
| 39 | 8 | 0 | -1.686111 | -1.664373 | -2.146513 |
| 40 | 1 | 0 | -2.137682 | -0.876517 | -2.483578 |
| 41 | 1 | 0 | 0.017849 | -0.744587 | 1.779461 |
| 42 | 8 | 0 | 0.823049 | -1.274294 | 1.933697 |
| 43 | 1 | 0 | 1.632187 | -0.659962 | 1.674424 |
| 44 | 1 | 0 | 0.462388 | -2.397574 | 3.200096 |
| 45 | 8 | 0 | 0.007611 | -3.079032 | 3.764885 |
| 46 | 1 | 0 | 0.610833 | -3.833971 | 3.827595 |
| 47 | 1 | 0 | 0.646923 | -2.487220 | 0.680153 |
| 48 | 8 | 0 | 0.290957 | -3.109437 | -0.007775 |
| 49 | 1 | 0 | 0.594249 | -2.751007 | -0.861667 |
| 50 | 1 | 0 | 1.490867 | 2.425855 | -1.056097 |
| 51 | 8 | 0 | 1.426309 | 3.363237 | -0.762349 |
| 52 | 1 | 0 | 2.031011 | 3.423942 | 0.007184 |
| 53 | 1 | 0 | -0.164626 | 4.134656 | -0.754499 |
| 54 | 8 | 0 | -1.040330 | 4.596148 | -0.769166 |
| 55 | 1 | 0 | -0.909698 | 5.353431 | -1.357957 |
| 56 | 1 | 0 | -1.492751 | -3.285656 | 2.935292 |
| 57 | 8 | 0 | -2.352253 | -3.174738 | 2.444087 |
| 58 | 1 | 0 | -2.853914 | -2.539089 | 2.976786 |
| 59 | 1 | 0 | -3.449711 | -4.032890 | 1.138784 |
| 60 | 8 | 0 | -3.742020 | -3.804454 | 0.232035 |
| 61 | 1 | 0 | -3.972780 | -4.628959 | -0.218871 |
| 62 | 11 | 0 | -1.905854 | -2.370958 | 0.061921 |
| 63 | 6 | 0 | -4.482974 | 2.450465 | -1.903970 |
| 64 | 6 | 0 | -5.378314 | 1.411853 | -2.168867 |
| 65 | 1 | 0 | -2.780829 | 3.101757 | -0.743116 |
| 66 | 1 | 0 | -4.225267 | -0.892731 | 0.048120 |
| 67 | 1 | 0 | -5.983564 | -0.600090 | -1.663333 |
| 68 | 1 | 0 | -4.553886 | 3.384508 | -2.453841 |
| 69 | 1 | 0 | -6.152222 | 1.539701 | -2.921085 |
| 70 | 1 | 0 | -0.524323 | 4.153528 | 1.957870 |
| 71 | 1 | 0 | -1.512827 | 3.683008 | 3.359218 |
| 72 | 1 | 0 | 0.250861 | 3.474529 | 3.413269 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.70791006    A.U. after   1 cycles

Convg  =    0.2288D-08         -V/T =  2.0090

S**2  =  0.0000

Zero-point correction=                        0.590376 (a.u.)

Thermal correction to Energy=                  0.645867

Thermal correction to Enthalpy=                0.646812

Thermal correction to Gibbs Free Energy=       0.493684

Sum of electronic and zero-point Energies=        -1960.117534

Sum of electronic and thermal Energies=           -1960.062043

Sum of electronic and thermal Enthalpies=      -1960.061098
Sum of electronic and thermal Free Energies=      -1960.214226


(7-2) TS1(es), OH- nucleophilic addition
  zuka02aana.chk   Stoichiometry C9H43NaO19
                Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic         Coordinates (Angstroms)
Number   Number    Type        X        Y        Z
-----------------------------------------------------------------------
    1       6        0      0.307003   2.434064  -0.649981
    2       6        0     -0.039039   1.416979   0.399734
    3       8        0     -1.111310   0.726106   0.327400
    4       8        0      0.465870   1.770505   1.597975
    5       6        0      0.190790   0.947973   2.746176
    6       6        0      1.450880   3.236588  -0.525369
    7       6        0     -0.533882   2.604280  -1.757718
    8       6        0     -0.238067   3.560779  -2.730258
    9       6        0      0.813526   1.628865   3.951502
   10       1        0     -0.893538   0.837768   2.860261
   11       1        0      0.623702  -0.042796   2.578692
   12       8        0      1.364728   0.042574  -0.066948
   13       1        0      1.459602  -0.001125  -1.037381
   14       1        0      1.352780  -1.422791   0.529554
   15       8        0      1.335465  -2.344875   0.986139
   16       1        0      1.951336  -2.266667   1.749352
   17       1        0      2.211709  -3.342379  -0.088741
   18       8        0      2.850575  -3.783706  -0.719985
   19       1        0      2.878676  -4.721486  -0.476102
   20       1        0      4.376333  -2.764187  -0.091233
   21       8        0      4.940931  -2.218541   0.496471
   22       1        0      4.707135  -1.281697   0.307410
   23       1        0      2.029979  -3.539780  -2.358036
   24       8        0      1.493255  -3.308313  -3.148191
   25       1        0      0.579394  -3.608661  -2.944265
   26       1        0      1.439290  -1.637557  -3.219106
   27       8        0      1.271327  -0.648180  -3.152109
   28       1        0      1.668727  -0.234600  -3.932385
   29       1        0      4.159936  -2.202203   2.028810
   30       8        0      3.504399  -1.961756   2.745050
   31       1        0      3.800435  -2.381609   3.565841
   32       1        0     -0.962030  -0.332835  -1.257498
   33       8        0     -1.203846  -0.711448  -2.132589
   34       1        0     -0.396857  -0.572487  -2.695143
   35       1        0     -1.272146  -2.562024  -2.286126
   36       8        0     -1.236488  -3.523409  -2.479851

| 37 | 1 | 0 | -1.881299 | -3.910900 | -1.861914 |
| 38 | 1 | 0 | -2.890572 | -0.482181 | -2.079582 |
| 39 | 8 | 0 | -3.755887 | -0.393960 | -1.594094 |
| 40 | 1 | 0 | -4.455372 | -0.296553 | -2.257172 |
| 41 | 1 | 0 | -1.191842 | -0.959464 | 1.090397 |
| 42 | 8 | 0 | -1.315889 | -1.897152 | 1.366054 |
| 43 | 1 | 0 | -0.394586 | -2.265387 | 1.338513 |
| 44 | 1 | 0 | -2.887247 | -2.205785 | 2.374631 |
| 45 | 8 | 0 | -3.868369 | -2.258479 | 2.423286 |
| 46 | 1 | 0 | -4.082209 | -2.729958 | 1.590193 |
| 47 | 1 | 0 | -2.464321 | -2.690492 | 0.167151 |
| 48 | 8 | 0 | -3.274739 | -3.038129 | -0.274740 |
| 49 | 1 | 0 | -3.605156 | -2.284894 | -0.800448 |
| 50 | 1 | 0 | 2.899772 | 0.325278 | 0.483661 |
| 51 | 8 | 0 | 3.832964 | 0.362917 | 0.875358 |
| 52 | 1 | 0 | 3.728315 | 0.020834 | 1.781537 |
| 53 | 1 | 0 | 4.339507 | 2.103914 | 0.943801 |
| 54 | 8 | 0 | 4.546532 | 3.067550 | 0.971050 |
| 55 | 1 | 0 | 5.464678 | 3.140876 | 0.673329 |
| 56 | 1 | 0 | -4.321219 | -0.663536 | 2.339607 |
| 57 | 8 | 0 | -4.420716 | 0.334917 | 2.241025 |
| 58 | 1 | 0 | -4.230066 | 0.696234 | 3.120000 |
| 59 | 1 | 0 | -5.587926 | 1.577745 | 1.195836 |
| 60 | 8 | 0 | -5.340789 | 2.122154 | 0.422273 |
| 61 | 1 | 0 | -6.095212 | 2.682442 | 0.192184 |
| 62 | 11 | 0 | -3.341114 | 0.999930 | 0.229325 |
| 63 | 6 | 0 | 1.743256 | 4.189217 | -1.499166 |
| 64 | 6 | 0 | 0.901875 | 4.355883 | -2.602297 |
| 65 | 1 | 0 | 2.120224 | 3.112790 | 0.317296 |
| 66 | 1 | 0 | -1.413730 | 1.978947 | -1.868271 |
| 67 | 1 | 0 | -0.897065 | 3.681710 | -3.586146 |
| 68 | 1 | 0 | 2.637084 | 4.796284 | -1.390464 |
| 69 | 1 | 0 | 1.134562 | 5.100015 | -3.359589 |
| 70 | 1 | 0 | 1.893080 | 1.746093 | 3.816955 |
| 71 | 1 | 0 | 0.378470 | 2.621146 | 4.109119 |
| 72 | 1 | 0 | 0.637763 | 1.024755 | 4.848561 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.67759746     A.U. after   1 cycles
         Convg  =    0.3766D-08            -V/T =  2.0090
         S**2   =   0.0000
Zero-point correction=                      0.594015 (a.u.)
Thermal correction to Energy=               0.647392
Thermal correction to Enthalpy=             0.648336
Thermal correction to Gibbs Free Energy=    0.503230
Sum of electronic and zero-point Energies=       -1960.083582
Sum of electronic and thermal Energies=          -1960.030206

Sum of electronic and thermal Enthalpies=      -1960.029262
Sum of electronic and thermal Free Energies=      -1960.174368


(7-3) The OH- adduct, Int1(es)( anionic tetrahedral intermediate )
    Ph-C(-O-)(OH)-OEt + Na+ +  (H2O)16
zuka02bbbna.rev.chk    Stoichiometry  C9H43NaO19
                Standard orientation:

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| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|------|------|------|
| Number | Number | Type | X | Y | Z |

---

| 1 | 6 | 0 | -0.939830 | 2.605122 | -0.499605 |
| 2 | 6 | 0 | -1.493055 | 1.172981 | -0.608753 |
| 3 | 8 | 0 | -1.272958 | 0.463764 | 0.526088 |
| 4 | 8 | 0 | -0.794882 | 0.427194 | -1.681365 |
| 5 | 6 | 0 | -1.021186 | 0.895391 | -3.033739 |
| 6 | 6 | 0 | -1.748580 | 3.604562 | 0.058031 |
| 7 | 6 | 0 | 0.384281 | 2.919901 | -0.830617 |
| 8 | 6 | 0 | 0.894123 | 4.199960 | -0.600066 |
| 9 | 6 | 0 | -0.053883 | 0.182859 | -3.964982 |
| 10 | 1 | 0 | -2.061355 | 0.689763 | -3.304049 |
| 11 | 1 | 0 | -0.869663 | 1.979919 | -3.067645 |
| 12 | 8 | 0 | -2.852544 | 1.261293 | -0.947596 |
| 13 | 1 | 0 | -3.343232 | 0.508789 | -0.553115 |
| 14 | 1 | 0 | -4.872912 | -3.430731 | -1.276191 |
| 15 | 8 | 0 | -4.732802 | -2.514010 | -1.554578 |
| 16 | 1 | 0 | -3.762347 | -2.433469 | -1.766643 |
| 17 | 1 | 0 | 0.922775 | -0.126772 | -1.155684 |
| 18 | 8 | 0 | 2.676310 | 1.029841 | 1.486470 |
| 19 | 1 | 0 | 1.824663 | 1.347740 | 1.875396 |
| 20 | 1 | 0 | 2.887379 | 0.232203 | 2.014796 |
| 21 | 8 | 0 | 2.507348 | -1.535128 | 2.793493 |
| 22 | 1 | 0 | 3.157680 | -1.883959 | 3.422000 |
| 23 | 1 | 0 | -4.909224 | -1.286519 | -0.391838 |
| 24 | 8 | 0 | -4.849650 | -0.493422 | 0.210116 |
| 25 | 1 | 0 | -5.615682 | 0.062279 | 0.001041 |
| 26 | 1 | 0 | -2.552232 | 0.289945 | 1.749155 |
| 27 | 8 | 0 | -3.204957 | 0.004744 | 2.439971 |
| 28 | 1 | 0 | -3.966154 | -0.302217 | 1.906129 |
| 29 | 1 | 0 | 2.690517 | -2.003081 | 1.917151 |
| 30 | 8 | 0 | 2.880282 | -2.538894 | 0.359649 |
| 31 | 1 | 0 | 3.826475 | -2.522328 | 0.052095 |
| 32 | 1 | 0 | 5.378856 | 2.619285 | 0.420472 |
| 33 | 8 | 0 | 4.581850 | 2.348101 | -0.057485 |
| 34 | 1 | 0 | 3.956146 | 1.996602 | 0.615917 |
| 35 | 1 | 0 | -0.957159 | -1.175078 | 0.726215 |

| 36 | 8 | 0 | -0.745815 | -2.027212 | 1.218041 |
|----|---|---|-----------|-----------|-----------|
| 37 | 1 | 0 | -1.614661 | -2.427100 | 1.380485 |
| 38 | 1 | 0 | 5.825087 | -2.664788 | -1.208474 |
| 39 | 8 | 0 | 5.393963 | -2.075362 | -0.572158 |
| 40 | 1 | 0 | 5.179014 | -1.236233 | -1.070529 |
| 41 | 1 | 0 | 1.573641 | -3.869709 | 0.068755 |
| 42 | 8 | 0 | 0.649709 | -4.185529 | -0.022179 |
| 43 | 1 | 0 | 0.124080 | -3.450350 | 0.363941 |
| 44 | 1 | 0 | -1.625558 | -1.324940 | -1.788027 |
| 45 | 8 | 0 | -2.083952 | -2.187755 | -1.861477 |
| 46 | 1 | 0 | -1.431650 | -2.841401 | -2.211608 |
| 47 | 1 | 0 | -0.457362 | -4.916626 | -2.933193 |
| 48 | 8 | 0 | -0.190627 | -4.051905 | -2.589330 |
| 49 | 1 | 0 | 0.181727 | -4.209129 | -1.678966 |
| 50 | 1 | 0 | -0.236603 | 1.889657 | 3.004690 |
| 51 | 8 | 0 | 0.170765 | 1.158183 | 2.516752 |
| 52 | 1 | 0 | -0.400361 | 1.028908 | 1.667945 |
| 53 | 1 | 0 | -2.098757 | -1.299918 | 5.135041 |
| 54 | 8 | 0 | -1.735837 | -1.332600 | 4.239125 |
| 55 | 1 | 0 | -2.398646 | -0.875947 | 3.644121 |
| 56 | 1 | 0 | 4.672354 | 0.967129 | -1.303807 |
| 57 | 8 | 0 | 4.506713 | 0.148645 | -1.824371 |
| 58 | 1 | 0 | 3.536789 | 0.019669 | -1.766585 |
| 59 | 1 | 0 | 2.434046 | -1.837945 | -0.182216 |
| 60 | 8 | 0 | 1.848894 | -0.305621 | -0.866324 |
| 61 | 1 | 0 | 2.015440 | 0.268775 | -0.084034 |
| 62 | 11 | 0 | 0.222065 | -1.112551 | 3.110585 |
| 63 | 6 | 0 | -1.239777 | 4.883045 | 0.292252 |
| 64 | 6 | 0 | 0.084322 | 5.185185 | -0.032984 |
| 65 | 1 | 0 | -2.780381 | 3.371456 | 0.298288 |
| 66 | 1 | 0 | 1.024894 | 2.170963 | -1.283624 |
| 67 | 1 | 0 | 1.924102 | 4.420084 | -0.867825 |
| 68 | 1 | 0 | -1.882946 | 5.646487 | 0.723023 |
| 69 | 1 | 0 | 0.479200 | 6.181788 | 0.146401 |
| 70 | 1 | 0 | -0.181111 | -0.904099 | -3.918771 |
| 71 | 1 | 0 | -0.239546 | 0.500678 | -4.997227 |
| 72 | 1 | 0 | 0.987006 | 0.419632 | -3.719404 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.70487010     A.U. after    1 cycles

      Convg  =    0.1911D-08          -V/T =  2.0090

      S**2  =   0.0000

Zero-point correction=                      0.596904 (a.u.)

Thermal correction to Energy=                0.648209

Thermal correction to Enthalpy=              0.649154

Thermal correction to Gibbs Free Energy=        0.510905

Sum of electronic and zero-point Energies=        -1960.107966

Sum of electronic and thermal Energies=        -1960.056661
Sum of electronic and thermal Enthalpies=       -1960.055717
Sum of electronic and thermal Free Energies=    -1960.193966

(7-4)  TS2(es), formation of EtOH, PhCOOH +  NaOH(H2O)15
zuka02bbbna.chk    Stoichiometry   C9H43NaO19
                  Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type        X        Y        Z
-----------------------------------------------------------------------
  1        6        0      0.264441   2.916402  -0.232370
  2        6        0      1.257926   1.797084  -0.243932
  3        8        0      1.159125   0.825579  -1.073173
  4        8        0      0.635771   0.830893   1.431269
  5        6        0      0.526279   1.645891   2.587959
  6        6        0      0.589225   4.159294   0.329195
  7        6        0     -1.000322   2.740334  -0.807394
  8        6        0     -1.932016   3.776178  -0.812193
  9        6        0      0.046353   0.856105   3.808637
 10        1        0      1.503749   2.105209   2.808844
 11        1        0     -0.180909   2.468332   2.401239
 12        8        0      2.479006   2.185882   0.162073
 13        1        0      3.165742   1.511820  -0.064035
 14        1        0      5.482759  -1.570803   1.725637
 15        8        0      5.076656  -0.691776   1.743120
 16        1        0      4.105769  -0.837641   1.931041
 17        1        0     -0.817335   0.172993   1.074750
 18        8        0     -2.692156  -0.401145  -1.982327
 19        1        0     -1.950520  -0.168428  -2.582546
 20        1        0     -2.680122  -1.380400  -1.978241
 21        8        0     -1.820411  -3.147246  -1.840365
 22        1        0     -2.309793  -3.896902  -2.212250
 23        1        0      4.986019   0.144147   0.289754
 24        8        0      4.759444   0.692146  -0.516380
 25        1        0      5.420904   1.399863  -0.557453
 26        1        0      2.520684   0.293141  -2.204987
 27        8        0      3.237797  -0.079116  -2.767764
 28        1        0      4.012895  -0.017598  -2.173387
 29        1        0     -2.031436  -3.144281  -0.850013
 30        8        0     -2.303888  -2.880519   0.747938
 31        1        0     -3.260141  -2.888675   1.021968
 32        1        0     -5.693636   0.942603  -1.624331
 33        8        0     -4.860014   1.154656  -1.179600
 34        1        0     -4.169902   0.595600  -1.602791
 35        1        0      1.063858  -0.892108  -0.472574

| 36 | 8 | 0 | 1.236812 | -1.859165 | -0.366078 |
| 37 | 1 | 0 | 1.866000 | -1.827916 | 0.398432 |
| 38 | 1 | 0 | -5.286512 | -2.761571 | 2.236269 |
| 39 | 8 | 0 | -4.917775 | -2.472563 | 1.388530 |
| 40 | 1 | 0 | -4.853511 | -1.474935 | 1.439483 |
| 41 | 1 | 0 | -0.833811 | -3.802958 | 1.364416 |
| 42 | 8 | 0 | 0.129664 | -3.998296 | 1.381131 |
| 43 | 1 | 0 | 0.487027 | -3.342186 | 0.750956 |
| 44 | 1 | 0 | 1.772745 | -0.327180 | 1.820711 |
| 45 | 8 | 0 | 2.432104 | -1.092440 | 1.936770 |
| 46 | 1 | 0 | 2.083560 | -1.676339 | 2.653869 |
| 47 | 1 | 0 | 1.841405 | -3.659512 | 4.097692 |
| 48 | 8 | 0 | 1.330838 | -2.993786 | 3.614923 |
| 49 | 1 | 0 | 0.840544 | -3.474665 | 2.897372 |
| 50 | 1 | 0 | 0.209302 | 0.043461 | -3.934952 |
| 51 | 8 | 0 | -0.185653 | -0.218469 | -3.088714 |
| 52 | 1 | 0 | 0.242186 | 0.353543 | -2.388821 |
| 53 | 1 | 0 | 2.767422 | -2.907516 | -4.255614 |
| 54 | 8 | 0 | 2.158542 | -2.359524 | -3.741568 |
| 55 | 1 | 0 | 2.683989 | -1.576840 | -3.409965 |
| 56 | 1 | 0 | -4.714001 | 0.616143 | 0.617708 |
| 57 | 8 | 0 | -4.452106 | 0.181811 | 1.459790 |
| 58 | 1 | 0 | -3.469115 | 0.197192 | 1.448271 |
| 59 | 1 | 0 | -2.011540 | -1.935291 | 0.890467 |
| 60 | 8 | 0 | -1.719650 | -0.243227 | 0.840172 |
| 61 | 1 | 0 | -1.884701 | -0.067001 | -0.106162 |
| 62 | 11 | 0 | 0.363636 | -2.451241 | -2.361502 |
| 63 | 6 | 0 | -0.339724 | 5.199915 | 0.316461 |
| 64 | 6 | 0 | -1.601747 | 5.011304 | -0.249161 |
| 65 | 1 | 0 | 1.569363 | 4.304924 | 0.768095 |
| 66 | 1 | 0 | -1.259096 | 1.786044 | -1.249338 |
| 67 | 1 | 0 | -2.913527 | 3.612502 | -1.248004 |
| 68 | 1 | 0 | -0.076053 | 6.159609 | 0.752821 |
| 69 | 1 | 0 | -2.326092 | 5.821373 | -0.250511 |
| 70 | 1 | 0 | -0.935428 | 0.406276 | 3.622159 |
| 71 | 1 | 0 | 0.741682 | 0.052042 | 4.073875 |
| 72 | 1 | 0 | -0.045775 | 1.522974 | 4.675485 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.69501668     A.U. after    1 cycles

     Convg  =    0.2003D-08          -V/T =  2.0090

     S**2  =   0.0000

Zero-point correction=                           0.595022 (a.u.)

Thermal correction to Energy=                    0.646997

Thermal correction to Enthalpy=                  0.647941

Thermal correction to Gibbs Free Energy=         0.507690

Sum of electronic and zero-point Energies=           -1960.099995

Sum of electronic and thermal Energies=          -1960.048019
Sum of electronic and thermal Enthalpies=        -1960.047075
Sum of electronic and thermal Free Energies=      -1960.187326


 (7-5)  Ph-COOH + EtOH +  NaOH(H2O)15  Int2(es)
 zuka02bbbna.for.chk   Stoichiometry C9H43NaO19
                 Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic          Coordinates (Angstroms)
Number   Number    Type       X         Y         Z
-----------------------------------------------------------------------
   1        6        0      -0.854018   2.991336  -0.585219
   2        6        0      -2.030787   2.312112  -0.003303
   3        8        0      -2.091434   1.929194   1.178325
   4        8        0      -0.033532  -0.328770  -2.745544
   5        6        0       0.745953  -0.419190  -3.941071
   6        6        0      -0.805551   3.290197  -1.956456
   7        6        0       0.245747   3.297046   0.233326
   8        6        0       1.386759   3.878497  -0.312404
   9        6        0       1.604723  -1.679355  -4.000044
  10        1        0       0.030323  -0.401059  -4.770692
  11        1        0       1.376461   0.476789  -4.029809
  12        8        0      -3.035321   2.131844  -0.848206
  13        1        0      -3.745550   1.534300  -0.475447
  14        1        0      -4.961317  -2.460160  -1.719194
  15        8        0      -4.539827  -1.603578  -1.882161
  16        1        0      -3.561506  -1.793544  -1.978529
  17        1        0       0.574809  -0.278849  -1.944496
  18        8        0       2.436430   0.984222   3.297074
  19        1        0       1.488677   1.222526   3.286624
  20        1        0       2.422123   0.004945   3.244550
  21        8        0       1.813071  -1.809457   3.081044
  22        1        0       2.196096  -2.395305   3.751272
  23        1        0      -4.851505  -0.385158  -0.801194
  24        8        0      -5.007699   0.381915  -0.169563
  25        1        0      -5.870498   0.754324  -0.409497
  26        1        0      -3.388605   0.933521   2.087491
  27        8        0      -4.013876   0.295415   2.493538
  28        1        0      -4.576034   0.047871   1.732884
  29        1        0       2.244581  -2.071681   2.198170
  30        8        0       2.739698  -2.326412   0.684084
  31        1        0       3.709304  -2.215542   0.514757
  32        1        0       4.814537   2.452636   1.785608
  33        8        0       3.943721   2.296703   1.390787
  34        1        0       3.423464   1.813563   2.082233
  35        1        0       0.162251  -1.158793   0.081002

| 36 | 8 | 0 | -0.596834 | -1.699517 | 0.507724 |
| 37 | 1 | 0 | -1.249021 | -1.813023 | -0.221526 |
| 38 | 1 | 0 | 5.792861 | -2.055912 | -0.669067 |
| 39 | 8 | 0 | 5.314287 | -1.598409 | 0.037491 |
| 40 | 1 | 0 | 4.968839 | -0.748790 | -0.361962 |
| 41 | 1 | 0 | 1.592838 | -3.828632 | 0.181441 |
| 42 | 8 | 0 | 0.676032 | -4.175354 | 0.138715 |
| 43 | 1 | 0 | 0.151790 | -3.371850 | 0.367815 |
| 44 | 1 | 0 | -1.266415 | -1.445652 | -2.365801 |
| 45 | 8 | 0 | -1.903051 | -2.090657 | -1.940235 |
| 46 | 1 | 0 | -1.539055 | -2.989037 | -2.140117 |
| 47 | 1 | 0 | -0.949770 | -5.386981 | -2.307042 |
| 48 | 8 | 0 | -0.575862 | -4.496364 | -2.244569 |
| 49 | 1 | 0 | -0.016392 | -4.483617 | -1.419515 |
| 50 | 1 | 0 | -0.934611 | 1.171466 | 3.954845 |
| 51 | 8 | 0 | -0.433695 | 0.992782 | 3.143173 |
| 52 | 1 | 0 | -0.940475 | 1.432094 | 2.416956 |
| 53 | 1 | 0 | -2.912554 | -2.058034 | 4.394003 |
| 54 | 8 | 0 | -2.421859 | -1.446301 | 3.827647 |
| 55 | 1 | 0 | -3.099060 | -0.884940 | 3.358917 |
| 56 | 1 | 0 | 4.051506 | 1.238247 | -0.158570 |
| 57 | 8 | 0 | 4.043918 | 0.585047 | -0.894002 |
| 58 | 1 | 0 | 3.112662 | 0.249019 | -0.919069 |
| 59 | 1 | 0 | 2.294276 | -1.556252 | 0.202008 |
| 60 | 8 | 0 | 1.406313 | -0.342454 | -0.492924 |
| 61 | 1 | 0 | 1.301202 | 0.503448 | -0.028468 |
| 62 | 11 | 0 | -0.445083 | -1.345807 | 2.700060 |
| 63 | 6 | 0 | 0.331573 | 3.886535 | -2.495505 |
| 64 | 6 | 0 | 1.427792 | 4.173588 | -1.678673 |
| 65 | 1 | 0 | -1.647318 | 3.034933 | -2.588937 |
| 66 | 1 | 0 | 0.205588 | 3.077386 | 1.294815 |
| 67 | 1 | 0 | 2.246220 | 4.075752 | 0.320012 |
| 68 | 1 | 0 | 0.368684 | 4.111896 | -3.557251 |
| 69 | 1 | 0 | 2.321195 | 4.619433 | -2.106704 |
| 70 | 1 | 0 | 2.333971 | -1.688499 | -3.182123 |
| 71 | 1 | 0 | 0.987406 | -2.580632 | -3.916646 |
| 72 | 1 | 0 | 2.156947 | -1.721714 | -4.947492 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.72805199     A.U. after    1 cycles

Convg  =    0.6559D-08           -V/T =  2.0091

S**2  =   0.0000

Zero-point correction=                       0.595573 (a.u.)

Thermal correction to Energy=                0.648765

Thermal correction to Enthalpy=              0.649710

Thermal correction to Gibbs Free Energy=       0.503345

Sum of electronic and zero-point Energies=        -1960.132479

Sum of electronic and thermal Energies=          -1960.079287
Sum of electronic and thermal Enthalpies=        -1960.078342
Sum of electronic and thermal Free Energies=     -1960.224707

(7-6) The electrolytic dissociation of Ph-COOH, TS3(es),
     the last step formation of the benzoate anion
  zukaphxnr.chk    Stoichiometry   C9H43NaO19
               Standard orientation:

---------------------------------------------------------------------
Center   Atomic   Atomic          Coordinates (Angstroms)
Number   Number   Type        X         Y         Z
---------------------------------------------------------------------
  1        6        0      -3.966833   1.204400  -0.337315
  2        6        0      -3.128389   0.276158  -1.148590
  3        8        0      -3.659693  -0.511334  -1.965825
  4        8        0       0.712398  -1.722139   2.029541
  5        6        0       1.284255  -2.242737   3.241788
  6        6        0      -5.178539   1.672897  -0.867483
  7        6        0      -5.972250   2.545033  -0.125863
  8        6        0      -5.571759   2.933098   1.156071
  9        1        0       1.193355  -1.490323   4.035969
 10        1        0       2.353349  -2.445997   3.084032
 11        6        0       0.548026  -3.514042   3.627848
 12        8        0      -1.844980   0.348396  -0.950741
 13        1        0       0.790563   1.526236  -1.457635
 14        1        0      -1.198817  -0.436070  -1.503114
 15        8        0      -0.336813  -1.195064  -2.093413
 16        1        0      -0.819893  -1.584231  -2.862457
 17        1        0      -1.123473  -1.143374   2.360783
 18        8        0      -1.977530  -0.770595   2.651136
 19        1        0      -2.659800  -1.402439   2.343316
 20        8        0       0.460353   2.014927  -0.632655
 21        1        0       1.316011   1.145833   0.679574
 22        1        0      -0.483841   1.765250  -0.566799
 23        8        0       1.347418   0.485332  -2.590009
 24        1        0       0.463177  -0.454584  -2.442779
 25        1        0       1.396917   0.797466  -3.505204
 26        1        0       0.481253  -2.444986  -1.052273
 27        8        0       0.950716  -3.050890  -0.428980
 28        1        0       0.821964  -2.657150   0.465661
 29        8        0       1.950003   0.589423   1.200152
 30        1        0       1.158408  -0.869028   1.800606
 31        1        0       2.403214   1.193629   1.839259
 32        1        0      -2.869523  -1.464471  -3.284748
 33        8        0      -2.266186  -1.944924  -3.901460
 34        1        0      -2.590971  -2.856780  -3.936525

| 35 | 8 | 0 | 3.332936 | 2.351976 | 2.803377 |
| 36 | 1 | 0 | 2.815500 | 2.893390 | 3.417854 |
| 37 | 1 | 0 | 3.725290 | 2.972608 | 2.145000 |
| 38 | 8 | 0 | 4.253881 | 3.887959 | 0.673613 |
| 39 | 1 | 0 | 3.400272 | 4.091015 | 0.196908 |
| 40 | 1 | 0 | 4.696466 | 4.739038 | 0.812000 |
| 41 | 1 | 0 | -4.857796 | -1.628458 | -1.185969 |
| 42 | 8 | 0 | -5.356830 | -2.296525 | -0.661589 |
| 43 | 1 | 0 | -6.222931 | -1.900426 | -0.484513 |
| 44 | 1 | 0 | -4.435882 | -2.566436 | 0.881547 |
| 45 | 8 | 0 | -3.928615 | -2.703946 | 1.715909 |
| 46 | 1 | 0 | -3.613073 | -3.618528 | 1.679738 |
| 47 | 1 | 0 | 2.707348 | 0.182231 | -1.769383 |
| 48 | 8 | 0 | 3.435080 | 0.049933 | -1.077702 |
| 49 | 1 | 0 | 2.973084 | 0.207585 | -0.216785 |
| 50 | 1 | 0 | 1.253075 | 3.561069 | -0.513407 |
| 51 | 8 | 0 | 1.840338 | 4.362123 | -0.470282 |
| 52 | 1 | 0 | 1.779401 | 4.778520 | -1.342688 |
| 53 | 11 | 0 | 4.751515 | -1.736215 | -0.948532 |
| 54 | 8 | 0 | 6.636007 | -0.578739 | -0.540176 |
| 55 | 1 | 0 | 7.597916 | -0.643514 | -0.465460 |
| 56 | 1 | 0 | 6.410009 | 0.392511 | -0.602031 |
| 57 | 8 | 0 | 3.505974 | -3.557284 | -0.885139 |
| 58 | 1 | 0 | 2.523302 | -3.368386 | -0.741173 |
| 59 | 1 | 0 | 3.582244 | -4.518222 | -0.964312 |
| 60 | 8 | 0 | 5.522432 | 1.826847 | -0.961152 |
| 61 | 1 | 0 | 4.677431 | 1.337732 | -1.118850 |
| 62 | 1 | 0 | 5.277289 | 2.553500 | -0.353497 |
| 63 | 6 | 0 | -3.565805 | 1.591968 | 0.949960 |
| 64 | 6 | 0 | -4.377641 | 2.448463 | 1.693902 |
| 65 | 1 | 0 | -5.477565 | 1.360849 | -1.863710 |
| 66 | 1 | 0 | -6.901647 | 2.921289 | -0.544906 |
| 67 | 1 | 0 | -6.196339 | 3.606046 | 1.738018 |
| 68 | 1 | 0 | -2.666211 | 1.168205 | 1.386717 |
| 69 | 1 | 0 | -4.079047 | 2.727261 | 2.700390 |
| 70 | 1 | 0 | -0.510690 | -3.303583 | 3.810567 |
| 71 | 1 | 0 | 0.623437 | -4.264417 | 2.832934 |
| 72 | 1 | 0 | 0.979055 | -3.936735 | 4.542467 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.71330345    A.U. after   2 cycles

      Convg  =   0.7316D-08         -V/T =  2.0090

      S**2  =  0.0000

Zero-point correction=                       0.587591 (a.u.)

Thermal correction to Energy=                0.641530

Thermal correction to Enthalpy=              0.642475

Thermal correction to Gibbs Free Energy=     0.491106

Sum of electronic and zero-point Energies=        -1960.125713
Sum of electronic and thermal Energies=           -1960.071773
Sum of electronic and thermal Enthalpies=         -1960.070829
Sum of electronic and thermal Free Energies=      -1960.222198


(7-7)  Product of Ph-COO-, EtOH, Na+ and (H2O)16, i.e.,
 after the  last step formation of the benzoate anion
 zukaphxnr.for.chk     Stoichiometry  C9H43NaO19
                Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic          Coordinates (Angstroms)
Number   Number   Type         X         Y         Z
-----------------------------------------------------------------------
   1       6        0      -3.827094   1.060530  -0.440231
   2       6        0      -3.032509  -0.006675  -1.142231
   3       8        0      -3.667233  -0.905291  -1.774267
   4       8        0       0.818185  -1.845972   1.845287
   5       6        0       1.393965  -2.218747   3.110160
   6       6        0      -5.038568   1.503655  -0.990081
   7       6        0      -5.772768   2.505019  -0.355368
   8       6        0      -5.314879   3.050969   0.846845
   9       1        0       1.203282  -1.422408   3.840613
  10       1        0       2.482573  -2.331295   2.999080
  11       6        0       0.764276  -3.522254   3.568671
  12       8        0      -1.763168   0.049983  -1.065950
  13       1        0       0.598967   1.436134  -1.743014
  14       1        0      -0.777784  -1.148457  -1.730344
  15       8        0      -0.156153  -1.729727  -2.263921
  16       1        0      -0.790605  -2.197928  -2.865725
  17       1        0      -0.990865  -1.133964   2.325539
  18       8        0      -1.685347  -0.620469   2.777104
  19       1        0      -2.519786  -1.111168   2.621939
  20       8        0       0.209193   1.783478  -0.909661
  21       1        0       1.166366   1.002401   0.380674
  22       1        0      -0.671588   1.307948  -0.850935
  23       8        0       1.365279   0.281846  -3.052643
  24       1        0       0.796129  -0.537663  -2.898384
  25       1        0       1.309661   0.494617  -3.996303
  26       1        0       0.819899  -2.803630  -1.161286
  27       8        0       1.366131  -3.275359  -0.487077
  28       1        0       1.121783  -2.866144   0.377242
  29       8        0       1.879595   0.525117   0.877813
  30       1        0       1.193310  -0.977534   1.561273
  31       1        0       2.213108   1.153720   1.568520
  32       1        0      -2.917238  -1.961840  -2.939868
  33       8        0      -2.399218  -2.545138  -3.561035

| 34 | 1 | 0 | -2.771299 | -3.433432 | -3.458531 |
|----|---|---|-----------|-----------|-----------|
| 35 | 8 | 0 | 2.864102 | 2.345595 | 2.676449 |
| 36 | 1 | 0 | 2.191196 | 2.721611 | 3.263923 |
| 37 | 1 | 0 | 3.175982 | 3.080041 | 2.098850 |
| 38 | 8 | 0 | 3.620864 | 4.133009 | 0.679069 |
| 39 | 1 | 0 | 2.744318 | 4.254688 | 0.220764 |
| 40 | 1 | 0 | 3.969678 | 5.021988 | 0.844391 |
| 41 | 1 | 0 | -4.867511 | -1.711868 | -0.758660 |
| 42 | 8 | 0 | -5.451899 | -2.153093 | -0.091111 |
| 43 | 1 | 0 | -6.223794 | -1.573694 | -0.007582 |
| 44 | 1 | 0 | -4.560804 | -2.154988 | 1.467144 |
| 45 | 8 | 0 | -4.084062 | -2.151124 | 2.333390 |
| 46 | 1 | 0 | -4.079987 | -3.071502 | 2.633029 |
| 47 | 1 | 0 | 2.844413 | 0.188550 | -2.044855 |
| 48 | 8 | 0 | 3.486943 | 0.208443 | -1.296142 |
| 49 | 1 | 0 | 2.923800 | 0.325422 | -0.482747 |
| 50 | 1 | 0 | 0.686249 | 3.416805 | -0.573836 |
| 51 | 8 | 0 | 1.121254 | 4.284173 | -0.359739 |
| 52 | 1 | 0 | 0.732827 | 4.942988 | -0.952947 |
| 53 | 11 | 0 | 4.956758 | -1.400259 | -0.750542 |
| 54 | 8 | 0 | 6.531922 | 0.029121 | -0.051781 |
| 55 | 1 | 0 | 7.424538 | 0.089187 | 0.315370 |
| 56 | 1 | 0 | 6.215897 | 0.962291 | -0.215170 |
| 57 | 8 | 0 | 3.983689 | -3.375337 | -0.773505 |
| 58 | 1 | 0 | 2.974564 | -3.346804 | -0.698288 |
| 59 | 1 | 0 | 4.219977 | -4.312846 | -0.804065 |
| 60 | 8 | 0 | 5.280166 | 2.279807 | -0.821593 |
| 61 | 1 | 0 | 4.557120 | 1.709954 | -1.169219 |
| 62 | 1 | 0 | 4.829244 | 2.953645 | -0.271432 |
| 63 | 6 | 0 | -3.369736 | 1.610352 | 0.766059 |
| 64 | 6 | 0 | -4.120722 | 2.594955 | 1.409395 |
| 65 | 1 | 0 | -5.386724 | 1.065788 | -1.921028 |
| 66 | 1 | 0 | -6.701931 | 2.857765 | -0.795869 |
| 67 | 1 | 0 | -5.892980 | 3.823518 | 1.347785 |
| 68 | 1 | 0 | -2.463269 | 1.224183 | 1.223651 |
| 69 | 1 | 0 | -3.775039 | 2.998610 | 2.357199 |
| 70 | 1 | 0 | -0.315189 | -3.398656 | 3.701120 |
| 71 | 1 | 0 | 0.937081 | -4.319031 | 2.836681 |
| 72 | 1 | 0 | 1.196351 | -3.833460 | 4.526447 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1960.72927973     A.U. after    1 cycles

$\quad\quad$ Convg  =    0.3955D-08            -V/T = 2.0090

$\quad\quad$ S**2   =   0.0000

Zero-point correction=                      0.594166 (a.u)

Thermal correction to Energy=               0.649193

Thermal correction to Enthalpy=             0.650137

Thermal correction to Gibbs Free Energy=        0.495482
Sum of electronic and zero-point Energies=       -1960.135114
Sum of electronic and thermal Energies=          -1960.080087
Sum of electronic and thermal Enthalpies=        -1960.079143
Sum of electronic and thermal Free Energies=     -1960.233798

======================================================================

[8] The Na^{+}-containing amide hydrolysis shown in Figure S4.

(8-1) Reactant-like complex (precursor) composed of
N-ethyl benzamide and NaOH(H2O)16
tuka02aana.rev.chk    Stoichiometry  C9H44NNaO18
standard orientation:

----------------------------------------------------------------------

| 1  | 6 | 0 | 2.204289  | 1.953649  | 0.663871  |
|----|---|---|-----------|-----------|-----------|
| 2  | 6 | 0 | 1.636890  | 1.521096  | -0.655192 |
| 3  | 8 | 0 | 1.973942  | 0.405934  | -1.142297 |
| 4  | 7 | 0 | 0.799702  | 2.360766  | -1.263101 |
| 5  | 6 | 0 | 0.138148  | 2.099224  | -2.544111 |
| 6  | 6 | 0 | 1.383618  | 2.446986  | 1.687239  |
| 7  | 6 | 0 | 3.582425  | 1.812315  | 0.886744  |
| 8  | 6 | 0 | 4.136364  | 2.174988  | 2.113843  |
| 9  | 1 | 0 | 0.540199  | 3.241249  | -0.801229 |
| 10 | 6 | 0 | 0.387100  | 3.233031  | -3.539564 |
| 11 | 1 | 0 | 0.517379  | 1.151044  | -2.927638 |
| 12 | 1 | 0 | -0.935674 | 1.981507  | -2.357706 |
| 13 | 8 | 0 | -1.738903 | 0.609911  | 1.144823  |
| 14 | 1 | 0 | -2.382778 | 0.349146  | 1.838150  |
| 15 | 1 | 0 | -2.031675 | 0.146298  | 0.269314  |
| 16 | 8 | 0 | -2.393217 | -0.525219 | -1.087587 |
| 17 | 1 | 0 | -2.707315 | 0.195540  | -1.660897 |
| 18 | 1 | 0 | -3.592077 | -1.315022 | -0.779296 |
| 19 | 8 | 0 | -4.500763 | -1.782953 | -0.501510 |
| 20 | 1 | 0 | -4.641810 | -2.515702 | -1.120353 |
| 21 | 1 | 0 | -5.577011 | -0.465841 | -0.768433 |
| 22 | 8 | 0 | -6.054796 | 0.388786  | -0.957963 |
| 23 | 1 | 0 | -6.476791 | 0.649516  | -0.126004 |
| 24 | 1 | 0 | -4.231667 | -2.407506 | 1.188931  |
| 25 | 8 | 0 | -3.975714 | -2.717921 | 2.089857  |
| 26 | 1 | 0 | -3.190253 | -3.297519 | 1.946276  |
| 27 | 1 | 0 | -3.346278 | -1.457859 | 2.971287  |
| 28 | 8 | 0 | -2.858922 | -0.692565 | 3.411497  |
| 29 | 1 | 0 | -3.418044 | -0.398972 | 4.145869  |
| 30 | 1 | 0 | -4.828108 | 1.461152  | -1.548474 |
| 31 | 8 | 0 | -4.056128 | 1.995423  | -1.879706 |
| 32 | 1 | 0 | -4.389514 | 2.508993  | -2.630283 |
| 33 | 1 | 0 | -0.629180 | -0.555808 | 1.818938  |
| 34 | 8 | 0 | -0.242687 | -1.259386 | 2.413908  |
| 35 | 1 | 0 | -0.789694 | -1.165892 | 3.218391  |
| 36 | 1 | 0 | -1.035491 | -2.975042 | 1.998939  |
| 37 | 8 | 0 | -1.450795 | -3.844658 | 1.822037  |
| 38 | 1 | 0 | -1.034575 | -4.118758 | 0.978832  |
| 39 | 1 | 0 | 1.290207  | -1.871653 | 1.964238  |

| 40 | 8 | 0 | 2.079119 | -2.293369 | 1.523281 |
| 41 | 1 | 0 | 2.564210 | -2.751614 | 2.225824 |
| 42 | 1 | 0 | 0.490271 | -0.821434 | -1.657110 |
| 43 | 8 | 0 | -0.146752 | -1.548633 | -1.801281 |
| 44 | 1 | 0 | -1.079142 | -1.148278 | -1.584089 |
| 45 | 1 | 0 | 0.645121 | -2.826686 | -2.928414 |
| 46 | 8 | 0 | 1.270547 | -3.576995 | -3.067192 |
| 47 | 1 | 0 | 1.085258 | -4.134437 | -2.283993 |
| 48 | 1 | 0 | 0.106065 | -2.955638 | -0.745093 |
| 49 | 8 | 0 | 0.397635 | -3.819869 | -0.351899 |
| 50 | 1 | 0 | 1.048488 | -3.565059 | 0.329834 |
| 51 | 1 | 0 | -2.314783 | 2.277040 | 0.677967 |
| 52 | 8 | 0 | -2.684065 | 3.121216 | 0.321576 |
| 53 | 1 | 0 | -3.213983 | 2.844058 | -0.459024 |
| 54 | 1 | 0 | -1.425873 | 4.175166 | -0.093917 |
| 55 | 8 | 0 | -0.598799 | 4.664752 | -0.371051 |
| 56 | 1 | 0 | -0.499165 | 5.408591 | 0.239793 |
| 57 | 1 | 0 | 2.739310 | -2.872481 | -2.757816 |
| 58 | 8 | 0 | 3.545348 | -2.339599 | -2.468406 |
| 59 | 1 | 0 | 3.722164 | -1.726105 | -3.197715 |
| 60 | 1 | 0 | 4.984998 | -2.659375 | -1.249859 |
| 61 | 8 | 0 | 5.194804 | -2.308867 | -0.358518 |
| 62 | 1 | 0 | 5.956795 | -2.795975 | -0.015218 |
| 63 | 11 | 0 | 3.084697 | -1.344755 | -0.318836 |
| 64 | 6 | 0 | 1.941459 | 2.792206 | 2.919668 |
| 65 | 6 | 0 | 3.314598 | 2.661927 | 3.133880 |
| 66 | 1 | 0 | 0.312653 | 2.524881 | 1.531384 |
| 67 | 1 | 0 | 4.221354 | 1.447922 | 0.085514 |
| 68 | 1 | 0 | 5.207683 | 2.084245 | 2.271465 |
| 69 | 1 | 0 | 1.298056 | 3.158362 | 3.714620 |
| 70 | 1 | 0 | 3.744743 | 2.938724 | 4.092523 |
| 71 | 1 | 0 | 0.030603 | 4.187966 | -3.140467 |
| 72 | 1 | 0 | 1.454727 | 3.328015 | -3.766772 |
| 73 | 1 | 0 | -0.147182 | 3.029733 | -4.474206 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1940.85272273     A.U. after    1 cycles

Convg  =    0.4247D-08          -V/T =  2.0091

S**2  =   0.0000

Zero-point correction=                        0.606447 (a.u.)

Thermal correction to Energy=                  0.660246

Thermal correction to Enthalpy=                0.661190

Thermal correction to Gibbs Free Energy=       0.513787

Sum of electronic and zero-point Energies=           -1940.246275

Sum of electronic and thermal Energies=              -1940.192477

Sum of electronic and thermal Enthalpies=            -1940.191532

Sum of electronic and thermal Free Energies=         -1940.338935

(8-2) TS1(am), OH- nucleophilic addition to the amide
tuka02aana.chk    Stoichiometry C9H44NNaO18
Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.403379 | 2.335923 | 1.008445 |
| 2 | 6 | 0 | 0.372184 | 1.347645 | -0.151082 |
| 3 | 8 | 0 | 1.144645 | 0.290813 | -0.067036 |
| 4 | 7 | 0 | 0.284650 | 1.971109 | -1.384197 |
| 5 | 6 | 0 | 0.235892 | 1.204183 | -2.627991 |
| 6 | 6 | 0 | -0.548705 | 3.358721 | 1.136122 |
| 7 | 6 | 0 | 1.425911 | 2.253064 | 1.960551 |
| 8 | 6 | 0 | 1.501630 | 3.165908 | 3.015343 |
| 9 | 1 | 0 | -0.323783 | 2.788791 | -1.413459 |
| 10 | 6 | 0 | 0.509204 | 2.109377 | -3.828406 |
| 11 | 1 | 0 | 0.987948 | 0.412987 | -2.571393 |
| 12 | 1 | 0 | -0.740864 | 0.711558 | -2.747194 |
| 13 | 8 | 0 | -1.338097 | 0.648278 | 0.123234 |
| 14 | 1 | 0 | -1.423954 | 0.465546 | 1.080531 |
| 15 | 1 | 0 | -1.842981 | -0.661631 | -0.615053 |
| 16 | 8 | 0 | -2.176464 | -1.480843 | -1.138284 |
| 17 | 1 | 0 | -2.828981 | -1.125414 | -1.779541 |
| 18 | 1 | 0 | -3.072689 | -2.507410 | -0.182803 |
| 19 | 8 | 0 | -3.719759 | -3.051370 | 0.363704 |
| 20 | 1 | 0 | -3.645117 | -3.965332 | 0.047700 |
| 21 | 1 | 0 | -5.252842 | -2.262051 | -0.121865 |
| 22 | 8 | 0 | -5.963265 | -1.723486 | -0.551028 |
| 23 | 1 | 0 | -6.368815 | -1.198873 | 0.155633 |
| 24 | 1 | 0 | -2.927729 | -2.957397 | 2.068388 |
| 25 | 8 | 0 | -2.394005 | -2.855231 | 2.884469 |
| 26 | 1 | 0 | -1.566032 | -3.365680 | 2.721939 |
| 27 | 1 | 0 | -1.905005 | -1.240893 | 3.029138 |
| 28 | 8 | 0 | -1.480499 | -0.332100 | 3.037976 |
| 29 | 1 | 0 | -1.865489 | 0.153691 | 3.782156 |
| 30 | 1 | 0 | -5.119247 | -0.789351 | -1.751103 |
| 31 | 8 | 0 | -4.468675 | -0.319251 | -2.338564 |
| 32 | 1 | 0 | -4.847916 | -0.307425 | -3.229932 |
| 33 | 1 | 0 | 0.926230 | -0.599304 | 1.397003 |
| 34 | 8 | 0 | 1.016331 | -1.097416 | 2.256593 |
| 35 | 1 | 0 | 0.280801 | -0.745766 | 2.811764 |
| 36 | 1 | 0 | 0.527606 | -2.870642 | 2.312846 |
| 37 | 8 | 0 | 0.194724 | -3.792773 | 2.392964 |
| 38 | 1 | 0 | 0.662411 | -4.266078 | 1.679762 |

| 39 | 1 | 0 | 2.698092 | -1.425989 | 2.030105 |
|----|---|---|----------|-----------|----------|
| 40 | 8 | 0 | 3.469709 | -1.586561 | 1.424391 |
| 41 | 1 | 0 | 4.247167 | -1.750511 | 1.978541 |
| 42 | 1 | 0 | 0.687778 | -1.157738 | -0.955686 |
| 43 | 8 | 0 | 0.498330 | -2.040663 | -1.372258 |
| 44 | 1 | 0 | -0.482944 | -2.042407 | -1.472808 |
| 45 | 1 | 0 | 1.821867 | -2.693038 | -2.473403 |
| 46 | 8 | 0 | 2.721585 | -3.055190 | -2.653722 |
| 47 | 1 | 0 | 2.850670 | -3.657713 | -1.893126 |
| 48 | 1 | 0 | 1.362191 | -3.263783 | -0.315437 |
| 49 | 8 | 0 | 2.048486 | -3.860496 | 0.066861 |
| 50 | 1 | 0 | 2.633082 | -3.264360 | 0.573424 |
| 51 | 1 | 0 | -2.740627 | 1.524095 | -0.423363 |
| 52 | 8 | 0 | -3.503929 | 1.995292 | -0.860857 |
| 53 | 1 | 0 | -3.923515 | 1.320886 | -1.430371 |
| 54 | 1 | 0 | -2.671709 | 3.223569 | -1.748664 |
| 55 | 8 | 0 | -1.999739 | 3.840008 | -2.148158 |
| 56 | 1 | 0 | -2.350517 | 4.735020 | -2.034813 |
| 57 | 1 | 0 | 3.665398 | -1.688044 | -2.566921 |
| 58 | 8 | 0 | 4.068046 | -0.773156 | -2.443554 |
| 59 | 1 | 0 | 3.886551 | -0.301751 | -3.270802 |
| 60 | 1 | 0 | 5.586630 | -0.043505 | -1.417909 |
| 61 | 8 | 0 | 5.603335 | 0.420594 | -0.556678 |
| 62 | 1 | 0 | 6.455618 | 0.870333 | -0.472403 |
| 63 | 11 | 0 | 3.342831 | 0.004586 | -0.301964 |
| 64 | 6 | 0 | -0.472637 | 4.271781 | 2.186664 |
| 65 | 6 | 0 | 0.552685 | 4.180460 | 3.131350 |
| 66 | 1 | 0 | -1.361550 | 3.434866 | 0.422380 |
| 67 | 1 | 0 | 2.159398 | 1.456930 | 1.890233 |
| 68 | 1 | 0 | 2.301095 | 3.078163 | 3.746712 |
| 69 | 1 | 0 | -1.222980 | 5.053460 | 2.270633 |
| 70 | 1 | 0 | 0.607470 | 4.891484 | 3.951419 |
| 71 | 1 | 0 | -0.231925 | 2.912876 | -3.884154 |
| 72 | 1 | 0 | 1.503995 | 2.565037 | -3.755393 |
| 73 | 1 | 0 | 0.458197 | 1.530627 | -4.758123 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1940.81514661    A.U. after   1 cycles

Convg  =    0.4804D-08          -V/T =  2.0091

S**2   =   0.0000

Zero-point correction=                    0.607715(a.u.)

Thermal correction to Energy=             0.660660

Thermal correction to Enthalpy=           0.661604

Thermal correction to Gibbs Free Energy=       0.518342

Sum of electronic and zero-point Energies=        -1940.207432

Sum of electronic and thermal Energies=           -1940.154487

Sum of electronic and thermal Enthalpies=         -1940.153543

Sum of electronic and thermal Free Energies=     -1940.296805

(8-3) Anionic tetrahedral intermediate, Int1(am),
    Ph-C(-O-)(OH)-NH-Et, Na+ and (H2O)16
    tuka02bbna.rev.chk     Stoichiometry C9H44NNaO18
                Standard orientation:

---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |
|--------|--------|-------|---|---|---|

---------------------------------------------------------------------

| 1 | 6 | 0 | -1.791021 | 2.297395 | -0.638961 |
| 2 | 6 | 0 | -1.357299 | 0.823551 | -0.780714 |
| 3 | 8 | 0 | -0.874477 | 0.298467 | 0.382438 |
| 4 | 7 | 0 | -0.342096 | 0.773146 | -1.865077 |
| 5 | 6 | 0 | -0.196663 | -0.503224 | -2.602118 |
| 6 | 6 | 0 | -2.900504 | 2.796507 | -1.334809 |
| 7 | 6 | 0 | -1.041992 | 3.179545 | 0.150352 |
| 8 | 6 | 0 | -1.402817 | 4.522968 | 0.258028 |
| 9 | 1 | 0 | -0.561207 | 1.506253 | -2.538813 |
| 10 | 6 | 0 | 0.816068 | -0.353251 | -3.736218 |
| 11 | 1 | 0 | 0.143684 | -1.266721 | -1.897497 |
| 12 | 1 | 0 | -1.156063 | -0.836871 | -3.014085 |
| 13 | 8 | 0 | -2.499129 | 0.034043 | -1.229856 |
| 14 | 1 | 0 | -3.214471 | 0.113322 | -0.561898 |
| 15 | 1 | 0 | -5.039611 | -3.492255 | 0.795528 |
| 16 | 8 | 0 | -5.007347 | -2.873888 | 0.050888 |
| 17 | 1 | 0 | -4.119822 | -3.004205 | -0.377563 |
| 18 | 1 | 0 | 1.340654 | 0.928848 | -1.162992 |
| 19 | 8 | 0 | 2.978583 | 1.267308 | 1.888880 |
| 20 | 1 | 0 | 2.086444 | 1.375804 | 2.292953 |
| 21 | 1 | 0 | 3.196819 | 0.329869 | 2.075065 |
| 22 | 8 | 0 | 2.923098 | -1.600259 | 2.197529 |
| 23 | 1 | 0 | 3.631136 | -2.090476 | 2.642837 |
| 24 | 1 | 0 | -4.932385 | -1.200359 | 0.461623 |
| 25 | 8 | 0 | -4.705302 | -0.246432 | 0.641379 |
| 26 | 1 | 0 | -5.508941 | 0.269450 | 0.478650 |
| 27 | 1 | 0 | -2.038238 | 0.140211 | 1.685544 |
| 28 | 8 | 0 | -2.598348 | 0.033691 | 2.504191 |
| 29 | 1 | 0 | -3.503320 | -0.059505 | 2.144168 |
| 30 | 1 | 0 | 3.086900 | -1.728202 | 1.208362 |
| 31 | 8 | 0 | 3.287169 | -1.699956 | -0.442474 |
| 32 | 1 | 0 | 4.245976 | -1.566959 | -0.668721 |
| 33 | 1 | 0 | 5.760349 | 3.006359 | 1.601294 |
| 34 | 8 | 0 | 4.988140 | 2.989756 | 1.017279 |
| 35 | 1 | 0 | 4.303466 | 2.450523 | 1.473858 |
| 36 | 1 | 0 | -0.482649 | -1.254429 | 0.473914 |

| 37 | 8 | 0 | -0.306716 | -2.210368 | 0.773288 |
|----|---|---|-----------|-----------|----------|
| 38 | 1 | 0 | -1.126425 | -2.660891 | 0.476324 |
| 39 | 1 | 0 | 6.346104 | -1.244974 | -1.741517 |
| 40 | 8 | 0 | 5.846979 | -0.922710 | -0.976678 |
| 41 | 1 | 0 | 5.634500 | 0.036776 | -1.165689 |
| 42 | 1 | 0 | 2.158057 | -3.176497 | -1.014152 |
| 43 | 8 | 0 | 1.341865 | -3.707223 | -0.908738 |
| 44 | 1 | 0 | 0.822267 | -3.187050 | -0.251181 |
| 45 | 1 | 0 | -2.425022 | -1.836365 | -1.183006 |
| 46 | 8 | 0 | -2.485910 | -2.788997 | -0.930670 |
| 47 | 1 | 0 | -1.980457 | -3.296930 | -1.614516 |
| 48 | 1 | 0 | -0.820632 | -5.032320 | -2.835289 |
| 49 | 8 | 0 | -0.733224 | -4.093222 | -2.617559 |
| 50 | 1 | 0 | 0.118260 | -4.000625 | -2.111419 |
| 51 | 1 | 0 | -0.271812 | 1.162553 | 3.173701 |
| 52 | 8 | 0 | 0.398963 | 0.816532 | 2.563469 |
| 53 | 1 | 0 | -0.056222 | 0.801195 | 1.654877 |
| 54 | 1 | 0 | -1.539654 | -1.721632 | 4.973594 |
| 55 | 8 | 0 | -1.210980 | -1.663613 | 4.066094 |
| 56 | 1 | 0 | -1.860818 | -1.101518 | 3.555133 |
| 57 | 1 | 0 | 5.117166 | 2.168687 | -0.650529 |
| 58 | 8 | 0 | 4.985663 | 1.589048 | -1.434779 |
| 59 | 1 | 0 | 4.014308 | 1.456671 | -1.477653 |
| 60 | 1 | 0 | 2.855685 | -0.843419 | -0.706487 |
| 61 | 8 | 0 | 2.298863 | 0.824921 | -0.878517 |
| 62 | 1 | 0 | 2.372907 | 1.118978 | 0.054409 |
| 63 | 11 | 0 | 0.629578 | -1.568228 | 2.734333 |
| 64 | 6 | 0 | -3.266680 | 4.139995 | -1.222749 |
| 65 | 6 | 0 | -2.520470 | 5.007128 | -0.424531 |
| 66 | 1 | 0 | -3.475866 | 2.126549 | -1.966012 |
| 67 | 1 | 0 | -0.168595 | 2.814991 | 0.680721 |
| 68 | 1 | 0 | -0.808124 | 5.191762 | 0.874750 |
| 69 | 1 | 0 | -4.134173 | 4.507957 | -1.764869 |
| 70 | 1 | 0 | -2.803330 | 6.052923 | -0.338661 |
| 71 | 1 | 0 | 0.488161 | 0.402858 | -4.461645 |
| 72 | 1 | 0 | 1.802152 | -0.058820 | -3.363328 |
| 73 | 1 | 0 | 0.917294 | -1.303504 | -4.270887 |

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SCF Done:  E(RB+HF-LYP) =  -1940.83625089     A.U. after    1 cycles

   Convg  =    0.4394D-08           -V/T =  2.0090

   S**2  =   0.0000

Zero-point correction=                    0.611283 (a.u.)

Thermal correction to Energy=                0.662859

Thermal correction to Enthalpy=             0.663803

Thermal correction to Gibbs Free Energy=       0.525100

Sum of electronic and zero-point Energies=        -1940.224968

Sum of electronic and thermal Energies=          -1940.173392
Sum of electronic and thermal Enthalpies=         -1940.172448
Sum of electronic and thermal Free Energies=      -1940.311151

(8-4) TS2(am) toward the zwitterion(i.e., Mulliken CT complex)
tuka02bbna.chk    Stoichiometry    C9H44NNaO18
                  Standard orientation:
---------------------------------------------------------------------
Center    Atomic    Atomic         Coordinates (Angstroms)
Number    Number    Type        X          Y          Z
---------------------------------------------------------------------
   1        6        0      -1.551473   2.424483  -0.531199
   2        6        0      -1.313474   0.907550  -0.654933
   3        8        0      -0.910598   0.312711   0.462612
   4        7        0      -0.208375   0.755758  -1.765704
   5        6        0      -0.184352  -0.499500  -2.587075
   6        6        0      -2.507446   3.073556  -1.324915
   7        6        0      -0.769676   3.184858   0.347811
   8        6        0      -0.949813   4.564911   0.443181
   9        1        0      -0.281057   1.557712  -2.396633
  10        6        0       0.887956  -0.407543  -3.668581
  11        1        0       0.029495  -1.322909  -1.905696
  12        1        0      -1.173143  -0.642183  -3.022472
  13        8        0      -2.452059   0.264234  -1.246000
  14        1        0      -3.204514   0.337994  -0.611699
  15        1        0      -5.483005  -3.154979   0.369861
  16        8        0      -5.263057  -2.479843  -0.288813
  17        1        0      -4.366788  -2.717394  -0.645024
  18        1        0       0.763353   0.812427  -1.270196
  19        8        0       3.059707   1.030320   2.108027
  20        1        0       2.199966   1.182437   2.549087
  21        1        0       3.156742   0.049702   2.131364
  22        8        0       2.817821  -1.788451   2.051135
  23        1        0       3.559836  -2.314165   2.386023
  24        1        0      -5.001909  -0.875531   0.265461
  25        8        0      -4.672675   0.032173   0.516745
  26        1        0      -5.418002   0.640248   0.398025
  27        1        0      -2.102390   0.115640   1.779962
  28        8        0      -2.673419  -0.030946   2.576732
  29        1        0      -3.572978  -0.047326   2.196516
  30        1        0       2.910733  -1.807996   0.984656
  31        8        0       2.943421  -1.684056  -0.462276
  32        1        0       3.883579  -1.695034  -0.749720
  33        1        0       5.875683   2.493941   1.457430
  34        8        0       5.036523   2.674591   1.009653
  35        1        0       4.360301   2.142547   1.488186

| | | | | | |
|---|---|---|---|---|---|
| 36 | 1 | 0 | -0.661745 | -1.340847 | 0.558695 |
| 37 | 8 | 0 | -0.572793 | -2.294001 | 0.854012 |
| 38 | 1 | 0 | -1.401600 | -2.693217 | 0.521032 |
| 39 | 1 | 0 | 6.086842 | -1.466537 | -1.983401 |
| 40 | 8 | 0 | 5.652046 | -1.148471 | -1.179020 |
| 41 | 1 | 0 | 5.448630 | -0.185417 | -1.340005 |
| 42 | 1 | 0 | 1.908369 | -2.972223 | -0.992803 |
| 43 | 8 | 0 | 1.124574 | -3.590290 | -1.009707 |
| 44 | 1 | 0 | 0.582081 | -3.246652 | -0.268082 |
| 45 | 1 | 0 | -2.527882 | -1.688582 | -1.258360 |
| 46 | 8 | 0 | -2.675545 | -2.639193 | -1.060281 |
| 47 | 1 | 0 | -2.146411 | -3.141818 | -1.734155 |
| 48 | 1 | 0 | -0.940882 | -4.712257 | -3.111974 |
| 49 | 8 | 0 | -0.875820 | -3.811329 | -2.763668 |
| 50 | 1 | 0 | -0.037244 | -3.778045 | -2.214506 |
| 51 | 1 | 0 | -0.297457 | 0.866091 | 3.372290 |
| 52 | 8 | 0 | 0.397187 | 0.599928 | 2.748994 |
| 53 | 1 | 0 | -0.021209 | 0.681243 | 1.845274 |
| 54 | 1 | 0 | -1.575838 | -1.918780 | 4.972407 |
| 55 | 8 | 0 | -1.256000 | -1.840503 | 4.062959 |
| 56 | 1 | 0 | -1.911944 | -1.274587 | 3.575751 |
| 57 | 1 | 0 | 5.008107 | 1.950281 | -0.746299 |
| 58 | 8 | 0 | 4.788791 | 1.408313 | -1.535879 |
| 59 | 1 | 0 | 3.826935 | 1.211116 | -1.414717 |
| 60 | 1 | 0 | 2.563296 | -0.510519 | -0.645636 |
| 61 | 8 | 0 | 2.229269 | 0.632403 | -0.754891 |
| 62 | 1 | 0 | 2.367477 | 0.984589 | 0.145662 |
| 63 | 11 | 0 | 0.630167 | -1.798902 | 2.732814 |
| 64 | 6 | 0 | -2.691321 | 4.454371 | -1.223705 |
| 65 | 6 | 0 | -1.913951 | 5.202972 | -0.339166 |
| 66 | 1 | 0 | -3.109967 | 2.492871 | -2.016642 |
| 67 | 1 | 0 | -0.015211 | 2.698236 | 0.956173 |
| 68 | 1 | 0 | -0.333468 | 5.140458 | 1.128149 |
| 69 | 1 | 0 | -3.441594 | 4.943649 | -1.839098 |
| 70 | 1 | 0 | -2.054609 | 6.277668 | -0.263034 |
| 71 | 1 | 0 | 0.681278 | 0.409679 | -4.371633 |
| 72 | 1 | 0 | 1.880449 | -0.255420 | -3.236513 |
| 73 | 1 | 0 | 0.896789 | -1.343166 | -4.235911 |

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SCF Done:  E(RB+HF-LYP) = -1940.81873868    A.U. after   1 cycles

      Convg  =   0.3382D-08          -V/T = 2.0090

      S**2  =  0.0000

Zero-point correction=                    0.605882 (a.u.)
Thermal correction to Energy=                0.656922
Thermal correction to Enthalpy=              0.657866
Thermal correction to Gibbs Free Energy=      0.519940

Sum of electronic and zero-point Energies=      -1940.212857
Sum of electronic and thermal Energies=      -1940.161817
Sum of electronic and thermal Enthalpies=      -1940.160873
Sum of electronic and thermal Free Energies=      -1940.298799


(8-5) The zwitterion (i.e., Mulliken CT complex), Int2(am),
   Ph-C(-O-)(OH)-N(H2+)-Et, NaOH and (H2O)15
   tuka02ccna.for.chk   Stoichiometry  C9H44NNaO18
                Standard orientation:
-----------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type        X        Y        Z
-----------------------------------------------------------------------
   1        6        0      0.172378   3.227014  -0.461961
   2        6        0     -0.671871   1.982132  -0.759646
   3        8        0     -0.856427   1.155739   0.254020
   4        7        0      0.226528   1.189659  -1.903986
   5        6        0     -0.489572   0.182972  -2.744242
   6        6        0     -0.268232   4.504579  -0.824314
   7        6        0      1.409428   3.087325   0.185285
   8        6        0      2.188609   4.208165   0.470508
   9        1        0      0.639382   1.902951  -2.510499
  10        6        0      0.402615  -0.329204  -3.872008
  11        1        0     -0.781340  -0.635931  -2.085192
  12        1        0     -1.388954   0.667878  -3.127739
  13        8        0     -1.841312   2.330378  -1.447723
  14        1        0     -2.606889   1.915643  -0.993056
  15        1        0     -6.367238  -0.793157   0.678381
  16        8        0     -5.907482  -0.600627  -0.152117
  17        1        0     -5.330145  -1.379769  -0.338729
  18        1        0      1.013468   0.702137  -1.411534
  19        8        0      2.820948  -0.506062   1.897592
  20        1        0      2.217680   0.107034   2.360062
  21        1        0      2.361495  -1.432806   2.017639
  22        8        0      1.450981  -2.673889   2.036052
  23        1        0      1.840303  -3.372411   2.581357
  24        1        0     -4.953358   0.854356  -0.209689
  25        8        0     -4.374046   1.661298  -0.178090
  26        1        0     -4.929340   2.401835  -0.466456
  27        1        0     -2.108523   1.434263   1.533559
  28        8        0     -2.830405   1.418081   2.206997
  29        1        0     -3.619714   1.580721   1.654395
  30        1        0      1.742508  -3.055862   0.476528
  31        8        0      1.873639  -3.109183  -0.533149
  32        1        0      2.777301  -3.469862  -0.698085
  33        1        0      6.018880  -0.868368   2.073861

| 34 | 8 | 0 | 5.520398 | -0.245923 | 1.524661 |
|---|---|---|---|---|---|
| 35 | 1 | 0 | 4.572878 | -0.337523 | 1.799309 |
| 36 | 1 | 0 | -1.426388 | -0.440571 | 0.170506 |
| 37 | 8 | 0 | -1.607502 | -1.405785 | 0.339109 |
| 38 | 1 | 0 | -2.534108 | -1.583991 | 0.076268 |
| 39 | 1 | 0 | 4.862587 | -4.122520 | -1.830384 |
| 40 | 8 | 0 | 4.554694 | -3.675943 | -1.028571 |
| 41 | 1 | 0 | 4.860229 | -2.729848 | -1.101195 |
| 42 | 1 | 0 | 0.291141 | -3.525493 | -1.244832 |
| 43 | 8 | 0 | -0.670682 | -3.377061 | -1.423584 |
| 44 | 1 | 0 | -0.893891 | -2.646780 | -0.804286 |
| 45 | 1 | 0 | -3.891541 | -2.223011 | -1.846927 |
| 46 | 8 | 0 | -3.997877 | -2.411440 | -0.900858 |
| 47 | 1 | 0 | -3.723252 | -3.370554 | -0.816814 |
| 48 | 1 | 0 | -2.784193 | -5.474718 | -0.263751 |
| 49 | 8 | 0 | -2.860201 | -4.829661 | -0.981552 |
| 50 | 1 | 0 | -1.940250 | -4.473656 | -1.152512 |
| 51 | 1 | 0 | -0.047622 | 1.219579 | 3.255021 |
| 52 | 8 | 0 | 0.349103 | 0.638616 | 2.588401 |
| 53 | 1 | 0 | 0.030180 | 0.981569 | 1.708428 |
| 54 | 1 | 0 | -2.668841 | -0.903165 | 4.415783 |
| 55 | 8 | 0 | -2.417794 | -0.979521 | 3.484323 |
| 56 | 1 | 0 | -2.677081 | -0.120057 | 3.056423 |
| 57 | 1 | 0 | 5.412331 | -0.722949 | -0.264372 |
| 58 | 8 | 0 | 5.105935 | -1.012488 | -1.155744 |
| 59 | 1 | 0 | 4.186229 | -0.674962 | -1.209208 |
| 60 | 1 | 0 | 2.073056 | -1.383406 | -0.852364 |
| 61 | 8 | 0 | 2.294767 | -0.412054 | -0.801266 |
| 62 | 1 | 0 | 2.486218 | -0.308637 | 0.169405 |
| 63 | 11 | 0 | -0.469578 | -1.632506 | 2.371546 |
| 64 | 6 | 0 | 0.511261 | 5.626385 | -0.531572 |
| 65 | 6 | 0 | 1.739172 | 5.481996 | 0.114349 |
| 66 | 1 | 0 | -1.223713 | 4.612156 | -1.324802 |
| 67 | 1 | 0 | 1.766982 | 2.102905 | 0.471714 |
| 68 | 1 | 0 | 3.145066 | 4.083543 | 0.970264 |
| 69 | 1 | 0 | 0.155335 | 6.614670 | -0.810401 |
| 70 | 1 | 0 | 2.344993 | 6.355759 | 0.338420 |
| 71 | 1 | 0 | 0.685238 | 0.477597 | -4.559969 |
| 72 | 1 | 0 | 1.314669 | -0.791623 | -3.483048 |
| 73 | 1 | 0 | -0.138720 | -1.086983 | -4.446996 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1940.82661398    A.U. after   1 cycles

    Convg  =    0.2289D-08         -V/T =  2.0091

    S**2  =   0.0000

Zero-point correction=                  0.610399 (a.u.)

Thermal correction to Energy=            0.662633

Thermal correction to Enthalpy=            0.663577
Thermal correction to Gibbs Free Energy=      0.521463
Sum of electronic and zero-point Energies=      -1940.216215
Sum of electronic and thermal Energies=       -1940.163981
Sum of electronic and thermal Enthalpies=      -1940.163037
Sum of electronic and thermal Free Energies=     -1940.305151


 (8-6) TS3(am),  C(2)----N(7) scission TS
tuka02ccna.chk     Stoichiometry C9H44NNaO18
                Standard orientation:

---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|--------|--------|--------|
| Number | Number | Type | X | Y | Z |

---------------------------------------------------------------------

|  1 | 6 | 0 |  0.341215 |  3.340841 | -0.237571 |
|  2 | 6 | 0 | -0.688319 |  2.253572 | -0.426717 |
|  3 | 8 | 0 | -0.834394 |  1.348779 |  0.474597 |
|  4 | 7 | 0 |  0.213532 |  1.326514 | -1.902647 |
|  5 | 6 | 0 | -0.675002 |  0.578657 | -2.812584 |
|  6 | 6 | 0 |  0.095049 |  4.651156 | -0.666318 |
|  7 | 6 | 0 |  1.563342 |  3.035026 |  0.378351 |
|  8 | 6 | 0 |  2.523606 |  4.027441 |  0.567184 |
|  9 | 1 | 0 |  0.727669 |  2.041673 | -2.418898 |
| 10 | 6 | 0 |  0.063411 | -0.052753 | -3.994641 |
| 11 | 1 | 0 | -1.163135 | -0.198727 | -2.217423 |
| 12 | 1 | 0 | -1.447475 |  1.272454 | -3.159770 |
| 13 | 8 | 0 | -1.812830 |  2.697591 | -1.060183 |
| 14 | 1 | 0 | -2.591914 |  2.177503 | -0.754611 |
| 15 | 1 | 0 | -6.612371 | -0.582273 |  0.091119 |
| 16 | 8 | 0 | -5.918137 | -0.329761 | -0.535132 |
| 17 | 1 | 0 | -5.329513 | -1.117564 | -0.638997 |
| 18 | 1 | 0 |  0.911386 |  0.692996 | -1.471032 |
| 19 | 8 | 0 |  2.787862 | -0.784736 |  1.873488 |
| 20 | 1 | 0 |  2.235732 | -0.175358 |  2.397406 |
| 21 | 1 | 0 |  2.301984 | -1.700737 |  1.965780 |
| 22 | 8 | 0 |  1.355166 | -2.913995 |  1.954594 |
| 23 | 1 | 0 |  1.716799 | -3.634609 |  2.489832 |
| 24 | 1 | 0 | -4.946897 |  1.063625 | -0.228862 |
| 25 | 8 | 0 | -4.338876 |  1.828047 | -0.038256 |
| 26 | 1 | 0 | -4.855911 |  2.630664 | -0.207986 |
| 27 | 1 | 0 | -2.163119 |  1.397518 |  1.777133 |
| 28 | 8 | 0 | -2.928581 |  1.275172 |  2.380968 |
| 29 | 1 | 0 | -3.680957 |  1.477219 |  1.789942 |
| 30 | 1 | 0 |  1.640567 | -3.278158 |  0.375265 |
| 31 | 8 | 0 |  1.752497 | -3.308148 | -0.634308 |
| 32 | 1 | 0 |  2.655137 | -3.654462 | -0.831672 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 1 | 0 | 5.972845 | -1.249573 | 1.871487 |
| 34 | 8 | 0 | 5.477768 | -0.563032 | 1.401096 |
| 35 | 1 | 0 | 4.537747 | -0.653255 | 1.700427 |
| 36 | 1 | 0 | -1.386021 | -0.297705 | 0.183041 |
| 37 | 8 | 0 | -1.563635 | -1.268074 | 0.246991 |
| 38 | 1 | 0 | -2.496379 | -1.415059 | -0.016428 |
| 39 | 1 | 0 | 4.684218 | -4.257200 | -2.063305 |
| 40 | 8 | 0 | 4.420661 | -3.837946 | -1.231450 |
| 41 | 1 | 0 | 4.714502 | -2.886862 | -1.294162 |
| 42 | 1 | 0 | 0.161091 | -3.556124 | -1.365646 |
| 43 | 8 | 0 | -0.786848 | -3.326532 | -1.537396 |
| 44 | 1 | 0 | -0.920618 | -2.540301 | -0.966175 |
| 45 | 1 | 0 | -3.774775 | -2.054748 | -1.949700 |
| 46 | 8 | 0 | -3.970777 | -2.175939 | -1.006448 |
| 47 | 1 | 0 | -3.770317 | -3.144901 | -0.847117 |
| 48 | 1 | 0 | -2.918803 | -5.226470 | -0.115371 |
| 49 | 8 | 0 | -3.000182 | -4.655883 | -0.893165 |
| 50 | 1 | 0 | -2.076017 | -4.346021 | -1.126488 |
| 51 | 1 | 0 | 0.021608 | 0.944551 | 3.474618 |
| 52 | 8 | 0 | 0.367966 | 0.440788 | 2.722626 |
| 53 | 1 | 0 | 0.068812 | 0.924331 | 1.910426 |
| 54 | 1 | 0 | -2.785846 | -1.299391 | 4.308511 |
| 55 | 8 | 0 | -2.471981 | -1.239895 | 3.395125 |
| 56 | 1 | 0 | -2.752146 | -0.347103 | 3.061738 |
| 57 | 1 | 0 | 5.295443 | -0.922445 | -0.416471 |
| 58 | 8 | 0 | 4.957785 | -1.170857 | -1.308402 |
| 59 | 1 | 0 | 4.034720 | -0.833913 | -1.312746 |
| 60 | 1 | 0 | 1.950829 | -1.545085 | -0.914562 |
| 61 | 8 | 0 | 2.182980 | -0.582171 | -0.832282 |
| 62 | 1 | 0 | 2.391653 | -0.511262 | 0.133818 |
| 63 | 11 | 0 | -0.505799 | -1.784496 | 2.275435 |
| 64 | 6 | 0 | 1.057340 | 5.643636 | -0.470236 |
| 65 | 6 | 0 | 2.271211 | 5.335278 | 0.145140 |
| 66 | 1 | 0 | -0.850910 | 4.887995 | -1.140103 |
| 67 | 1 | 0 | 1.767719 | 2.019103 | 0.700970 |
| 68 | 1 | 0 | 3.468653 | 3.776716 | 1.040271 |
| 69 | 1 | 0 | 0.855425 | 6.659590 | -0.798668 |
| 70 | 1 | 0 | 3.019820 | 6.108726 | 0.293233 |
| 71 | 1 | 0 | 0.557332 | 0.711276 | -4.607535 |
| 72 | 1 | 0 | 0.820886 | -0.764727 | -3.652830 |
| 73 | 1 | 0 | -0.643057 | -0.592438 | -4.635091 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1940.82510814    A.U. after   1 cycles

Convg  =    0.1902D-08         -V/T =  2.0091

S**2  =   0.0000

Zero-point correction=                    0.608575 (a.u.)

Thermal correction to Energy=                0.661088
Thermal correction to Enthalpy=              0.662033
Thermal correction to Gibbs Free Energy=     0.518382
Sum of electronic and zero-point Energies=        -1940.216533
Sum of electronic and thermal Energies=           -1940.164020
Sum of electronic and thermal Enthalpies=         -1940.163076
Sum of electronic and thermal Free Energies=      -1940.306726


 (8-7)  Ph-COOH,  Et-NH2 and NaOH(H2O)15, Int3(am)
tuka02ccna.rev.chk    Stoichiometry  C9H44NNaO18
                 Standard orientation:
---------------------------------------------------------------------
Center    Atomic    Atomic          Coordinates (Angstroms)
Number    Number    Type         X         Y         Z
---------------------------------------------------------------------
   1        6        0       2.826328   2.482038  -0.369214
   2        6        0       3.336563   1.174327  -0.848041
   3        8        0       2.913825   0.618036  -1.872172
   4        7        0      -0.568908   1.573708   1.698476
   5        6        0      -0.821301   1.686200   3.150100
   6        6        0       3.254453   3.020308   0.854745
   7        6        0       1.889640   3.179165  -1.147857
   8        6        0       1.381860   4.398028  -0.704570
   9        1        0      -0.064728   2.395455   1.364235
  10        6        0      -1.620924   2.924516   3.561571
  11        1        0      -1.352463   0.777553   3.454216
  12        1        0       0.148662   1.673892   3.663873
  13        8        0       4.286898   0.648805  -0.088564
  14        1        0       4.553914  -0.273882  -0.379679
  15        1        0       2.584163  -3.556360  -0.136786
  16        8        0       3.310273  -3.504204   0.522702
  17        1        0       2.894071  -3.177909   1.355208
  18        1        0      -1.467918   1.545185   1.195649
  19        8        0      -2.589387   0.345022  -2.393845
  20        1        0      -1.687962   0.566376  -2.683566
  21        1        0      -2.552685  -0.671875  -2.158665
  22        8        0      -2.338387  -2.073810  -1.606828
  23        1        0      -2.756896  -2.743253  -2.165639
  24        1        0       4.440323  -2.512416  -0.108547
  25        8        0       5.049814  -1.889061  -0.622994
  26        1        0       5.960286  -2.109529  -0.372945
  27        1        0       3.270286  -1.036855  -2.686504
  28        8        0       3.418013  -1.977961  -2.920289
  29        1        0       4.215159  -2.193790  -2.395965
  30        1        0      -3.264037  -1.913585  -0.241429
  31        8        0      -3.694815  -1.646133   0.635079

| 32 | 1 | 0 | -4.672149 | -1.641651 | 0.498499 |
|----|---|---|-----------|-----------|----------|
| 33 | 1 | 0 | -5.457405 | 0.748478 | -3.778029 |
| 34 | 8 | 0 | -4.998507 | 1.394572 | -3.221606 |
| 35 | 1 | 0 | -4.104393 | 1.010154 | -3.043475 |
| 36 | 1 | 0 | 0.106882 | 0.080105 | 1.253595 |
| 37 | 8 | 0 | 0.334309 | -0.874754 | 0.969509 |
| 38 | 1 | 0 | 1.012746 | -1.219161 | 1.586406 |
| 39 | 1 | 0 | -7.063391 | -1.217566 | 0.796981 |
| 40 | 8 | 0 | -6.390808 | -1.184193 | 0.101413 |
| 41 | 1 | 0 | -6.297770 | -0.221577 | -0.145444 |
| 42 | 1 | 0 | -2.607442 | -2.070444 | 1.977590 |
| 43 | 8 | 0 | -1.773482 | -2.071578 | 2.510667 |
| 44 | 1 | 0 | -1.122804 | -1.613646 | 1.936289 |
| 45 | 1 | 0 | 2.476048 | -2.130222 | 3.495460 |
| 46 | 8 | 0 | 1.983669 | -2.447574 | 2.723461 |
| 47 | 1 | 0 | 1.245372 | -3.025739 | 3.083973 |
| 48 | 1 | 0 | -0.273896 | -4.734804 | 3.345353 |
| 49 | 8 | 0 | -0.121189 | -3.819907 | 3.622674 |
| 50 | 1 | 0 | -0.878701 | -3.277096 | 3.253780 |
| 51 | 1 | 0 | 0.462028 | -0.410160 | -3.621708 |
| 52 | 8 | 0 | 0.348220 | -0.082734 | -2.715981 |
| 53 | 1 | 0 | 1.205746 | 0.329549 | -2.471729 |
| 54 | 1 | 0 | 1.182333 | -4.103277 | -2.081065 |
| 55 | 8 | 0 | 1.453818 | -3.291236 | -1.625903 |
| 56 | 1 | 0 | 2.145582 | -2.857015 | -2.204976 |
| 57 | 1 | 0 | -5.715070 | 1.486136 | -1.488885 |
| 58 | 8 | 0 | -5.871942 | 1.412354 | -0.519797 |
| 59 | 1 | 0 | -4.970543 | 1.480450 | -0.130919 |
| 60 | 1 | 0 | -3.337763 | 0.128983 | 0.536035 |
| 61 | 8 | 0 | -3.148776 | 1.061604 | 0.257050 |
| 62 | 1 | 0 | -2.892415 | 0.950794 | -0.690105 |
| 63 | 11 | 0 | -0.250299 | -1.731991 | -1.066629 |
| 64 | 6 | 0 | 2.743856 | 4.240296 | 1.293916 |
| 65 | 6 | 0 | 1.807294 | 4.928648 | 0.517084 |
| 66 | 1 | 0 | 3.978090 | 2.478393 | 1.452784 |
| 67 | 1 | 0 | 1.568113 | 2.764743 | -2.097224 |
| 68 | 1 | 0 | 0.656757 | 4.933656 | -1.309808 |
| 69 | 1 | 0 | 3.076386 | 4.655160 | 2.240948 |
| 70 | 1 | 0 | 1.410671 | 5.879667 | 0.861585 |
| 71 | 1 | 0 | -1.091903 | 3.846489 | 3.287487 |
| 72 | 1 | 0 | -2.598927 | 2.936021 | 3.067893 |
| 73 | 1 | 0 | -1.785690 | 2.941381 | 4.645814 |

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SCF Done:  E(RB+HF-LYP) =  -1940.86175587     A.U. after    1 cycles

      Convg  =    0.3267D-08          -V/T =  2.0091

      S**2  =   0.0000

Zero-point correction=        0.609265 (a.u.)
Thermal correction to Energy=       0.662209
Thermal correction to Enthalpy=      0.663154
Thermal correction to Gibbs Free Energy=    0.516907
Sum of electronic and zero-point Energies=     -1940.252491
Sum of electronic and thermal Energies=      -1940.199546
Sum of electronic and thermal Enthalpies=     -1940.198602
Sum of electronic and thermal Free Energies=    -1940.344849

 (8-8)   TS4(am) leading to the product
 tuka02d1na.chk     Stoichiometry C9H44NNaO18
        standard orientation:

----------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|------|------|------|
| Number | Number | Type | X | Y | Z |

----------------------------------------------------------------------

| 1 | 6 | 0 | -3.860491 | 1.431750 | -0.164245 |
| 2 | 6 | 0 | -3.029012 | 0.591816 | -1.086420 |
| 3 | 8 | 0 | -3.618275 | -0.102505 | -1.970087 |
| 4 | 7 | 0 | 0.488601 | -1.994185 | 1.951954 |
| 5 | 6 | 0 | 1.085603 | -2.770489 | 3.054300 |
| 6 | 6 | 0 | -5.140265 | 1.851105 | -0.553490 |
| 7 | 6 | 0 | -5.905779 | 2.646213 | 0.298036 |
| 8 | 6 | 0 | -5.403400 | 3.013954 | 1.549022 |
| 9 | 1 | 0 | 1.016195 | -2.238240 | 4.016295 |
| 10 | 1 | 0 | 2.154952 | -2.893270 | 2.838703 |
| 11 | 6 | 0 | 0.423456 | -4.140462 | 3.184241 |
| 12 | 8 | 0 | -1.763980 | 0.623440 | -0.930314 |
| 13 | 1 | 0 | 0.939378 | 1.690490 | -1.394268 |
| 14 | 1 | 0 | -0.971497 | -0.327957 | -1.698092 |
| 15 | 8 | 0 | -0.313844 | -0.950633 | -2.249761 |
| 16 | 1 | 0 | -0.856245 | -1.196169 | -3.054691 |
| 17 | 8 | 0 | -2.508375 | -1.483868 | 2.504951 |
| 18 | 1 | 0 | -3.103060 | -2.071697 | 1.978168 |
| 19 | 1 | 0 | -2.970295 | -1.341844 | 3.343750 |
| 20 | 8 | 0 | 0.586076 | 2.177442 | -0.586725 |
| 21 | 1 | 0 | 1.389765 | 1.264163 | 0.800637 |
| 22 | 1 | 0 | -0.362256 | 1.925555 | -0.550525 |
| 23 | 8 | 0 | 1.503318 | 0.619762 | -2.546073 |
| 24 | 1 | 0 | 0.581205 | -0.241184 | -2.507945 |
| 25 | 1 | 0 | 1.647983 | 0.950968 | -3.444386 |
| 26 | 1 | 0 | 0.436637 | -2.445168 | -1.158654 |
| 27 | 8 | 0 | 0.831471 | -3.089504 | -0.539272 |
| 28 | 1 | 0 | 0.665558 | -2.710322 | 0.391477 |
| 29 | 8 | 0 | 1.978088 | 0.666988 | 1.320205 |
| 30 | 1 | 0 | 0.962862 | -1.090744 | 1.867214 |

| 31 | 1 | 0 | 2.479509 | 1.238343 | 1.947583 |
| 32 | 1 | 0 | -2.849481 | -0.852959 | -3.333691 |
| 33 | 8 | 0 | -2.254590 | -1.265015 | -4.019875 |
| 34 | 1 | 0 | -2.637192 | -2.130410 | -4.227290 |
| 35 | 8 | 0 | 3.524987 | 2.360446 | 2.916114 |
| 36 | 1 | 0 | 3.062030 | 2.931319 | 3.546754 |
| 37 | 1 | 0 | 3.928800 | 2.958229 | 2.244851 |
| 38 | 8 | 0 | 4.462658 | 3.849413 | 0.756689 |
| 39 | 1 | 0 | 3.607051 | 4.093891 | 0.303840 |
| 40 | 1 | 0 | 4.952110 | 4.677271 | 0.875814 |
| 41 | 1 | 0 | -4.754232 | -1.344454 | -1.495584 |
| 42 | 8 | 0 | -5.311936 | -2.101224 | -1.183973 |
| 43 | 1 | 0 | -6.201633 | -1.740871 | -1.057356 |
| 44 | 1 | 0 | -4.605921 | -2.815337 | 0.273750 |
| 45 | 8 | 0 | -4.180047 | -3.208742 | 1.076010 |
| 46 | 1 | 0 | -3.715539 | -3.999139 | 0.763039 |
| 47 | 1 | 0 | 2.742720 | 0.189284 | -1.624507 |
| 48 | 8 | 0 | 3.430271 | 0.003697 | -0.908822 |
| 49 | 1 | 0 | 2.957872 | 0.192409 | -0.054693 |
| 50 | 1 | 0 | 1.427836 | 3.685178 | -0.404805 |
| 51 | 8 | 0 | 2.044012 | 4.461704 | -0.319635 |
| 52 | 1 | 0 | 1.995398 | 4.925377 | -1.168660 |
| 53 | 11 | 0 | 4.655898 | -1.844704 | -0.812225 |
| 54 | 8 | 0 | 6.604719 | -0.770917 | -0.470758 |
| 55 | 1 | 0 | 7.558673 | -0.878232 | -0.355369 |
| 56 | 1 | 0 | 6.422594 | 0.209837 | -0.526289 |
| 57 | 8 | 0 | 3.371374 | -3.632474 | -0.932766 |
| 58 | 1 | 0 | 2.384571 | -3.428887 | -0.800745 |
| 59 | 1 | 0 | 3.429338 | -4.589631 | -1.058174 |
| 60 | 8 | 0 | 5.586438 | 1.685418 | -0.856063 |
| 61 | 1 | 0 | 4.717042 | 1.224927 | -0.964455 |
| 62 | 1 | 0 | 5.397012 | 2.426810 | -0.246620 |
| 63 | 6 | 0 | -3.361391 | 1.800481 | 1.092054 |
| 64 | 6 | 0 | -4.134998 | 2.584229 | 1.947000 |
| 65 | 1 | 0 | -5.515522 | 1.563318 | -1.531067 |
| 66 | 1 | 0 | -6.891752 | 2.981313 | -0.013652 |
| 67 | 1 | 0 | -6.001033 | 3.631689 | 2.214597 |
| 68 | 1 | 0 | -2.385264 | 1.436990 | 1.395829 |
| 69 | 1 | 0 | -3.749632 | 2.858711 | 2.925320 |
| 70 | 1 | 0 | -0.644970 | -4.033873 | 3.407160 |
| 71 | 1 | 0 | 0.517267 | -4.707230 | 2.251732 |
| 72 | 1 | 0 | 0.881950 | -4.721408 | 3.993559 |
| 73 | 1 | 0 | -0.497130 | -1.805011 | 2.160492 |

---------------------------------------------------------------------

SCF Done:  E(RB3LYP) = -1940.84877758    A.U. after   13 cycles

Convg  =    0.3257D-08        -V/T =  2.0090

Zero-point correction=                      0.600769 (a.u.)
Thermal correction to Energy=               0.655273
Thermal correction to Enthalpy=             0.656217
Thermal correction to Gibbs Free Energy=    0.501791
Sum of electronic and zero-point Energies=      -1940.248009
Sum of electronic and thermal Energies=         -1940.193504
Sum of electronic and thermal Enthalpies=       -1940.192560
Sum of electronic and thermal Free Energies=    -1940.346986


 (8-9) Product, Ph-COONa + Et-NH2 + (H2O)16
tuka02d1na.for.chk    Stoichiometry C9H44NNaO18
                Standard orientation:

---------------------------------------------------------------------
Center    Atomic    Atomic          Coordinates (Angstroms)
Number    Number    Type        X         Y         Z
---------------------------------------------------------------------
  1        6         0      -3.777219   1.546187   0.016509
  2        6         0      -3.033283   0.803052  -1.064867
  3        8         0      -3.706599   0.077296  -1.855905
  4        7         0       0.319939  -1.423436   2.070731
  5        6         0       0.972902  -2.010179   3.256207
  6        6         0      -5.171959   1.672506  -0.048555
  7        6         0      -5.865958   2.346251   0.955239
  8        6         0      -5.175151   2.887256   2.042635
  9        1         0       0.953480  -1.320388   4.114519
 10        1         0       2.030078  -2.179195   3.010658
 11        6         0       0.313839  -3.330177   3.651094
 12        8         0      -1.766550   0.927134  -1.113166
 13        1         0       0.891791   1.767196  -1.919826
 14        1         0      -0.966141  -0.398911  -1.804425
 15        8         0      -0.446723  -1.125641  -2.260586
 16        1         0      -1.105339  -1.480475  -2.916379
 17        8         0      -2.664059  -1.358445   2.444086
 18        1         0      -2.750497  -2.092507   1.784443
 19        1         0      -3.178626  -0.617329   2.090336
 20        8         0       0.567353   2.293513  -1.153266
 21        1         0       1.377778   1.494793   0.286168
 22        1         0      -0.382048   2.021500  -1.055862
 23        8         0       1.494893   0.429711  -3.074469
 24        1         0       0.752220  -0.237124  -2.908896
 25        1         0       1.566710   0.553896  -4.032768
 26        1         0      -0.023940  -2.323033  -0.922338
 27        8         0       0.159919  -2.941456  -0.175330
 28        1         0       0.233191  -2.362179   0.669072
 29        8         0       1.949852   0.922329   0.849543
 30        1         0       0.776643  -0.546719   1.808243

| 31 | 1 | 0 | 2.465227 | 1.517848 | 1.445185 |
|----|---|---|----------|----------|----------|
| 32 | 1 | 0 | -3.023530 | -0.857199 | -3.306890 |
| 33 | 8 | 0 | -2.623424 | -1.608481 | -3.809009 |
| 34 | 1 | 0 | -3.131847 | -2.372274 | -3.483082 |
| 35 | 8 | 0 | 3.527759 | 2.603698 | 2.394495 |
| 36 | 1 | 0 | 3.087123 | 3.260909 | 2.953018 |
| 37 | 1 | 0 | 4.022886 | 3.105645 | 1.707352 |
| 38 | 8 | 0 | 4.676723 | 3.714374 | 0.121062 |
| 39 | 1 | 0 | 3.847364 | 3.988587 | -0.354537 |
| 40 | 1 | 0 | 5.269532 | 4.480692 | 0.100004 |
| 41 | 1 | 0 | -4.261787 | -1.577386 | -1.548182 |
| 42 | 8 | 0 | -4.334724 | -2.563820 | -1.578223 |
| 43 | 1 | 0 | -5.265043 | -2.779000 | -1.415501 |
| 44 | 1 | 0 | -3.182407 | -3.192787 | -0.229994 |
| 45 | 8 | 0 | -2.619295 | -3.390722 | 0.548263 |
| 46 | 1 | 0 | -1.690900 | -3.386118 | 0.229621 |
| 47 | 1 | 0 | 2.796394 | -0.072286 | -1.946586 |
| 48 | 8 | 0 | 3.354352 | -0.228309 | -1.148910 |
| 49 | 1 | 0 | 2.855899 | 0.204166 | -0.397864 |
| 50 | 1 | 0 | 1.559838 | 3.738914 | -1.011263 |
| 51 | 8 | 0 | 2.258768 | 4.437690 | -0.936862 |
| 52 | 1 | 0 | 2.101868 | 5.055307 | -1.665759 |
| 53 | 11 | 0 | 4.062780 | -2.185965 | -0.307848 |
| 54 | 8 | 0 | 5.986802 | -1.279728 | 0.423242 |
| 55 | 1 | 0 | 6.778262 | -1.472058 | 0.944670 |
| 56 | 1 | 0 | 6.060674 | -0.333885 | 0.117054 |
| 57 | 8 | 0 | 2.628172 | -3.864122 | -0.377350 |
| 58 | 1 | 0 | 1.658061 | -3.574699 | -0.336042 |
| 59 | 1 | 0 | 2.622624 | -4.831343 | -0.360966 |
| 60 | 8 | 0 | 5.737701 | 1.125525 | -0.785589 |
| 61 | 1 | 0 | 4.877754 | 0.778684 | -1.118223 |
| 62 | 1 | 0 | 5.522854 | 2.007808 | -0.421872 |
| 63 | 6 | 0 | -3.089455 | 2.097960 | 1.107143 |
| 64 | 6 | 0 | -3.786266 | 2.759089 | 2.119062 |
| 65 | 1 | 0 | -5.694618 | 1.242277 | -0.896428 |
| 66 | 1 | 0 | -6.946315 | 2.446729 | 0.892793 |
| 67 | 1 | 0 | -5.717784 | 3.404897 | 2.829337 |
| 68 | 1 | 0 | -2.010601 | 1.991961 | 1.156384 |
| 69 | 1 | 0 | -3.246448 | 3.173117 | 2.966434 |
| 70 | 1 | 0 | -0.744985 | -3.178819 | 3.888439 |
| 71 | 1 | 0 | 0.373719 | -4.058515 | 2.834453 |
| 72 | 1 | 0 | 0.803505 | -3.758738 | 4.533336 |
| 73 | 1 | 0 | -0.664818 | -1.218325 | 2.280361 |

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SCF Done:  E(RB+HF-LYP) = -1940.86925259    A.U. after    1 cycles

Convg  =    0.2598D-08         -V/T =  2.0090

S**2  =  0.0000
Zero-point correction=                    0.608875 (a.u.)
Thermal correction to Energy=            0.663116
Thermal correction to Enthalpy=          0.664060
Thermal correction to Gibbs Free Energy=      0.513287
Sum of electronic and zero-point Energies=      -1940.260378
Sum of electronic and thermal Energies=         -1940.206137
Sum of electronic and thermal Enthalpies=       -1940.205192
Sum of electronic and thermal Free Energies=    -1940.355966


===================================================================

[9] B3LYP/6-311+G(d,p) geometries of the reactant-like complex (precursor), TS1(am) and T2(am)

(9-1) precursor composed of Ph-C(=O)-NH-Et + HO-(H2O)16
     Stoichiometry   C9H44NO18(1-)
   tuka02aaA.for.log    Standard orientation:
---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|-------|-------|-------|
| Number | Number | Type | X | Y | Z |
| 1 | 6 | 0 | -0.499203 | 2.783375 | -0.571371 |
| 2 | 6 | 0 | -0.563601 | 1.822573 | 0.581891 |
| 3 | 8 | 0 | -1.436696 | 0.923726 | 0.591115 |
| 4 | 7 | 0 | 0.288228 | 2.006528 | 1.596346 |
| 5 | 6 | 0 | 0.347439 | 1.114923 | 2.757416 |
| 6 | 6 | 0 | -1.659104 | 2.960325 | -1.334224 |
| 7 | 6 | 0 | -1.670162 | 3.844240 | -2.408862 |
| 8 | 6 | 0 | 0.659105 | 3.491095 | -0.913722 |
| 9 | 1 | 0 | 1.075540 | 2.641784 | 1.486252 |
| 10 | 6 | 0 | 0.930000 | 1.835791 | 3.969091 |
| 11 | 1 | 0 | -0.663937 | 0.767788 | 2.965835 |
| 12 | 1 | 0 | 0.945263 | 0.234130 | 2.502918 |
| 13 | 8 | 0 | 1.993131 | 0.066980 | -0.704809 |
| 14 | 1 | 0 | 1.509488 | -0.125856 | -1.524185 |
| 15 | 1 | 0 | 1.797081 | -0.670779 | -0.058179 |
| 16 | 8 | 0 | 1.616962 | -2.027926 | 0.916532 |
| 17 | 1 | 0 | 2.139710 | -1.995038 | 1.723520 |
| 18 | 1 | 0 | 2.382696 | -2.686338 | -0.111899 |
| 19 | 8 | 0 | 2.970959 | -3.041976 | -0.922012 |
| 20 | 1 | 0 | 3.190156 | -2.228318 | -1.393267 |
| 21 | 1 | 0 | 4.448113 | -3.356543 | -0.139911 |
| 22 | 8 | 0 | 5.314639 | -3.381441 | 0.351728 |
| 23 | 1 | 0 | 5.176650 | -3.984340 | 1.087597 |
| 24 | 1 | 0 | 1.564848 | -3.487153 | -2.147377 |
| 25 | 8 | 0 | 0.906618 | -3.369448 | -2.860526 |
| 26 | 1 | 0 | 0.033077 | -3.637931 | -2.499690 |
| 27 | 1 | 0 | 0.698553 | -1.749733 | -3.085895 |
| 28 | 8 | 0 | 0.525596 | -0.761310 | -3.109130 |
| 29 | 1 | 0 | 0.766548 | -0.460814 | -3.990038 |
| 30 | 1 | 0 | 5.827765 | -1.699501 | 0.670593 |
| 31 | 8 | 0 | 6.145613 | -0.771523 | 0.747579 |
| 32 | 1 | 0 | 6.919548 | -0.732537 | 0.178390 |
| 33 | 1 | 0 | -1.841434 | -0.103503 | -1.078641 |
| 34 | 8 | 0 | -2.033456 | -0.575727 | -1.907067 |
| 35 | 1 | 0 | -1.208350 | -0.516302 | -2.425955 |
| 36 | 1 | 0 | -1.901697 | -2.617156 | -2.026373 |
| 37 | 8 | 0 | -1.723681 | -3.571888 | -2.062985 |

| 38 | 1 | 0 | -2.133766 | -3.895922 | -1.239788 |
|----|---|---|-----------|-----------|-----------|
| 39 | 1 | 0 | -3.905841 | -1.226164 | -1.516707 |
| 40 | 8 | 0 | -4.610180 | -1.671153 | -1.020936 |
| 41 | 1 | 0 | -5.081313 | -0.970691 | -0.531714 |
| 42 | 1 | 0 | -1.063967 | -0.963393 | 1.128015 |
| 43 | 8 | 0 | -0.927002 | -1.876642 | 1.424373 |
| 44 | 1 | 0 | 0.060017 | -2.042088 | 1.256273 |
| 45 | 1 | 0 | -2.113373 | -2.095439 | 2.817379 |
| 46 | 8 | 0 | -3.006608 | -2.128746 | 3.219791 |
| 47 | 1 | 0 | -3.454406 | -2.769657 | 2.647780 |
| 48 | 1 | 0 | -2.275817 | -2.964499 | 0.725137 |
| 49 | 8 | 0 | -3.049473 | -3.512371 | 0.482712 |
| 50 | 1 | 0 | -3.671803 | -2.903675 | 0.034060 |
| 51 | 1 | 0 | 3.512323 | 0.848359 | -0.348028 |
| 52 | 8 | 0 | 4.294916 | 1.315487 | 0.026204 |
| 53 | 1 | 0 | 4.900148 | 0.616294 | 0.335252 |
| 54 | 1 | 0 | 3.589365 | 2.459625 | 1.047183 |
| 55 | 8 | 0 | 3.050855 | 3.134302 | 1.542943 |
| 56 | 1 | 0 | 3.599937 | 3.920325 | 1.600558 |
| 57 | 1 | 0 | -3.546792 | -0.427349 | 2.755902 |
| 58 | 8 | 0 | -3.719761 | 0.461568 | 2.373986 |
| 59 | 1 | 0 | -2.945266 | 0.649910 | 1.817980 |
| 60 | 1 | 0 | -5.094614 | 0.387309 | 1.319521 |
| 61 | 8 | 0 | -5.806707 | 0.293799 | 0.639446 |
| 62 | 1 | 0 | -6.065554 | 1.189219 | 0.406994 |
| 63 | 6 | 0 | 0.647266 | 4.367100 | -1.996397 |
| 64 | 6 | 0 | -0.515789 | 4.550835 | -2.743058 |
| 65 | 1 | 0 | -2.544843 | 2.393836 | -1.078168 |
| 66 | 1 | 0 | -2.576739 | 3.973660 | -2.989441 |
| 67 | 1 | 0 | 1.577457 | 3.349942 | -0.357645 |
| 68 | 1 | 0 | 1.554275 | 4.898622 | -2.262484 |
| 69 | 1 | 0 | -0.519599 | 5.233576 | -3.586054 |
| 70 | 1 | 0 | 1.934352 | 2.208652 | 3.757056 |
| 71 | 1 | 0 | 0.300028 | 2.680310 | 4.262979 |
| 72 | 1 | 0 | 0.987069 | 1.144435 | 4.813701 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1779.27977846    A.U. after   2 cycles

Convg  =   0.2767D-08        -V/T = 2.0045

Zero-point correction=                     0.603199 (a.u.)

Thermal correction to Energy=              0.656616

Thermal correction to Enthalpy=            0.657561

Thermal correction to Gibbs Free Energy=        0.509767

Sum of electronic and zero-point Energies=        -1778.676579

Sum of electronic and thermal Energies=           -1778.623162

Sum of electronic and thermal Enthalpies=         -1778.622218

Sum of electronic and thermal Free Energies=      -1778.770011

(9-2) TS1(am), OH- addition step
Stoichiometry   C9H44NO18(1-)
tuka02aaA.chk    Stoichiometry   C9H44NO18(1-)
                 Standard orientation:

---------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type        X        Y        Z
---------------------------------------------------------------------
| 1 | 6 | 0 | -0.546702 | 2.408401 | -0.831962 |
| 2 | 6 | 0 | -0.209949 | 1.375026 | 0.257308 |
| 3 | 8 | 0 | -1.125726 | 0.463377 | 0.478868 |
| 4 | 7 | 0 | 0.301276 | 2.043319 | 1.396386 |
| 5 | 6 | 0 | 0.634211 | 1.289941 | 2.600510 |
| 6 | 6 | 0 | -1.881039 | 2.592709 | -1.197450 |
| 7 | 6 | 0 | -2.233385 | 3.546036 | -2.151956 |
| 8 | 6 | 0 | 0.431856 | 3.201553 | -1.440976 |
| 9 | 1 | 0 | 1.010526 | 2.734234 | 1.173419 |
| 10 | 6 | 0 | 0.858024 | 2.240735 | 3.775115 |
| 11 | 1 | 0 | -0.192119 | 0.614631 | 2.818619 |
| 12 | 1 | 0 | 1.531606 | 0.666739 | 2.461492 |
| 13 | 8 | 0 | 1.121639 | 0.568736 | -0.417193 |
| 14 | 1 | 0 | 0.860888 | 0.294566 | -1.315446 |
| 15 | 1 | 0 | 1.607333 | -0.819542 | 0.319802 |
| 16 | 8 | 0 | 1.998575 | -1.670110 | 0.688231 |
| 17 | 1 | 0 | 2.728946 | -1.390079 | 1.264102 |
| 18 | 1 | 0 | 2.793948 | -2.337676 | -0.641024 |
| 19 | 8 | 0 | 3.365370 | -2.673046 | -1.387501 |
| 20 | 1 | 0 | 3.513611 | -1.901171 | -1.946388 |
| 21 | 1 | 0 | 4.852117 | -3.010882 | -0.475095 |
| 22 | 8 | 0 | 5.587670 | -3.031905 | 0.181550 |
| 23 | 1 | 0 | 5.598775 | -3.928715 | 0.528516 |
| 24 | 1 | 0 | 1.757882 | -3.264009 | -2.567282 |
| 25 | 8 | 0 | 1.032144 | -3.086498 | -3.183682 |
| 26 | 1 | 0 | 0.210423 | -3.437763 | -2.757331 |
| 27 | 1 | 0 | 0.683750 | -1.409044 | -3.216648 |
| 28 | 8 | 0 | 0.423586 | -0.454962 | -3.119057 |
| 29 | 1 | 0 | 0.665185 | -0.013971 | -3.938400 |
| 30 | 1 | 0 | 5.107086 | -1.635362 | 1.206116 |
| 31 | 8 | 0 | 4.622429 | -0.874253 | 1.596727 |
| 32 | 1 | 0 | 5.065706 | -0.643693 | 2.418170 |
| 33 | 1 | 0 | -1.778238 | -0.392603 | -0.923320 |
| 34 | 8 | 0 | -2.097343 | -0.851482 | -1.740641 |
| 35 | 1 | 0 | -1.475221 | -0.556005 | -2.424074 |
| 36 | 1 | 0 | -1.673092 | -2.688066 | -1.979117 |
| 37 | 8 | 0 | -1.374879 | -3.612286 | -2.086363 |

| 38 | 1 | 0 | -1.663946 | -4.019150 | -1.244492 |
| 39 | 1 | 0 | -3.804403 | -1.690584 | -1.155424 |
| 40 | 8 | 0 | -4.423265 | -2.200765 | -0.608196 |
| 41 | 1 | 0 | -4.854338 | -1.542844 | -0.029421 |
| 42 | 1 | 0 | -0.837649 | -1.074203 | 1.177763 |
| 43 | 8 | 0 | -0.708531 | -1.964996 | 1.601204 |
| 44 | 1 | 0 | 0.237441 | -2.144265 | 1.470175 |
| 45 | 1 | 0 | -1.647388 | -1.876565 | 3.120108 |
| 46 | 8 | 0 | -2.330903 | -1.686780 | 3.799909 |
| 47 | 1 | 0 | -2.996484 | -2.369190 | 3.665412 |
| 48 | 1 | 0 | -1.878575 | -3.319194 | 0.883835 |
| 49 | 8 | 0 | -2.480781 | -3.968026 | 0.476440 |
| 50 | 1 | 0 | -3.255652 | -3.438323 | 0.196266 |
| 51 | 1 | 0 | 2.796548 | 1.095316 | -0.306049 |
| 52 | 8 | 0 | 3.738024 | 1.356855 | -0.155809 |
| 53 | 1 | 0 | 4.116631 | 0.651618 | 0.392087 |
| 54 | 1 | 0 | 3.511585 | 2.861746 | 0.771118 |
| 55 | 8 | 0 | 3.215843 | 3.642466 | 1.291451 |
| 56 | 1 | 0 | 3.454365 | 4.407839 | 0.761732 |
| 57 | 1 | 0 | -2.953921 | -0.053862 | 2.955328 |
| 58 | 8 | 0 | -3.219356 | 0.640946 | 2.324632 |
| 59 | 1 | 0 | -2.474904 | 0.696379 | 1.684448 |
| 60 | 1 | 0 | -4.666479 | 0.137711 | 1.572729 |
| 61 | 8 | 0 | -5.476559 | -0.209855 | 1.116665 |
| 62 | 1 | 0 | -5.923894 | 0.562893 | 0.761917 |
| 63 | 6 | 0 | 0.082329 | 4.155879 | -2.394399 |
| 64 | 6 | 0 | -1.253637 | 4.332345 | -2.754799 |
| 65 | 1 | 0 | -2.637856 | 1.975520 | -0.731725 |
| 66 | 1 | 0 | -3.275703 | 3.671106 | -2.426061 |
| 67 | 1 | 0 | 1.473342 | 3.062727 | -1.179526 |
| 68 | 1 | 0 | 0.855204 | 4.758811 | -2.860362 |
| 69 | 1 | 0 | -1.526431 | 5.072735 | -3.499576 |
| 70 | 1 | 0 | 1.675998 | 2.934771 | 3.562019 |
| 71 | 1 | 0 | -0.046519 | 2.821763 | 3.971965 |
| 72 | 1 | 0 | 1.111236 | 1.677335 | 4.678692 |

---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1779.24427796    A.U. after    1 cycles

Convg  =    0.5611D-08         -V/T = 2.0045

Zero-point correction=                    0.604806 (a.u.)

Thermal correction to Energy=                  0.656899

Thermal correction to Enthalpy=               0.657843

Thermal correction to Gibbs Free Energy=       0.515283

Sum of electronic and zero-point Energies=        -1778.639472

Sum of electronic and thermal Energies=           -1778.587379

Sum of electronic and thermal Enthalpies=         -1778.586435

Sum of electronic and thermal Free Energies=       -1778.728995

(9-3) TS2(am) toward the Mulliken CT complex
stoichiometry    C9H44NO18(1-)

tuka02bzA.chk   Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic            Coordinates (Angstroms)
Number     Number     Type        X          Y          Z
---------------------------------------------------------------------
   1          6          0      -1.443656   0.990498   -0.999210
   2          6          0      -1.791453   -0.411947  -0.447736
   3          8          0      -2.584070   -0.398194   0.624447
   4          7          0      -0.470538   -1.114289  -0.103050
   5          6          0      -0.669353   -2.502998   0.399191
   6          6          0      -1.828564   2.139827   -0.307919
   7          6          0      -1.540028   3.405764   -0.822096
   8          6          0      -0.852669   3.534761   -2.028604
   9          1          0       0.145875   -1.138798  -0.920861
  10          1          0      -1.208909   -2.422750   1.342605
  11          1          0      -1.309554   -3.031360  -0.308311
  12          6          0       0.651852   -3.238935   0.591269
  13          8          0      -2.312465   -1.205766  -1.528189
  14          1          0      -3.218896   -0.894619  -1.699995
  15          1          0      -5.117214   -2.941092  -0.067859
  16          8          0      -5.469911   -3.203265  -0.959763
  17          1          0      -4.811419   -3.806810  -1.317445
  18          1          0       0.108696   -0.455394   0.719120
  19          8          0       0.814315   0.257266   1.589525
  20          1          0       0.250461   0.422462   2.356999
  21          1          0       2.326631   -0.367400   1.560439
  22          8          0       3.213875   -0.622913   1.168182
  23          1          0       3.601832   -1.417014   1.576851
  24          1          0      -5.390228   -1.599809  -1.704926
  25          8          0      -5.173813   -0.672625   -1.963034
  26          1          0      -5.525008   -0.545474  -2.848888
  27          1          0      -4.157340   0.355077   0.641001
  28          8          0      -5.103201   0.605779   0.783094
  29          1          0      -5.479731   0.530321   -0.103874
  30          1          0       2.691415   -1.032795  -0.553052
  31          8          0       2.442011   -1.151552  -1.493693
  32          1          0       2.614915   -0.260466  -1.862471
  33          1          0       4.372986   0.542163   0.665524
  34          8          0       5.053236   1.138073   0.264900
  35          1          0       4.939936   1.984273   0.739591
  36          1          0      -3.658827   -1.723308   1.053009
  37          8          0      -4.468830   -2.214279   1.346311
  38          1          0      -5.071408   -1.475843   1.526009

| 39 | 1 | 0 | 6.285004 | -0.077804 | 0.014015 |
|----|---|---|----------|-----------|----------|
| 40 | 8 | 0 | 6.744118 | -0.939674 | -0.126338 |
| 41 | 1 | 0 | 7.650624 | -0.726389 | -0.363065 |
| 42 | 1 | 0 | 3.993645 | -2.310323 | -1.635425 |
| 43 | 8 | 0 | 4.798664 | -2.814112 | -1.405079 |
| 44 | 1 | 0 | 5.486305 | -2.142847 | -1.273310 |
| 45 | 1 | 0 | -2.230074 | -0.185115 | 3.665892 |
| 46 | 8 | 0 | -1.929972 | 0.503325 | 3.064547 |
| 47 | 1 | 0 | -2.120134 | 0.150431 | 2.152881 |
| 48 | 1 | 0 | -3.361699 | 1.949393 | 3.028162 |
| 49 | 8 | 0 | -4.121165 | 2.524217 | 2.838823 |
| 50 | 1 | 0 | -4.627122 | 2.032616 | 2.173134 |
| 51 | 1 | 0 | 3.946429 | 1.490369 | -1.361438 |
| 52 | 8 | 0 | 3.121761 | 1.560063 | -1.873405 |
| 53 | 1 | 0 | 2.501311 | 1.932843 | -1.218734 |
| 54 | 1 | 0 | 0.835104 | 2.964259 | 0.207811 |
| 55 | 8 | 0 | 1.622229 | 2.462171 | 0.450445 |
| 56 | 1 | 0 | 1.276656 | 1.626957 | 0.920326 |
| 57 | 6 | 0 | -0.767392 | 1.128796 | -2.216768 |
| 58 | 6 | 0 | -0.464659 | 2.389462 | -2.724794 |
| 59 | 1 | 0 | -2.361890 | 2.050475 | 0.628394 |
| 60 | 1 | 0 | -1.860218 | 4.286999 | -0.276375 |
| 61 | 1 | 0 | -0.621584 | 4.517988 | -2.424493 |
| 62 | 1 | 0 | -0.483813 | 0.244445 | -2.775389 |
| 63 | 1 | 0 | 0.078681 | 2.477408 | -3.658864 |
| 64 | 1 | 0 | 1.207456 | -3.320466 | -0.345496 |
| 65 | 1 | 0 | 1.288395 | -2.736532 | 1.321116 |
| 66 | 1 | 0 | 0.451637 | -4.249970 | 0.956985 |
| 67 | 1 | 0 | 3.073120 | 3.165430 | 1.159617 |
| 68 | 8 | 0 | 3.958605 | 3.404437 | 1.523716 |
| 69 | 1 | 0 | 3.840266 | 3.411894 | 2.477877 |
| 70 | 1 | 0 | 5.762698 | -2.274896 | 1.325989 |
| 71 | 8 | 0 | 4.974374 | -2.823117 | 1.450224 |
| 72 | 1 | 0 | 4.776221 | -3.088526 | 0.530558 |

---------------------------------------------------------------------

 SCF Done:  E(RB+HF-LYP) = -1779.23815810    A.U. after   3 cycles

        Convg  =   0.1606D-08          -V/T = 2.0045

Zero-point correction=                        0.602525 (a.u.)

Thermal correction to Energy=                 0.654001

Thermal correction to Enthalpy=               0.654945

Thermal correction to Gibbs Free Energy=      0.513845

Sum of electronic and zero-point Energies=        -1778.635633

Sum of electronic and thermal Energies=           -1778.584157

Sum of electronic and thermal Enthalpies=         -1778.583213

Sum of electronic and thermal Free Energies=      -1778.724313

=======================================================================

[10] para-Y-substituted N-ethylbenzamide + OH⁻(H₂O)₁₆, Y = MeO and NO₂.  precursor, TS1(am) and TS2(am)


(10-1) Y= MeO(CH3O), precursor
tuka02aaome.for.chk  Stoichiometry  C10H46NO19(1-)


Largest concise Abelian subgroup C1     NOp   1
                    Standard orientation:
---------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|------|------|------|
| Number | Number | Type | X | Y | Z |

---------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|------|------|------|------|------|------|
| 1 | 6 | 0 | -2.121205 | -1.104406 | 0.561960 |
| 2 | 6 | 0 | -0.858666 | -0.836162 | 1.316489 |
| 3 | 8 | 0 | 0.198429 | -1.454504 | 1.008143 |
| 4 | 7 | 0 | -0.906565 | 0.021432 | 2.346483 |
| 5 | 6 | 0 | 0.269557 | 0.407911 | 3.130060 |
| 6 | 6 | 0 | -2.248104 | -2.332274 | -0.110292 |
| 7 | 6 | 0 | -3.395233 | -2.638525 | -0.827170 |
| 8 | 6 | 0 | -3.173580 | -0.185155 | 0.480778 |
| 9 | 1 | 0 | -1.727718 | 0.614137 | 2.467119 |
| 10 | 6 | 0 | -0.136295 | 0.855323 | 4.532484 |
| 11 | 1 | 0 | 0.937957 | -0.453527 | 3.180197 |
| 12 | 1 | 0 | 0.806351 | 1.208956 | 2.607015 |
| 13 | 8 | 0 | -0.594346 | 1.825607 | -0.552651 |
| 14 | 1 | 0 | -0.605331 | 1.389401 | -1.427901 |
| 15 | 1 | 0 | 0.373937 | 1.939839 | -0.295468 |
| 16 | 8 | 0 | 1.956832 | 2.301001 | 0.073792 |
| 17 | 1 | 0 | 1.971109 | 2.910850 | 0.826735 |
| 18 | 1 | 0 | 2.005118 | 3.059483 | -1.135009 |
| 19 | 8 | 0 | 1.934498 | 3.629905 | -2.043114 |
| 20 | 1 | 0 | 0.978889 | 3.667837 | -2.214814 |
| 21 | 1 | 0 | 2.207290 | 5.154184 | -1.339487 |
| 22 | 8 | 0 | 2.270420 | 5.988585 | -0.786614 |
| 23 | 1 | 0 | 3.114301 | 5.918002 | -0.316293 |
| 24 | 1 | 0 | 2.225437 | 2.214550 | -3.245660 |
| 25 | 8 | 0 | 2.051800 | 1.448420 | -3.840387 |
| 26 | 1 | 0 | 2.663539 | 0.717080 | -3.570213 |
| 27 | 1 | 0 | 0.587467 | 0.830694 | -3.424762 |
| 28 | 8 | 0 | -0.271728 | 0.420457 | -3.081049 |
| 29 | 1 | 0 | -0.886024 | 0.400455 | -3.829257 |
| 30 | 1 | 0 | 0.868253 | 5.967973 | 0.296873 |
| 31 | 8 | 0 | 0.075713 | 5.994197 | 0.893560 |
| 32 | 1 | 0 | -0.354788 | 6.840111 | 0.702322 |
| 33 | 1 | 0 | 0.604790 | -1.730384 | -0.894551 |
| 34 | 8 | 0 | 0.765543 | -1.898588 | -1.846936 |
| 35 | 1 | 0 | 0.264850 | -1.192192 | -2.314512 |

| 36 | 1 | 0 | 2.443601 | -1.300192 | -2.693732 |
|---|---|---|---|---|---|
| 37 | 8 | 0 | 3.243931 | -0.909600 | -3.103282 |
| 38 | 1 | 0 | 3.942571 | -1.112848 | -2.443743 |
| 39 | 1 | 0 | 1.951495 | -3.498974 | -1.674756 |
| 40 | 8 | 0 | 2.731992 | -4.000252 | -1.371301 |
| 41 | 1 | 0 | 2.433064 | -4.559694 | -0.619157 |
| 42 | 1 | 0 | 1.899366 | -0.501092 | 0.854495 |
| 43 | 8 | 0 | 2.779854 | -0.085258 | 0.773131 |
| 44 | 1 | 0 | 2.573679 | 0.869623 | 0.489714 |
| 45 | 1 | 0 | 3.868413 | -1.018090 | 1.990280 |
| 46 | 8 | 0 | 4.301093 | -1.857311 | 2.268127 |
| 47 | 1 | 0 | 4.693223 | -2.157155 | 1.422944 |
| 48 | 1 | 0 | 3.793749 | -1.199837 | -0.289845 |
| 49 | 8 | 0 | 4.417210 | -1.856387 | -0.681074 |
| 50 | 1 | 0 | 3.879829 | -2.664527 | -0.867243 |
| 51 | 1 | 0 | -1.461468 | 3.194538 | 0.073681 |
| 52 | 8 | 0 | -1.883669 | 3.916115 | 0.610343 |
| 53 | 1 | 0 | -1.187059 | 4.597619 | 0.737046 |
| 54 | 1 | 0 | -2.371112 | 3.039357 | 1.975774 |
| 55 | 8 | 0 | -2.683796 | 2.405947 | 2.687382 |
| 56 | 1 | 0 | -3.560620 | 2.719673 | 2.950326 |
| 57 | 1 | 0 | 2.783950 | -2.825873 | 2.528141 |
| 58 | 8 | 0 | 1.887829 | -3.248968 | 2.553964 |
| 59 | 1 | 0 | 1.300729 | -2.631290 | 2.072375 |
| 60 | 1 | 0 | 1.957535 | -4.673945 | 1.590327 |
| 61 | 8 | 0 | 1.984657 | -5.428645 | 0.938584 |
| 62 | 1 | 0 | 1.126889 | -5.870758 | 1.010864 |
| 63 | 6 | 0 | -4.327885 | -0.478526 | -0.246282 |
| 64 | 6 | 0 | -4.442719 | -1.710318 | -0.900161 |
| 65 | 1 | 0 | -1.430749 | -3.043589 | -0.067284 |
| 66 | 1 | 0 | -3.497477 | -3.586894 | -1.345219 |
| 67 | 1 | 0 | -3.096148 | 0.785570 | 0.958805 |
| 68 | 1 | 0 | -5.116348 | 0.262836 | -0.302714 |
| 69 | 8 | 0 | -5.534090 | -2.095642 | -1.636651 |
| 70 | 1 | 0 | -0.828031 | 1.702829 | 4.490303 |
| 71 | 1 | 0 | -0.619028 | 0.037276 | 5.079587 |
| 72 | 1 | 0 | 0.754187 | 1.161742 | 5.092037 |
| 73 | 6 | 0 | -6.612404 | -1.180835 | -1.767982 |
| 74 | 1 | 0 | -7.057469 | -0.943758 | -0.792926 |
| 75 | 1 | 0 | -6.291289 | -0.251401 | -2.255209 |
| 76 | 1 | 0 | -7.353119 | -1.681455 | -2.393620 |

-----------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1893.08683444    A.U. after   1 cycles

Convg  =    0.7549D-08          -V/T =  2.0093

Zero-point correction=                  0.639390 (a.u.)

Thermal correction to Energy=            0.693874

Thermal correction to Enthalpy=          0.694819
Thermal correction to Gibbs Free Energy=       0.544924
Sum of electronic and zero-point Energies=        -1892.447444
Sum of electronic and thermal Energies=          -1892.392960
Sum of electronic and thermal Enthalpies=         -1892.392016
Sum of electronic and thermal Free Energies=       -1892.541911

 (10-2)  TS1(am), Y=MeO
 tuka02aaome.chk     Stoichiometry C10H46NO19(1-)
              Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic          Coordinates (Angstroms)
Number     Number     Type          X          Y          Z
---------------------------------------------------------------------
   1          6          0      2.172861    0.058594    0.234528
   2          6          0      0.812803    0.124968    0.929476
   3          8          0      0.091952    1.188496    0.696395
   4          7          0      0.890573   -0.333708    2.246646
   5          6          0     -0.283766   -0.323108    3.116851
   6          6          0      2.787366    1.254191   -0.165048
   7          6          0      4.042373    1.254738   -0.764537
   8          6          0      2.862398   -1.138233    0.020446
   9          1          0      1.441978   -1.182993    2.357910
  10          6          0      0.126205   -0.595898    4.563394
  11          1          0     -0.754516    0.658896    3.044809
  12          1          0     -1.029223   -1.065950    2.793046
  13          8          0     -0.059621   -1.213592    0.059029
  14          1          0      0.056722   -1.025648   -0.893422
  15          1          0     -1.673030   -1.386550    0.301184
  16          8          0     -2.662542   -1.525711    0.477696
  17          1          0     -2.710533   -2.366829    0.973108
  18          1          0     -3.464060   -1.962792   -1.048497
  19          8          0     -3.856420   -2.374867   -1.861085
  20          1          0     -3.369959   -1.968071   -2.610926
  21          1          0     -3.788129   -4.009488   -1.540388
  22          8          0     -3.816458   -4.940410   -1.160711
  23          1          0     -4.759877   -5.148773   -1.093634
  24          8          0     -2.343846   -0.954929   -3.787750
  25          1          0     -2.532241    0.017605   -3.543483
  26          1          0     -2.535240   -1.025764   -4.734683
  27          1          0     -0.602169   -0.956750   -3.276992
  28          8          0      0.288856   -0.761069   -2.896859
  29          1          0      0.862427   -1.508434   -3.120233
  30          1          0     -2.978011   -4.680293    0.350975
  31          8          0     -2.484939   -4.357026    1.153269
  32          1          0     -2.747172   -4.922112    1.894214

| 33 | 1 | 0 | -0.033074 | 1.684112 | -0.976854 |
|----|---|---|-----------|-----------|-----------|
| 34 | 8 | 0 | -0.061275 | 1.956127 | -1.937384 |
| 35 | 1 | 0 | 0.408515 | 1.236411 | -2.399159 |
| 36 | 1 | 0 | -1.661753 | 1.743254 | -2.783386 |
| 37 | 8 | 0 | -2.541017 | 1.568907 | -3.199017 |
| 38 | 1 | 0 | -3.165608 | 1.975519 | -2.541827 |
| 39 | 1 | 0 | -0.773072 | 3.814799 | -1.790150 |
| 40 | 8 | 0 | -1.377273 | 4.535344 | -1.525749 |
| 41 | 1 | 0 | -0.956204 | 4.962762 | -0.744509 |
| 42 | 1 | 0 | -1.637181 | 1.193209 | 0.884483 |
| 43 | 8 | 0 | -2.629958 | 1.224922 | 0.976383 |
| 44 | 1 | 0 | -2.899600 | 0.280368 | 0.934554 |
| 45 | 1 | 0 | -2.845359 | 2.301293 | 2.355945 |
| 46 | 8 | 0 | -2.744178 | 3.014261 | 3.037903 |
| 47 | 1 | 0 | -3.226191 | 3.773022 | 2.675654 |
| 48 | 1 | 0 | -3.319061 | 2.306428 | -0.382586 |
| 49 | 8 | 0 | -3.643969 | 2.912318 | -1.086252 |
| 50 | 1 | 0 | -2.942234 | 3.601917 | -1.171187 |
| 51 | 1 | 0 | 0.196318 | -2.862525 | 0.383005 |
| 52 | 8 | 0 | 0.333404 | -3.814204 | 0.667140 |
| 53 | 1 | 0 | -0.570584 | -4.150450 | 0.830235 |
| 54 | 1 | 0 | 1.237201 | -3.605389 | 2.132123 |
| 55 | 8 | 0 | 1.788653 | -3.330240 | 2.914233 |
| 56 | 1 | 0 | 2.657108 | -3.732609 | 2.771380 |
| 57 | 1 | 0 | -0.908819 | 3.332806 | 2.731217 |
| 58 | 8 | 0 | -0.006130 | 3.444174 | 2.354913 |
| 59 | 1 | 0 | 0.138695 | 2.633822 | 1.807579 |
| 60 | 1 | 0 | -0.074751 | 4.820476 | 1.371096 |
| 61 | 8 | 0 | -0.155805 | 5.611678 | 0.763531 |
| 62 | 1 | 0 | 0.744954 | 5.946737 | 0.648835 |
| 63 | 6 | 0 | 4.125371 | -1.154874 | -0.579728 |
| 64 | 6 | 0 | 4.718378 | 0.048198 | -0.974282 |
| 65 | 1 | 0 | 2.265107 | 2.191047 | -0.005005 |
| 66 | 1 | 0 | 4.514546 | 2.181434 | -1.076904 |
| 67 | 1 | 0 | 2.406593 | -2.079613 | 0.306795 |
| 68 | 1 | 0 | 4.624286 | -2.105130 | -0.735279 |
| 69 | 8 | 0 | 5.955644 | 0.144245 | -1.575842 |
| 70 | 1 | 0 | 0.622144 | -1.568853 | 4.652187 |
| 71 | 1 | 0 | 0.814829 | 0.178603 | 4.918934 |
| 72 | 1 | 0 | -0.757378 | -0.597768 | 5.212832 |
| 73 | 6 | 0 | 6.677161 | -1.053499 | -1.803470 |
| 74 | 1 | 0 | 6.896062 | -1.577383 | -0.863246 |
| 75 | 1 | 0 | 6.131742 | -1.731750 | -2.473489 |
| 76 | 1 | 0 | 7.614259 | -0.754492 | -2.277311 |

-----------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1893.05649779     A.U. after    1 cycles

Convg = 0.5166D-08          -V/T = 2.0093
Zero-point correction=                      0.640600 (a.u.)
Thermal correction to Energy=               0.693667
Thermal correction to Enthalpy=             0.694611
Thermal correction to Gibbs Free Energy=    0.551135
Sum of electronic and zero-point Energies=        -1892.415898
Sum of electronic and thermal Energies=           -1892.362831
Sum of electronic and thermal Enthalpies=         -1892.361887
Sum of electronic and thermal Free Energies=      -1892.505363


 (10-3) TS2(am), Y=MeO
tuka02bzome.chk    Stoichiometry C10H46NO19(1-)


              Standard orientation:
---------------------------------------------------------------------
Center   Atomic   Atomic         Coordinates (Angstroms)
Number   Number   Type        X        Y        Z
---------------------------------------------------------------------
   1       6       0     -1.397385   0.904052  -0.604076
   2       6       0     -1.803341  -0.572130  -0.470918
   3       8       0     -2.601009  -0.845862   0.560041
   4       7       0     -0.482102  -1.399609  -0.312873
   5       6       0     -0.714152  -2.874418  -0.237084
   6       6       0     -1.747948   1.842297   0.375732
   7       6       0     -1.375411   3.177837   0.251619
   8       6       0     -0.627349   3.598593  -0.855539
   9       1       0      0.194294  -1.189325  -1.065292
  10       1       0     -1.358156  -3.041969   0.627935
  11       1       0     -1.269354  -3.154679  -1.133666
  12       6       0      0.586761  -3.662176  -0.120593
  13       8       0     -2.295874  -1.054548  -1.725308
  14       1       0     -3.185170  -0.656743  -1.852954
  15       1       0     -5.215271  -2.952568  -0.871838
  16       8       0     -5.533779  -2.929595  -1.821782
  17       1       0     -4.858969  -3.410962  -2.323763
  18       1       0     -0.005909  -1.055216   0.578291
  19       8       0      0.842890  -0.513251   1.916253
  20       1       0      0.185315  -0.472247   2.634968
  21       1       0      2.369367  -1.281169   1.627565
  22       8       0      3.177492  -1.402067   1.059480
  23       1       0      3.592739  -2.289187   1.151878
  24       1       0     -5.336154  -1.210129  -2.066358
  25       8       0     -5.046694  -0.257901  -2.048659
  26       1       0     -5.334590   0.139307  -2.883421
  27       1       0     -4.147067  -0.054429   0.739275
  28       8       0     -5.101473   0.157840   0.917126

| | | | | | |
|---|---|---|---|---|---|
| 29 | 1 | 0 | -5.445819 | 0.366424 | 0.030613 |
| 30 | 1 | 0 | 2.509875 | -1.212165 | -0.607819 |
| 31 | 8 | 0 | 2.233777 | -1.011017 | -1.535373 |
| 32 | 1 | 0 | 2.420756 | -0.035091 | -1.583586 |
| 33 | 1 | 0 | 4.332422 | -0.089548 | 0.886273 |
| 34 | 8 | 0 | 5.020612 | 0.585727 | 0.659180 |
| 35 | 1 | 0 | 4.896414 | 1.287251 | 1.347518 |
| 36 | 1 | 0 | -3.747260 | -2.196696 | 0.568665 |
| 37 | 8 | 0 | -4.598657 | -2.695630 | 0.700340 |
| 38 | 1 | 0 | -5.173787 | -1.983092 | 1.043882 |
| 39 | 1 | 0 | 6.192343 | -0.502188 | 0.001599 |
| 40 | 8 | 0 | 6.626953 | -1.286876 | -0.429827 |
| 41 | 1 | 0 | 7.517096 | -1.001035 | -0.680478 |
| 42 | 1 | 0 | 3.760928 | -1.998921 | -2.096879 |
| 43 | 8 | 0 | 4.573521 | -2.556457 | -2.094880 |
| 44 | 1 | 0 | 5.293110 | -1.967659 | -1.791142 |
| 45 | 1 | 0 | -2.213372 | -1.359863 | 3.588360 |
| 46 | 8 | 0 | -1.912082 | -0.550360 | 3.149166 |
| 47 | 1 | 0 | -2.126232 | -0.678973 | 2.180408 |
| 48 | 1 | 0 | -3.437144 | 0.719799 | 3.523370 |
| 49 | 8 | 0 | -4.269583 | 1.232089 | 3.552200 |
| 50 | 1 | 0 | -4.725788 | 1.005585 | 2.718831 |
| 51 | 1 | 0 | 3.813782 | 1.422389 | -0.730520 |
| 52 | 8 | 0 | 2.922552 | 1.613553 | -1.087191 |
| 53 | 1 | 0 | 2.382801 | 1.706975 | -0.250465 |
| 54 | 1 | 0 | 0.986301 | 2.343897 | 1.358152 |
| 55 | 8 | 0 | 1.714887 | 1.704341 | 1.374334 |
| 56 | 1 | 0 | 1.221333 | 0.579346 | 1.690672 |
| 57 | 6 | 0 | -0.674625 | 1.345314 | -1.716871 |
| 58 | 6 | 0 | -0.280800 | 2.676830 | -1.849442 |
| 59 | 1 | 0 | -2.315382 | 1.530253 | 1.244844 |
| 60 | 1 | 0 | -1.649715 | 3.905526 | 1.009435 |
| 61 | 8 | 0 | -0.284704 | 4.927151 | -0.886056 |
| 62 | 1 | 0 | -0.409449 | 0.641310 | -2.500478 |
| 63 | 1 | 0 | 0.305822 | 2.973465 | -2.710276 |
| 64 | 1 | 0 | 1.238781 | -3.495270 | -0.983472 |
| 65 | 1 | 0 | 1.140504 | -3.395342 | 0.784238 |
| 66 | 1 | 0 | 0.353878 | -4.731871 | -0.071693 |
| 67 | 1 | 0 | 3.083132 | 2.202230 | 2.105864 |
| 68 | 8 | 0 | 4.011861 | 2.391658 | 2.472080 |
| 69 | 1 | 0 | 3.983732 | 2.099576 | 3.394759 |
| 70 | 1 | 0 | 5.668998 | -3.032670 | 0.605462 |
| 71 | 8 | 0 | 4.845301 | -3.547525 | 0.528642 |
| 72 | 1 | 0 | 4.631193 | -3.436063 | -0.429066 |
| 73 | 6 | 0 | 0.679305 | 5.341403 | -1.846791 |
| 74 | 1 | 0 | 1.595821 | 4.744561 | -1.768361 |

| 75 | 1 | 0 | 0.283322 | 5.272648 | -2.868872 |
|----|---|---|----------|----------|-----------|
| 76 | 1 | 0 | 0.896998 | 6.386036 | -1.616685 |

------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1893.04834908     A.U. after    1 cycles

Convg  =    0.3567D-08           -V/T =  2.0093

Zero-point correction=                       0.638580 (a.u.)

Thermal correction to Energy=                0.691004

Thermal correction to Enthalpy=              0.691948

Thermal correction to Gibbs Free Energy=       0.548583

Sum of electronic and zero-point Energies=      -1892.409769

Sum of electronic and thermal Energies=         -1892.357345

Sum of electronic and thermal Enthalpies=       -1892.356401

Sum of electronic and thermal Free Energies=      -1892.499766

 (10-4) precursor, Y=NO2

tuka02aano2.for.chk   Stoichiometry   C9H43N2O20(1-)

Standard orientation:

------------------------------------------------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|-----|-----|-----|
| Number | Number | Type | X | Y | Z |

------------------------------------------------------------------

| 1 | 6 | 0 | 2.212908 | -0.020542 | 0.713925 |
|----|---|---|----------|-----------|-----------|
| 2 | 6 | 0 | 0.917334 | 0.306723 | 1.408306 |
| 3 | 8 | 0 | 0.280904 | 1.336460 | 1.064696 |
| 4 | 7 | 0 | 0.534228 | -0.479950 | 2.419459 |
| 5 | 6 | 0 | -0.712623 | -0.273779 | 3.163853 |
| 6 | 6 | 0 | 2.909068 | 1.038319 | 0.111856 |
| 7 | 6 | 0 | 4.121385 | 0.817040 | -0.532495 |
| 8 | 6 | 0 | 2.736304 | -1.321147 | 0.646108 |
| 9 | 1 | 0 | 0.980568 | -1.389207 | 2.552533 |
| 10 | 6 | 0 | -0.615780 | -0.879567 | 4.561686 |
| 11 | 1 | 0 | -0.895826 | 0.800986 | 3.220731 |
| 12 | 1 | 0 | -1.542485 | -0.718355 | 2.601157 |
| 13 | 8 | 0 | -0.395642 | -1.834101 | -0.503284 |
| 14 | 1 | 0 | -0.200809 | -1.480738 | -1.394625 |
| 15 | 1 | 0 | -1.334789 | -1.540270 | -0.274459 |
| 16 | 8 | 0 | -2.924274 | -1.179194 | 0.008993 |
| 17 | 1 | 0 | -3.262842 | -1.715951 | 0.741256 |
| 18 | 1 | 0 | -3.282388 | -1.823078 | -1.230109 |
| 19 | 8 | 0 | -3.464434 | -2.347640 | -2.143184 |
| 20 | 1 | 0 | -2.630700 | -2.815516 | -2.315096 |
| 21 | 1 | 0 | -4.407591 | -3.611465 | -1.493162 |
| 22 | 8 | 0 | -4.826067 | -4.370878 | -0.991079 |
| 23 | 1 | 0 | -5.598046 | -3.993229 | -0.544586 |
| 24 | 1 | 0 | -3.056305 | -0.940108 | -3.326297 |

| 25 | 8 | 0 | -2.525446 | -0.343817 | -3.902945 |
| 26 | 1 | 0 | -2.738894 | 0.588980 | -3.644827 |
| 27 | 1 | 0 | -0.964126 | -0.479204 | -3.437347 |
| 28 | 8 | 0 | -0.022271 | -0.516443 | -3.064848 |
| 29 | 1 | 0 | 0.549735 | -0.802081 | -3.792417 |
| 30 | 1 | 0 | -3.580467 | -5.037624 | 0.081210 |
| 31 | 8 | 0 | -2.867240 | -5.459764 | 0.625679 |
| 32 | 1 | 0 | -2.791150 | -6.361416 | 0.280528 |
| 33 | 1 | 0 | 0.110887 | 1.774979 | -0.884830 |
| 34 | 8 | 0 | 0.118365 | 2.014814 | -1.833534 |
| 35 | 1 | 0 | 0.228718 | 1.159626 | -2.309122 |
| 36 | 1 | 0 | -1.636588 | 2.288643 | -2.753461 |
| 37 | 8 | 0 | -2.520261 | 2.298953 | -3.175415 |
| 38 | 1 | 0 | -3.064649 | 2.790969 | -2.521838 |
| 39 | 1 | 0 | -0.219229 | 3.990133 | -1.637095 |
| 40 | 8 | 0 | -0.711675 | 4.778026 | -1.339868 |
| 41 | 1 | 0 | -0.218423 | 5.151263 | -0.575260 |
| 42 | 1 | 0 | -1.666333 | 1.289717 | 0.839749 |
| 43 | 8 | 0 | -2.634455 | 1.320178 | 0.717286 |
| 44 | 1 | 0 | -2.869245 | 0.374248 | 0.422292 |
| 45 | 1 | 0 | -3.223505 | 2.651107 | 1.908281 |
| 46 | 8 | 0 | -3.225271 | 3.592897 | 2.193459 |
| 47 | 1 | 0 | -3.409042 | 4.048884 | 1.347520 |
| 48 | 1 | 0 | -2.982400 | 2.775072 | -0.363027 |
| 49 | 8 | 0 | -3.216809 | 3.643529 | -0.766480 |
| 50 | 1 | 0 | -2.361550 | 4.116986 | -0.910460 |
| 51 | 1 | 0 | -0.295412 | -3.483622 | 0.052127 |
| 52 | 8 | 0 | -0.242817 | -4.331327 | 0.566987 |
| 53 | 1 | 0 | -1.162935 | -4.673327 | 0.624574 |
| 54 | 1 | 0 | 0.504273 | -3.799593 | 1.975477 |
| 55 | 8 | 0 | 1.031507 | -3.372082 | 2.715910 |
| 56 | 1 | 0 | 1.622224 | -4.060026 | 3.054036 |
| 57 | 1 | 0 | -1.454281 | 3.757186 | 2.526007 |
| 58 | 8 | 0 | -0.465064 | 3.721719 | 2.592956 |
| 59 | 1 | 0 | -0.207372 | 2.912740 | 2.108714 |
| 60 | 1 | 0 | 0.153072 | 5.037815 | 1.664442 |
| 61 | 8 | 0 | 0.479111 | 5.727902 | 1.023574 |
| 62 | 1 | 0 | 1.426559 | 5.827758 | 1.192293 |
| 63 | 6 | 0 | 3.944767 | -1.557972 | -0.001654 |
| 64 | 6 | 0 | 4.625430 | -0.483303 | -0.575786 |
| 65 | 1 | 0 | 2.486564 | 2.035645 | 0.148151 |
| 66 | 1 | 0 | 4.670088 | 1.627022 | -0.996530 |
| 67 | 1 | 0 | 2.198116 | -2.157935 | 1.077495 |
| 68 | 1 | 0 | 4.356615 | -2.557105 | -0.070600 |
| 69 | 7 | 0 | 5.909405 | -0.728589 | -1.247297 |
| 70 | 1 | 0 | -0.408251 | -1.953213 | 4.512387 |

| 71 | 1 | 0 | 0.177207 | -0.396406 | 5.143901 |
|---|---|---|---|---|---|
| 72 | 1 | 0 | -1.564007 | -0.733438 | 5.089800 |
| 73 | 8 | 0 | 6.340082 | -1.885082 | -1.272623 |
| 74 | 8 | 0 | 6.495113 | 0.234387 | -1.749959 |

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SCF Done:  E(RB+HF-LYP) =  -1983.07780819     A.U. after    1 cycles

      Convg  =    0.3822D-08          -V/T =  2.0093

      S**2   =   0.0000

Zero-point correction=                          0.609038(a.u.)

Thermal correction to Energy=                    0.663442

Thermal correction to Enthalpy=                  0.664386

Thermal correction to Gibbs Free Energy=        0.514915

Sum of electronic and zero-point Energies=        -1982.468770

Sum of electronic and thermal Energies=           -1982.414366

Sum of electronic and thermal Enthalpies=         -1982.413422

Sum of electronic and thermal Free Energies=      -1982.562893


 (10-5) TS1(am), Y=NO2

  tuka02aano2.chk Stoichiometry    C9H43N2O20(1-)


              Standard orientation:

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| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| Number | Number | Type | X | Y | Z |

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| 1 | 6 | 0 | 2.003506 | -0.382541 | 0.325705 |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 0.596931 | -0.193648 | 0.909974 |
| 3 | 8 | 0 | 0.070439 | 0.989661 | 0.770460 |
| 4 | 7 | 0 | 0.509247 | -0.805230 | 2.167612 |
| 5 | 6 | 0 | -0.694690 | -0.672563 | 2.984689 |
| 6 | 6 | 0 | 2.767614 | 0.754171 | 0.032045 |
| 7 | 6 | 0 | 4.068817 | 0.638487 | -0.448776 |
| 8 | 6 | 0 | 2.568593 | -1.652578 | 0.124662 |
| 9 | 1 | 0 | 0.898806 | -1.745621 | 2.205278 |
| 10 | 6 | 0 | -0.416350 | -1.124921 | 4.417407 |
| 11 | 1 | 0 | -0.999270 | 0.375196 | 2.977277 |
| 12 | 1 | 0 | -1.531640 | -1.257010 | 2.568429 |
| 13 | 8 | 0 | -0.329607 | -1.268323 | -0.163109 |
| 14 | 1 | 0 | -0.151828 | -0.987166 | -1.085665 |
| 15 | 1 | 0 | -1.930816 | -1.144181 | -0.005323 |
| 16 | 8 | 0 | -2.949570 | -1.146586 | 0.027441 |
| 17 | 1 | 0 | -3.189496 | -1.898198 | 0.606302 |
| 18 | 1 | 0 | -3.342257 | -1.707211 | -1.497842 |
| 19 | 8 | 0 | -3.565829 | -2.137946 | -2.378265 |
| 20 | 1 | 0 | -2.740546 | -2.562874 | -2.663358 |

| 21 | 1 | 0 | -4.607579 | -3.428673 | -1.796403 |
|----|---|---|-----------|-----------|-----------|
| 22 | 8 | 0 | -5.082680 | -4.123620 | -1.266840 |
| 23 | 1 | 0 | -6.011817 | -3.850657 | -1.249148 |
| 24 | 1 | 0 | -3.118304 | -0.479956 | -3.472258 |
| 25 | 8 | 0 | -2.477799 | 0.054683 | -3.978478 |
| 26 | 1 | 0 | -2.594543 | 1.006748 | -3.699132 |
| 27 | 1 | 0 | -0.931554 | -0.264463 | -3.399787 |
| 28 | 8 | 0 | -0.030234 | -0.407570 | -2.978972 |
| 29 | 1 | 0 | 0.516582 | -0.852129 | -3.643222 |
| 30 | 1 | 0 | -4.147658 | -4.039452 | 0.234317 |
| 31 | 8 | 0 | -3.503515 | -3.797407 | 0.949318 |
| 32 | 1 | 0 | -3.775627 | -4.261579 | 1.754389 |
| 33 | 1 | 0 | 0.103519 | 1.782480 | -0.852436 |
| 34 | 8 | 0 | 0.181671 | 2.167570 | -1.762875 |
| 35 | 1 | 0 | 0.375457 | 1.386371 | -2.320615 |
| 36 | 1 | 0 | -1.439766 | 2.538668 | -2.721959 |
| 37 | 8 | 0 | -2.314482 | 2.614358 | -3.162820 |
| 38 | 1 | 0 | -2.855636 | 3.062768 | -2.467751 |
| 39 | 1 | 0 | -0.141590 | 4.105151 | -1.359424 |
| 40 | 8 | 0 | -0.586903 | 4.894459 | -0.996021 |
| 41 | 1 | 0 | -0.113969 | 5.112318 | -0.160411 |
| 42 | 1 | 0 | -1.637798 | 1.313400 | 0.807197 |
| 43 | 8 | 0 | -2.610187 | 1.525413 | 0.846978 |
| 44 | 1 | 0 | -3.036134 | 0.670705 | 0.623256 |
| 45 | 1 | 0 | -2.766730 | 2.487882 | 2.333226 |
| 46 | 8 | 0 | -2.597779 | 3.116427 | 3.078388 |
| 47 | 1 | 0 | -2.883804 | 3.978905 | 2.740159 |
| 48 | 1 | 0 | -3.015318 | 3.021419 | -0.250561 |
| 49 | 8 | 0 | -3.175950 | 3.812212 | -0.808993 |
| 50 | 1 | 0 | -2.325067 | 4.313550 | -0.791848 |
| 51 | 1 | 0 | -0.503920 | -2.991522 | 0.000438 |
| 52 | 8 | 0 | -0.671717 | -3.954771 | 0.196756 |
| 53 | 1 | 0 | -1.615733 | -4.005354 | 0.445772 |
| 54 | 1 | 0 | 0.302514 | -4.085958 | 1.643634 |
| 55 | 8 | 0 | 0.878957 | -3.942784 | 2.440170 |
| 56 | 1 | 0 | 1.574185 | -4.614490 | 2.393433 |
| 57 | 1 | 0 | -0.718467 | 3.074966 | 2.978792 |
| 58 | 8 | 0 | 0.228983 | 3.019308 | 2.716871 |
| 59 | 1 | 0 | 0.268817 | 2.272816 | 2.072801 |
| 60 | 1 | 0 | 0.587813 | 4.488026 | 1.934424 |
| 61 | 8 | 0 | 0.730664 | 5.346195 | 1.443065 |
| 62 | 1 | 0 | 1.687829 | 5.487874 | 1.425320 |
| 63 | 6 | 0 | 3.867200 | -1.788960 | -0.350757 |
| 64 | 6 | 0 | 4.606752 | -0.636364 | -0.631667 |
| 65 | 1 | 0 | 2.328446 | 1.733388 | 0.180273 |
| 66 | 1 | 0 | 4.664400 | 1.513608 | -0.678016 |

| 67 | 1 | 0 | 1.985117 | -2.540782 | 0.337578 |
|----|---|---|----------|-----------|----------|
| 68 | 1 | 0 | 4.310836 | -2.764439 | -0.507828 |
| 69 | 7 | 0 | 5.976647 | -0.771853 | -1.128211 |
| 70 | 1 | 0 | -0.084840 | -2.169225 | 4.441419 |
| 71 | 1 | 0 | 0.363143 | -0.502944 | 4.870182 |
| 72 | 1 | 0 | -1.325103 | -1.037697 | 5.024636 |
| 73 | 8 | 0 | 6.431629 | -1.911096 | -1.286579 |
| 74 | 8 | 0 | 6.618638 | 0.257120 | -1.365377 |

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SCF Done:  E(RB+HF-LYP) =  -1983.04975966    A.U. after    1 cycles

      Convg  =    0.4205D-08          -V/T =  2.0092

      S**2  =   0.0000

Zero-point correction=                        0.610950 (a.u.)

Thermal correction to Energy=                 0.664146

Thermal correction to Enthalpy=               0.665090

Thermal correction to Gibbs Free Energy=      0.519627

Sum of electronic and zero-point Energies=       -1982.438810

Sum of electronic and thermal Energies=          -1982.385614

Sum of electronic and thermal Enthalpies=        -1982.384669

Sum of electronic and thermal Free Energies=     -1982.530133


 (10-6) TS2(am),  Y=NO2

tuka02bzno2.chk   Stoichiometry   C9H43N2O20(1-)


                Standard orientation:

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| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|--------|--------|--------|------|------|------|
| Number | Number | Type | X | Y | Z |

---------------------------------------------------------------------

| 1 | 6 | 0 | -1.374096 | 0.701285 | -0.568993 |
|----|---|---|-----------|-----------|-----------|
| 2 | 6 | 0 | -1.660668 | -0.813886 | -0.448966 |
| 3 | 8 | 0 | -2.444876 | -1.148457 | 0.571402 |
| 4 | 7 | 0 | -0.290762 | -1.540934 | -0.293374 |
| 5 | 6 | 0 | -0.431687 | -3.030150 | -0.236717 |
| 6 | 6 | 0 | -1.831543 | 1.589505 | 0.412093 |
| 7 | 6 | 0 | -1.643488 | 2.963112 | 0.270112 |
| 8 | 6 | 0 | -0.985472 | 3.437181 | -0.865226 |
| 9 | 1 | 0 | 0.382446 | -1.281021 | -1.037491 |
| 10 | 1 | 0 | -1.041056 | -3.250115 | 0.641344 |
| 11 | 1 | 0 | -0.991340 | -3.328439 | -1.124476 |
| 12 | 6 | 0 | 0.915759 | -3.741006 | -0.166367 |
| 13 | 8 | 0 | -2.114684 | -1.293362 | -1.714211 |
| 14 | 1 | 0 | -3.057095 | -1.024925 | -1.806088 |
| 15 | 1 | 0 | -4.944193 | -3.479657 | -0.795196 |
| 16 | 8 | 0 | -5.316589 | -3.470844 | -1.724377 |
| 17 | 1 | 0 | -4.699339 | -3.995800 | -2.255293 |

| 18 | 1 | 0 | 0.156441 | -1.181639 | 0.609113 |
|----|---|---|----------|-----------|----------|
| 19 | 8 | 0 | 0.956969 | -0.617156 | 1.954490 |
| 20 | 1 | 0 | 0.311533 | -0.655044 | 2.683969 |
| 21 | 1 | 0 | 2.543655 | -1.282626 | 1.609646 |
| 22 | 8 | 0 | 3.334032 | -1.337066 | 1.010575 |
| 23 | 1 | 0 | 3.820162 | -2.190704 | 1.078355 |
| 24 | 1 | 0 | -5.163186 | -1.753275 | -2.003597 |
| 25 | 8 | 0 | -4.916197 | -0.789425 | -1.986392 |
| 26 | 1 | 0 | -5.224908 | -0.405386 | -2.820122 |
| 27 | 1 | 0 | -4.055888 | -0.504299 | 0.774341 |
| 28 | 8 | 0 | -5.016519 | -0.375520 | 0.990299 |
| 29 | 1 | 0 | -5.411918 | -0.190223 | 0.120418 |
| 30 | 1 | 0 | 2.625995 | -1.165680 | -0.633031 |
| 31 | 8 | 0 | 2.295278 | -0.950086 | -1.539844 |
| 32 | 1 | 0 | 2.406822 | 0.040746 | -1.549852 |
| 33 | 1 | 0 | 4.402271 | 0.048803 | 0.799000 |
| 34 | 8 | 0 | 5.037392 | 0.769017 | 0.559448 |
| 35 | 1 | 0 | 4.922154 | 1.427338 | 1.290423 |
| 36 | 1 | 0 | -3.480034 | -2.609892 | 0.600579 |
| 37 | 8 | 0 | -4.284817 | -3.171255 | 0.755589 |
| 38 | 1 | 0 | -4.905724 | -2.504784 | 1.112230 |
| 39 | 1 | 0 | 6.260191 | -0.231398 | -0.137814 |
| 40 | 8 | 0 | 6.733948 | -0.983019 | -0.587597 |
| 41 | 1 | 0 | 7.595073 | -0.636754 | -0.862515 |
| 42 | 1 | 0 | 3.875413 | -1.832963 | -2.179818 |
| 43 | 8 | 0 | 4.713138 | -2.349430 | -2.198157 |
| 44 | 1 | 0 | 5.411805 | -1.725692 | -1.914935 |
| 45 | 1 | 0 | -2.064821 | -1.708956 | 3.612514 |
| 46 | 8 | 0 | -1.785686 | -0.888315 | 3.179543 |
| 47 | 1 | 0 | -1.987939 | -1.014204 | 2.209637 |
| 48 | 1 | 0 | -3.278227 | 0.421373 | 3.487604 |
| 49 | 8 | 0 | -4.060150 | 1.005299 | 3.428060 |
| 50 | 1 | 0 | -4.578837 | 0.650459 | 2.680520 |
| 51 | 1 | 0 | 3.688071 | 1.580625 | -0.722635 |
| 52 | 8 | 0 | 2.761963 | 1.686186 | -1.020824 |
| 53 | 1 | 0 | 2.269453 | 1.750435 | -0.154325 |
| 54 | 1 | 0 | 0.969725 | 2.301528 | 1.625861 |
| 55 | 8 | 0 | 1.694062 | 1.669078 | 1.507769 |
| 56 | 1 | 0 | 1.262685 | 0.502237 | 1.782022 |
| 57 | 6 | 0 | -0.709519 | 1.207858 | -1.695887 |
| 58 | 6 | 0 | -0.503554 | 2.574440 | -1.851015 |
| 59 | 1 | 0 | -2.354742 | 1.217885 | 1.284838 |
| 60 | 1 | 0 | -2.009752 | 3.656521 | 1.017447 |
| 61 | 7 | 0 | -0.809552 | 4.884515 | -1.036683 |
| 62 | 1 | 0 | -0.360234 | 0.529266 | -2.467124 |
| 63 | 1 | 0 | 0.022661 | 2.971734 | -2.709390 |

| 64 | 1 | 0 | 1.532004 | -3.528502 | -1.045215 |
| 65 | 1 | 0 | 1.479222 | -3.454075 | 0.725958 |
| 66 | 1 | 0 | 0.744671 | -4.822483 | -0.124727 |
| 67 | 1 | 0 | 3.096944 | 2.174387 | 2.198699 |
| 68 | 8 | 0 | 4.030077 | 2.391326 | 2.529826 |
| 69 | 1 | 0 | 4.065985 | 2.047686 | 3.434202 |
| 70 | 1 | 0 | 5.919154 | -2.788761 | 0.461685 |
| 71 | 8 | 0 | 5.122593 | -3.347296 | 0.404418 |
| 72 | 1 | 0 | 4.875286 | -3.241522 | -0.545865 |
| 73 | 8 | 0 | -0.354410 | 5.292478 | -2.109257 |
| 74 | 8 | 0 | -1.133369 | 5.624433 | -0.102598 |

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SCF Done:  E(RB+HF-LYP) =  -1983.04011267     A.U. after    1 cycles

       Convg  =    0.6356D-08          -V/T =  2.0092

       S**2  =   0.0000

 Zero-point correction=                    0.607971 (a.u.)

Thermal correction to Energy=                0.660482

Thermal correction to Enthalpy=              0.661426

Thermal correction to Gibbs Free Energy=      0.516834

Sum of electronic and zero-point Energies=       -1982.432141

Sum of electronic and thermal Energies=          -1982.379631

Sum of electronic and thermal Enthalpies=        -1982.378686

Sum of electronic and thermal Free Energies=      -1982.523279