Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Supporting Information

# Tuning the optical and electrochemical properties of core-substituted naphthalenediimides with styryl imide substituent

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**Table S1:** Reaction conditions tested for Chan-Lam coupling reaction of RF8H with trans-phenylvinylboronic acid

| Entry | Catalyst | Additive | Solvent / Temperature | Yield (%) |
|---|---|---|---|---|
| **1** | $Cu(OAc)_2$ | $Et_3N$ | $CHCl_3$ / 65 °C | 8.6 |
| **2** | $Cu(OAc)_2$ | $Et_3N$ | THF / 70 °C | 10 |
| **3** | $Cu(OAc)_2$ | Pyridine | Toluene / 110 °C | No reaction |
| **4[a]** | $Cu(OAc)_2$ | Pyridine | DMAc / 110 °C | 13 |
| **5** | $Cu(OAc)_2$ | $Et_3N$ | Ethyl acetate / 70 °C | No reaction |
| **6[a]** | $Cu(OAc)_2$ | $Et_3N$ | Dioxane / 70 °C | 12.5 |
| **7** | $Cu(OTf)_2$ | $Et_3N$ | THF / 70 °C | No reaction |
| **8** | $Cu(OTf)_2$ | 1,10-phenanthroline | $CHCl_3$ / 60 °C | No reaction |
| **9** | $Cu(OTf)_2$ | No additive | Dioxane / 70 °C | No reaction |
| **10** | $Cu(OAc)_2$ | No additive | THF: dioxane (3:1) / 70 °C | No reaction |
| **11** | $Cu(OTf)_2$ | $Et_3N$ | Dioxane / 70 °C | No reaction |
| **12** | $Cu(OAc)_2$ | Urea | Dioxane / 70 °C | No reaction |
| **13** | $Cu(OAc)_2$ | Urea | Dioxane / 70 °C | No reaction |

a. reaction time 7 days with three time addition of reactants

*Note: reactant ratio imide: boronic acid: catalyst: additive is 1:2.5:2.5 and reaction time is 48 hrs except for entries 4 and 6. The second portion (same initial amounts) of reactants (boronic acid, catalyst and additive) was added after 24 hrs. For entries 4 and 6 the third portion was added after 4 days.*

# $^{1}$H NMR spectra

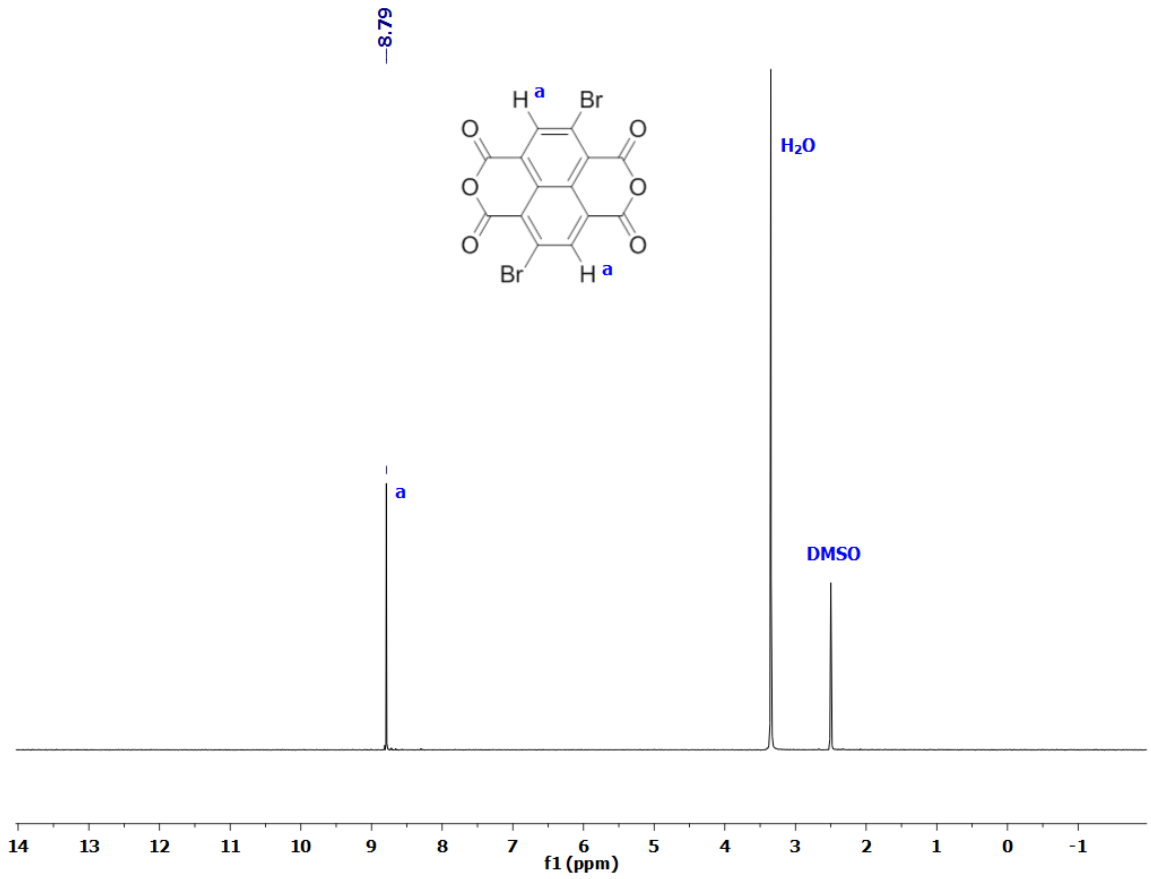


**Figure S1:** $^{1}$H NMR Spectrum (400 MHz, $d^{6}$-DMSO) of **26BrNDA**.

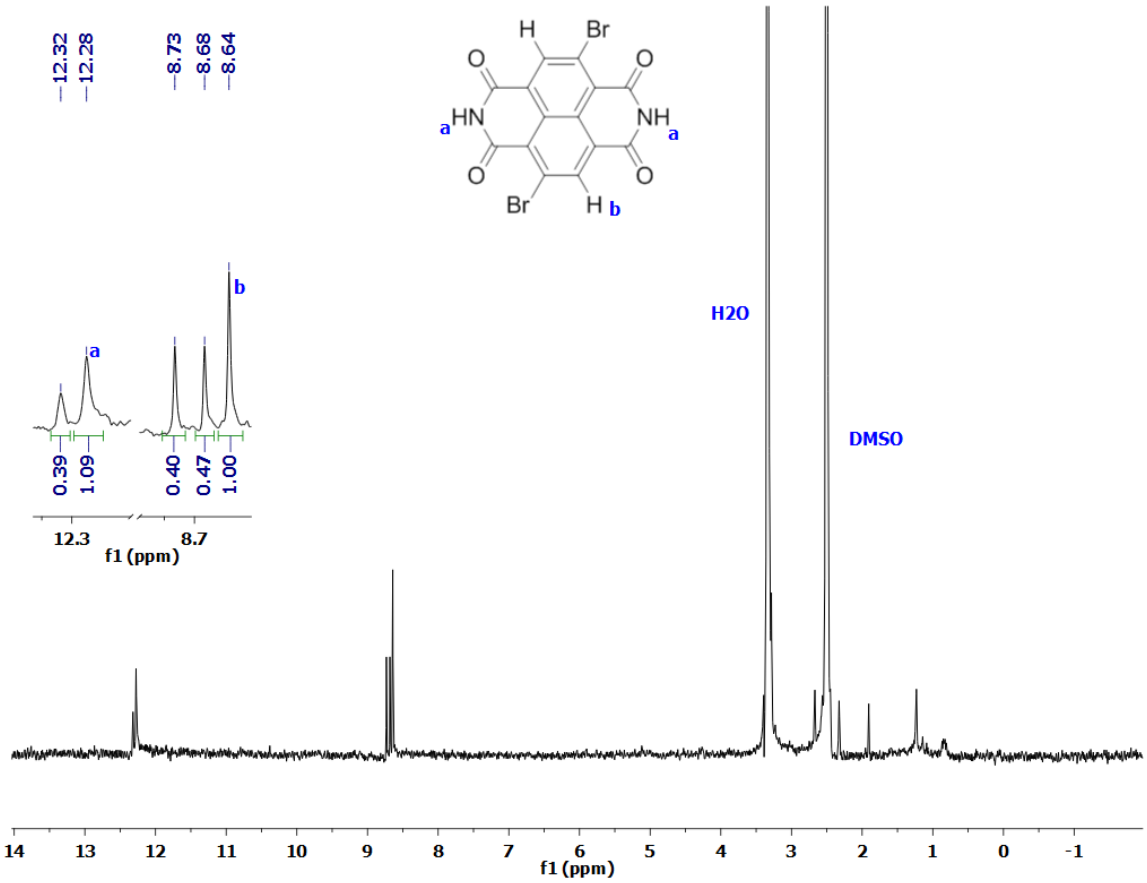


**Figure S2:** $^{1}$H NMR Spectrum (400 MHz, $d^{6}$-DMSO) of **26BrNDI**.

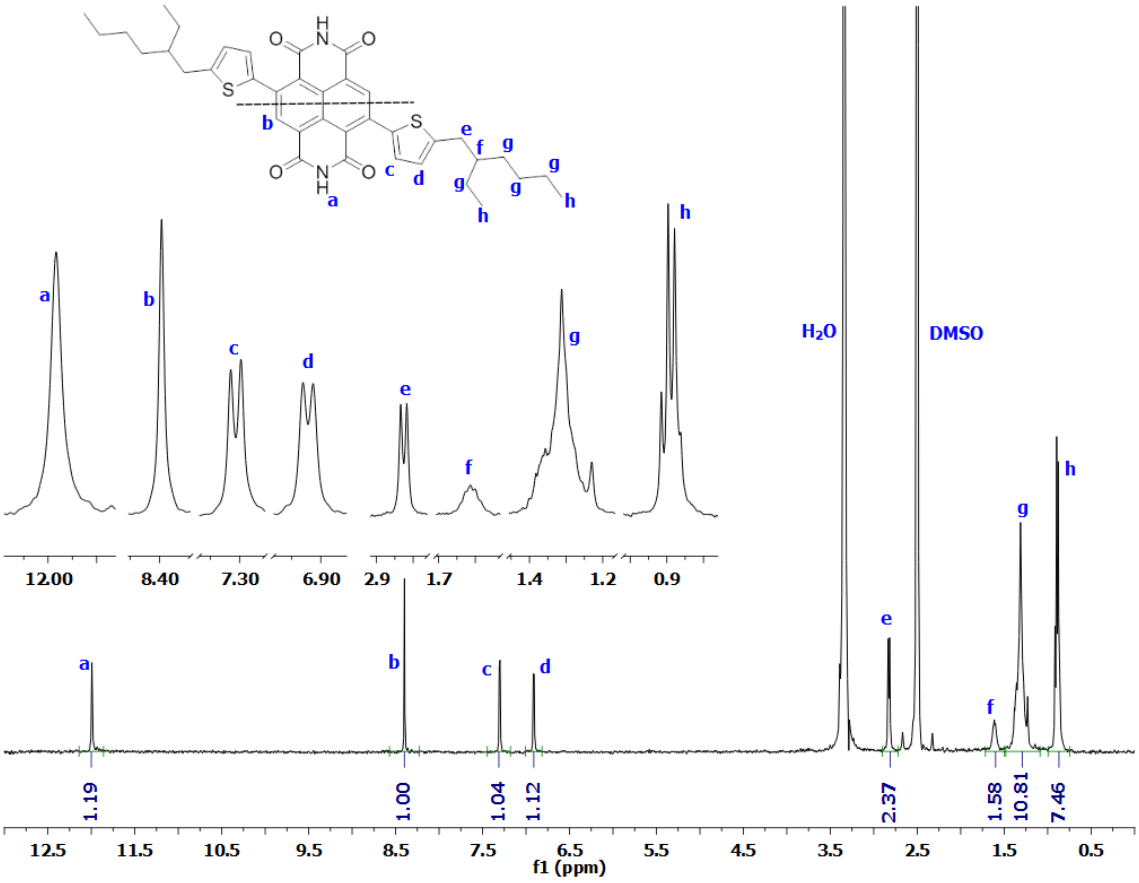


**Figure S3:** $^{1}$H NMR Spectrum (400 MHz, $d^{6}$-DMSO) of **RF7H**.

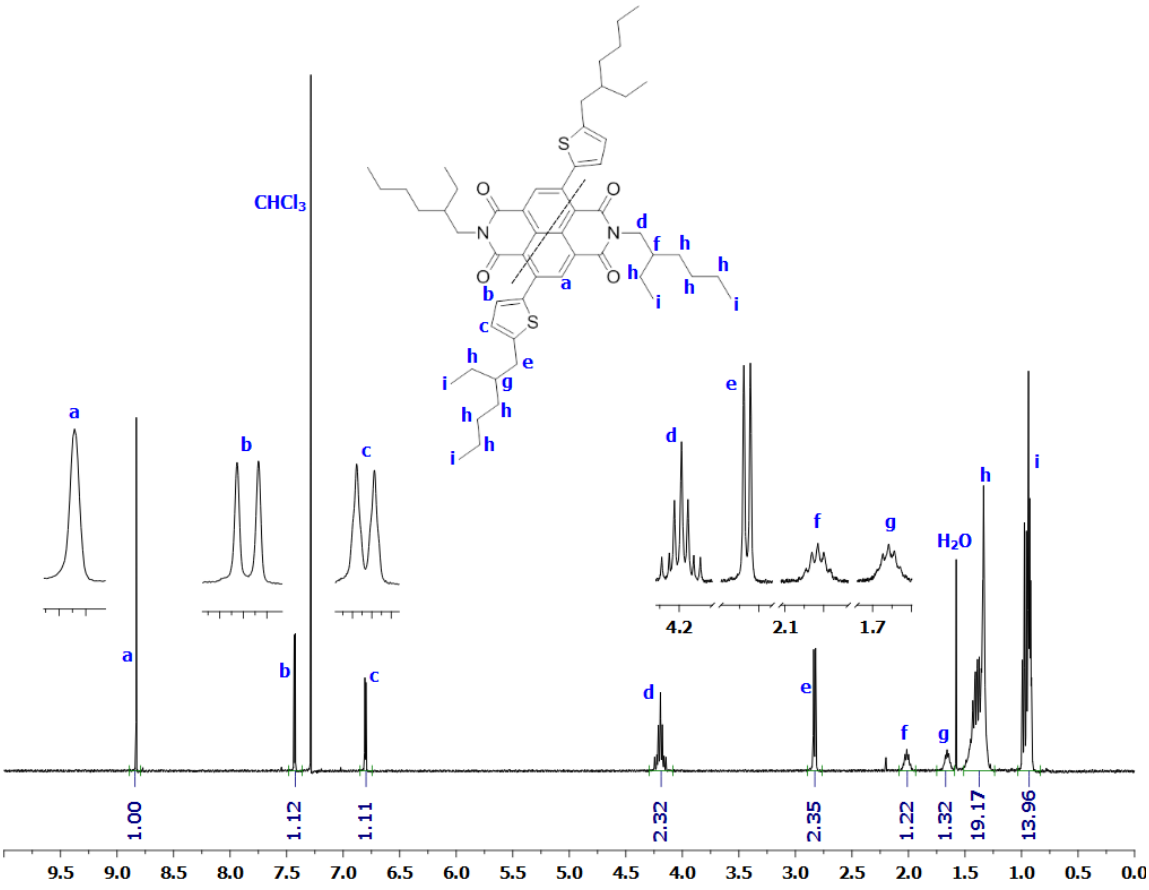


**Figure S4:** $^{1}$H NMR Spectrum (400 MHz, $CDCl_3$) of **RF7a**.

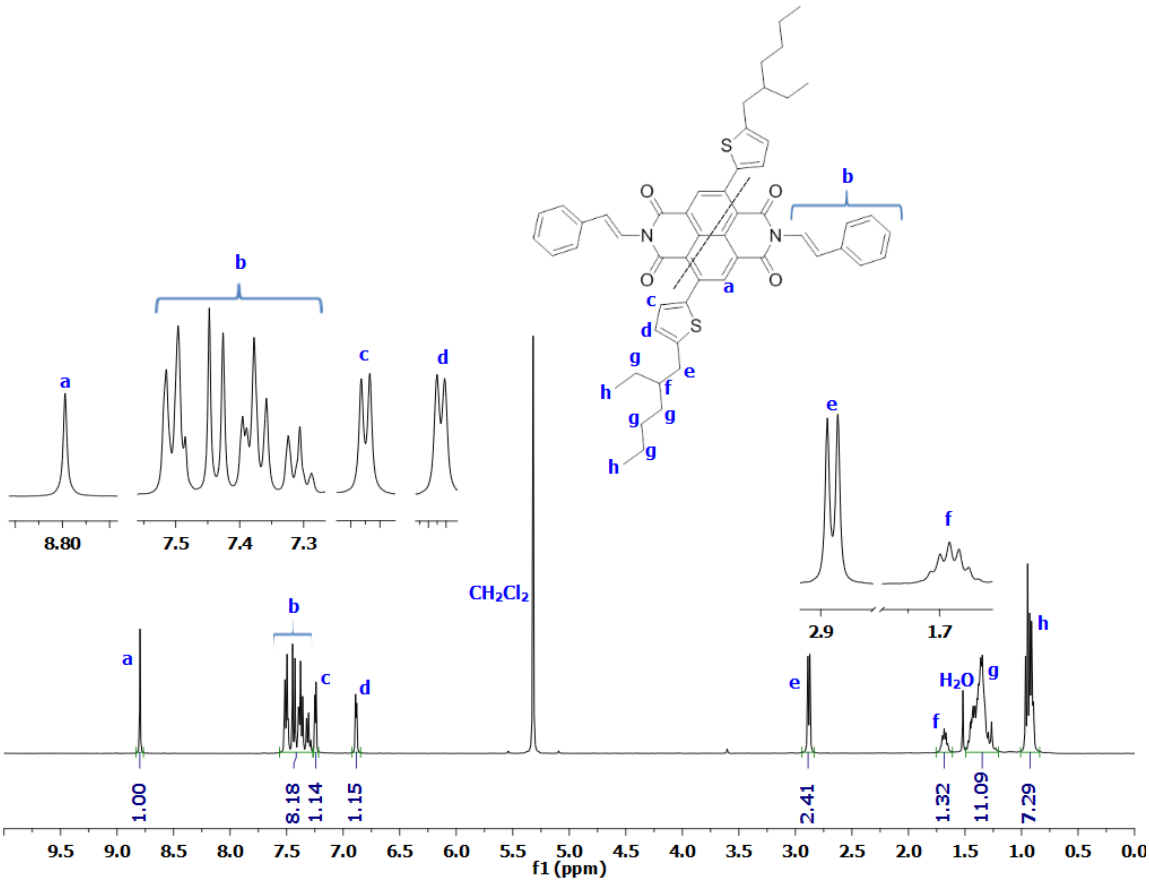


**Figure S5:** $^{1}$H NMR Spectrum (400 MHz, $CD_2Cl_2$) of **RF7b**.

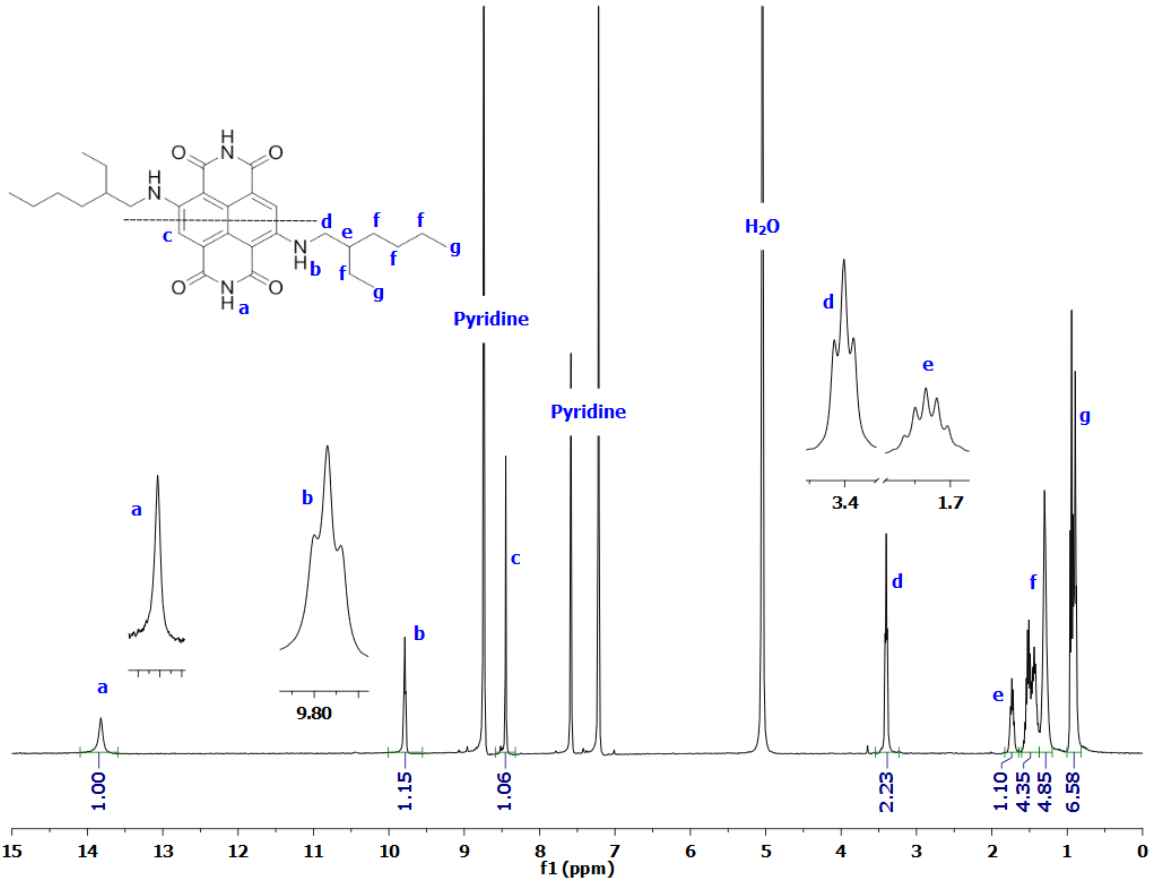


**Figure S6:** $^{1}$H NMR Spectrum (400 MHz, $d^{5}$-pyridine) of **RF8H**.

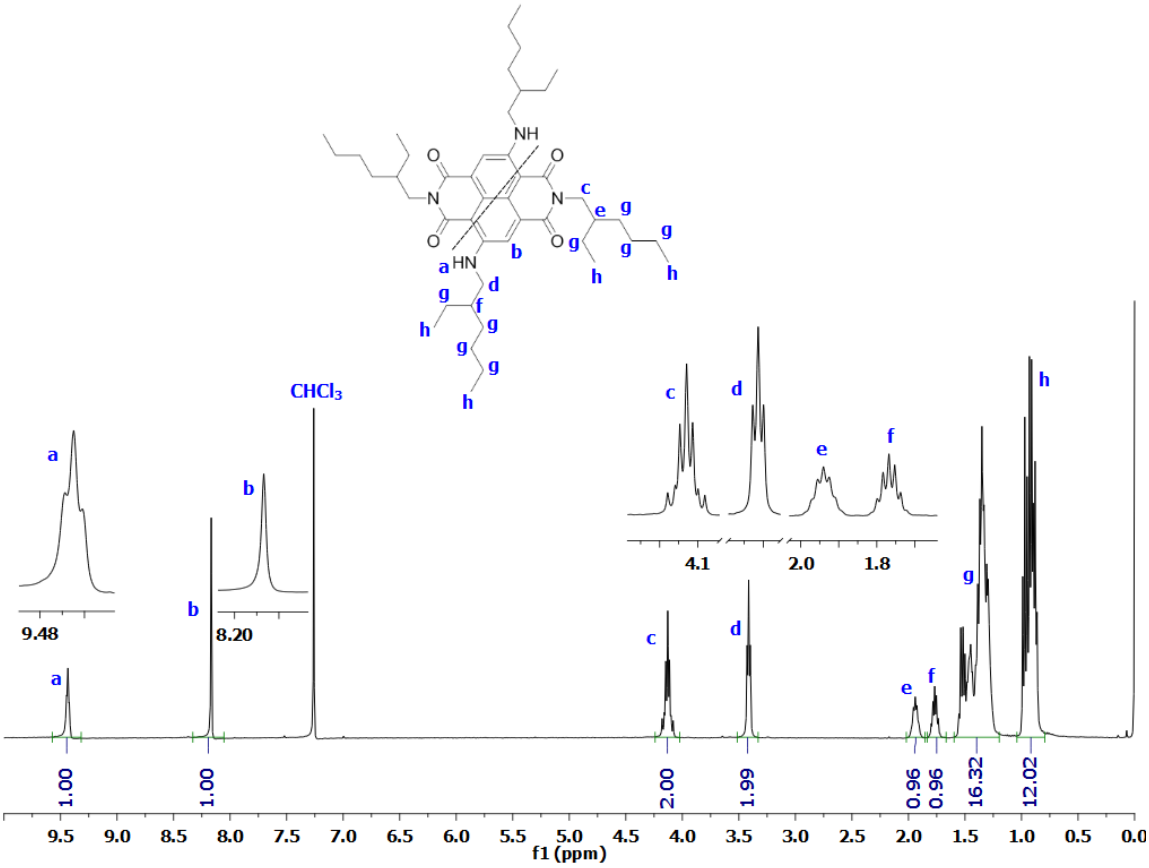


**Figure S7:** $^{1}$H NMR Spectrum (400 MHz, $CDCl_3$) of **RF8a**.

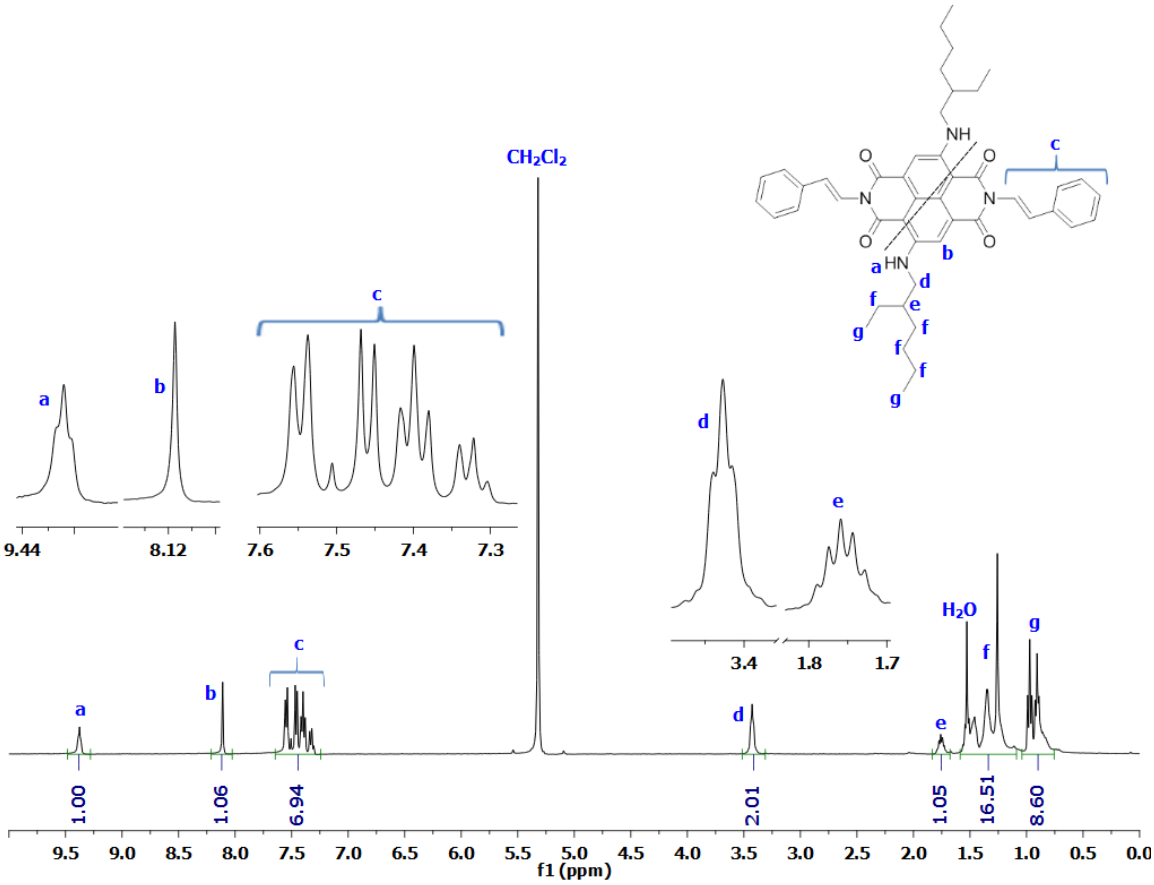


**Figure S8:** $^{1}$H NMR Spectrum (400 MHz, $CD_2Cl_2$) of **RF8b**.

## MALDI-TOF Mass Spectra

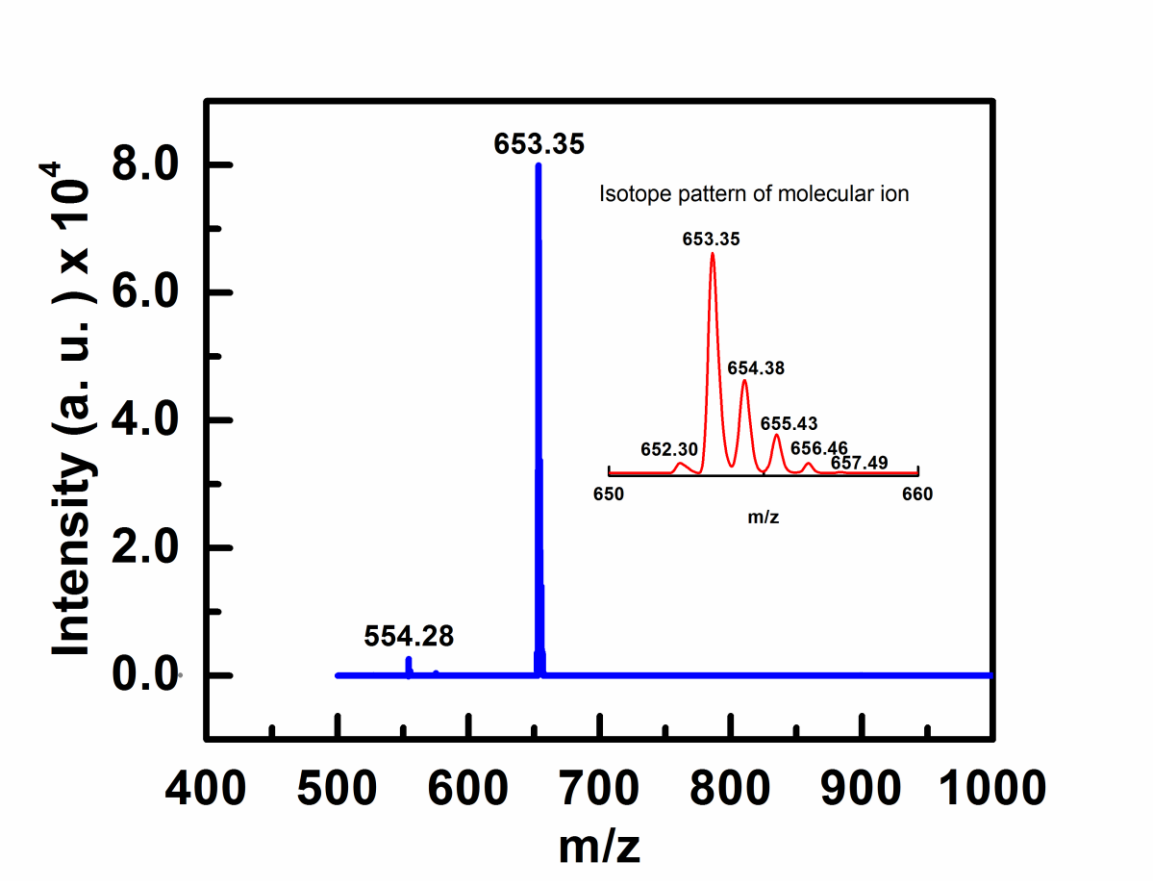


**Figure S9:** MALDI-TOF Mass Spectrum of **RF7H** (Insert: Isotope pattern of the molecular ion in reflective negative ion mode).

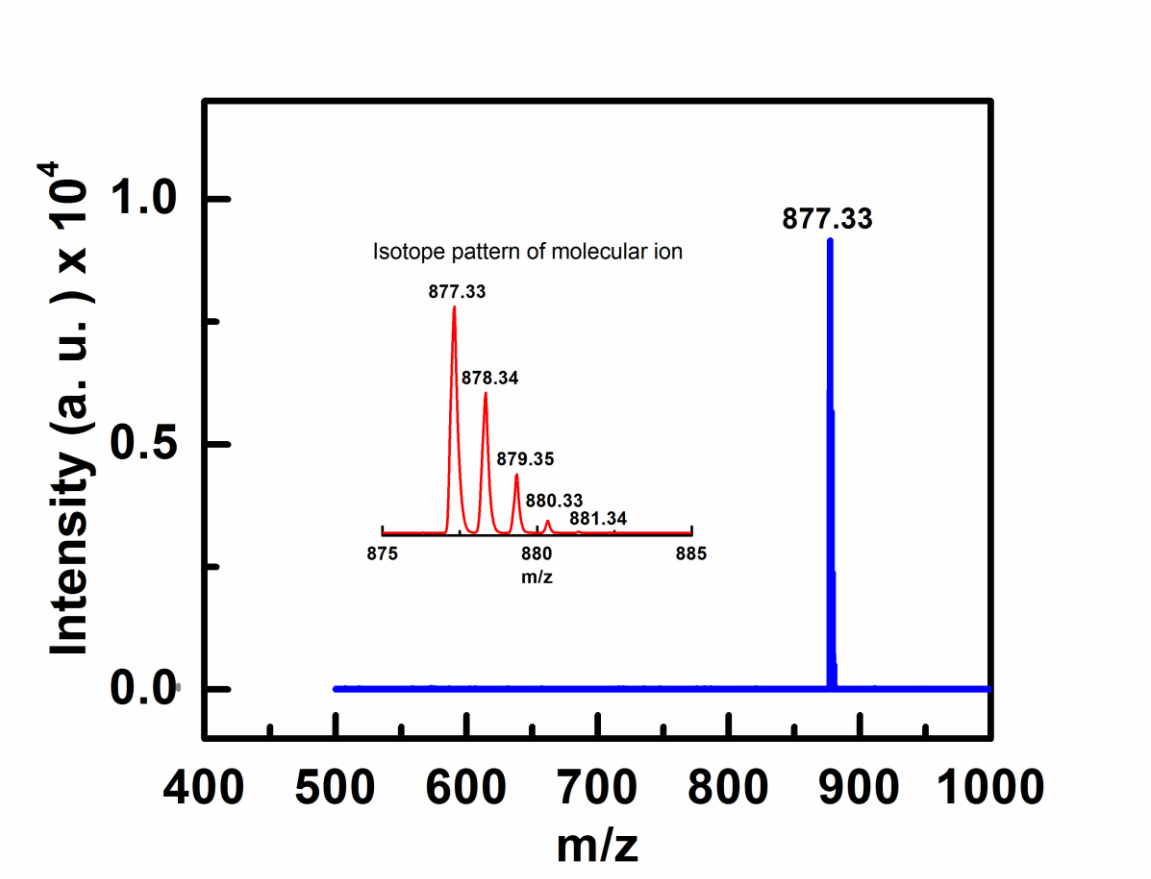


**Figure S10:** MALDI-TOF Mass Spectrum of **RF7a** (Insert: Isotope pattern of the molecular ion in reflective negative ion mode).

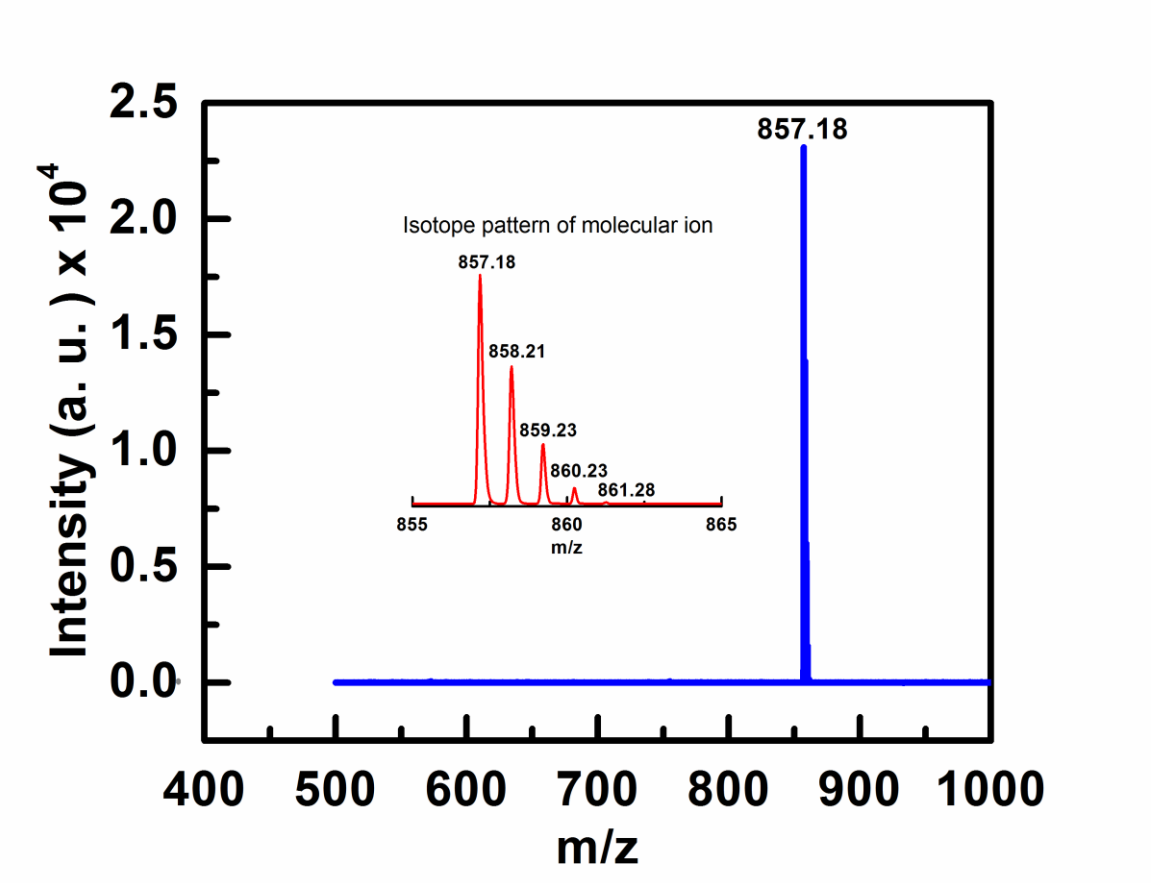


**Figure S11:** MALDI-TOF Mass Spectrum of **RF7b** (Insert: Isotope pattern of the molecular ion in reflective negative ion mode).

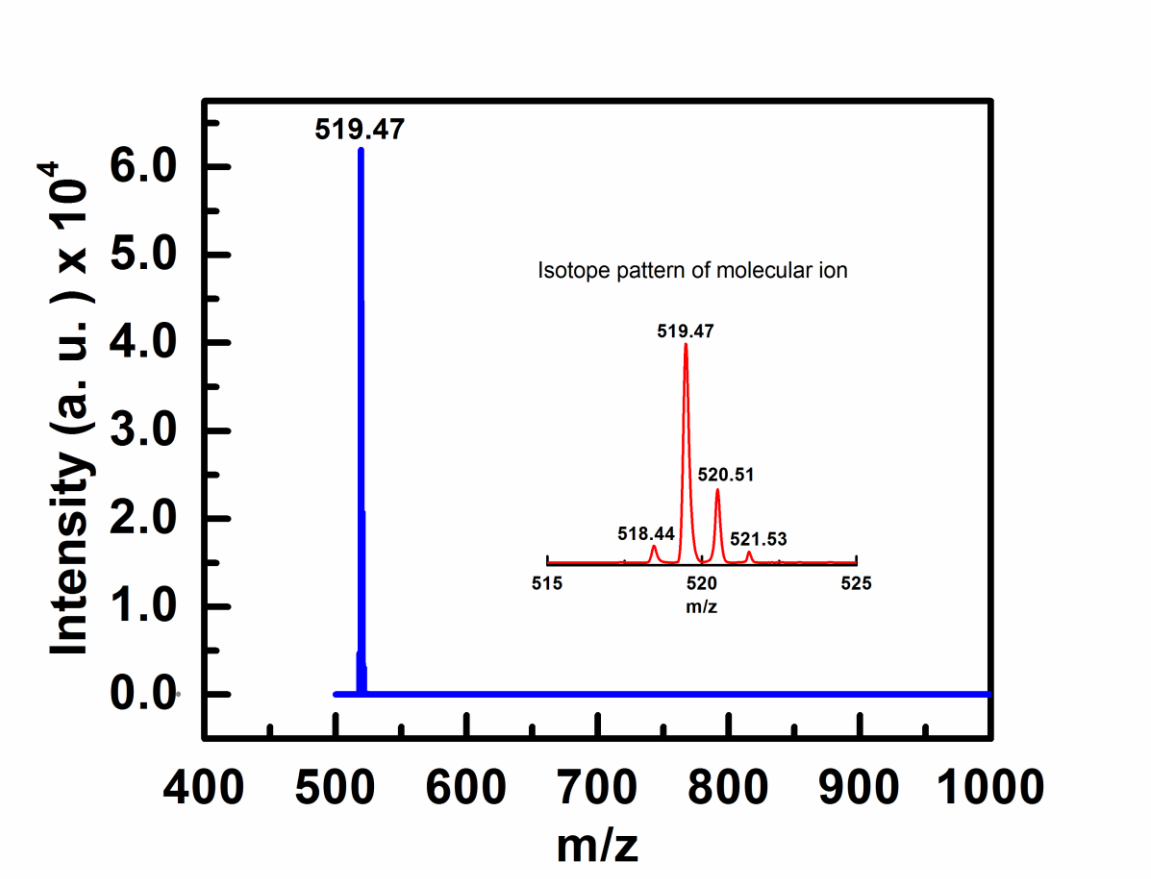


**Figure S12:** MALDI-TOF Mass Spectrum of **RF8H** (Insert: Isotope pattern of the molecular ion in reflective negative ion mode).

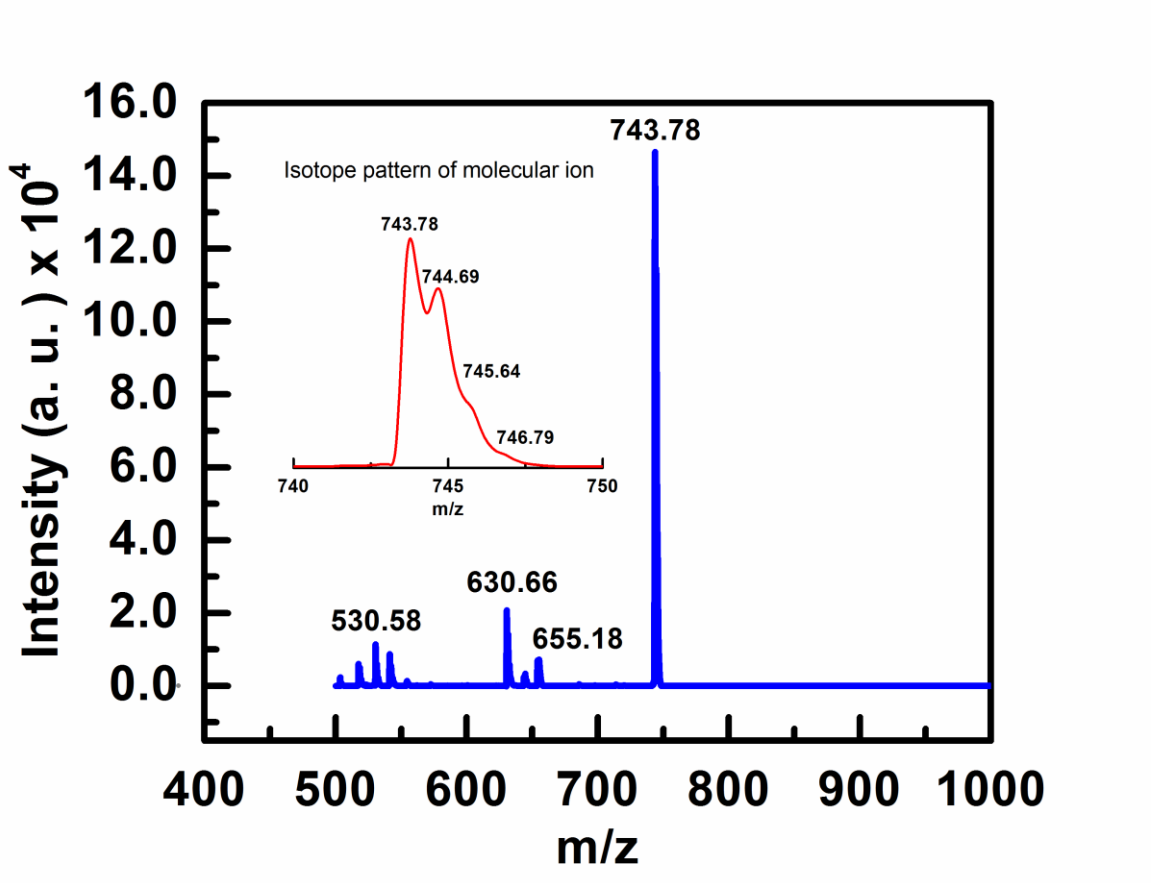


**Figure S13:** MALDI-TOF Mass Spectrum of **RF8a** (Insert: Isotope pattern of the molecular ion in reflective negative ion mode).

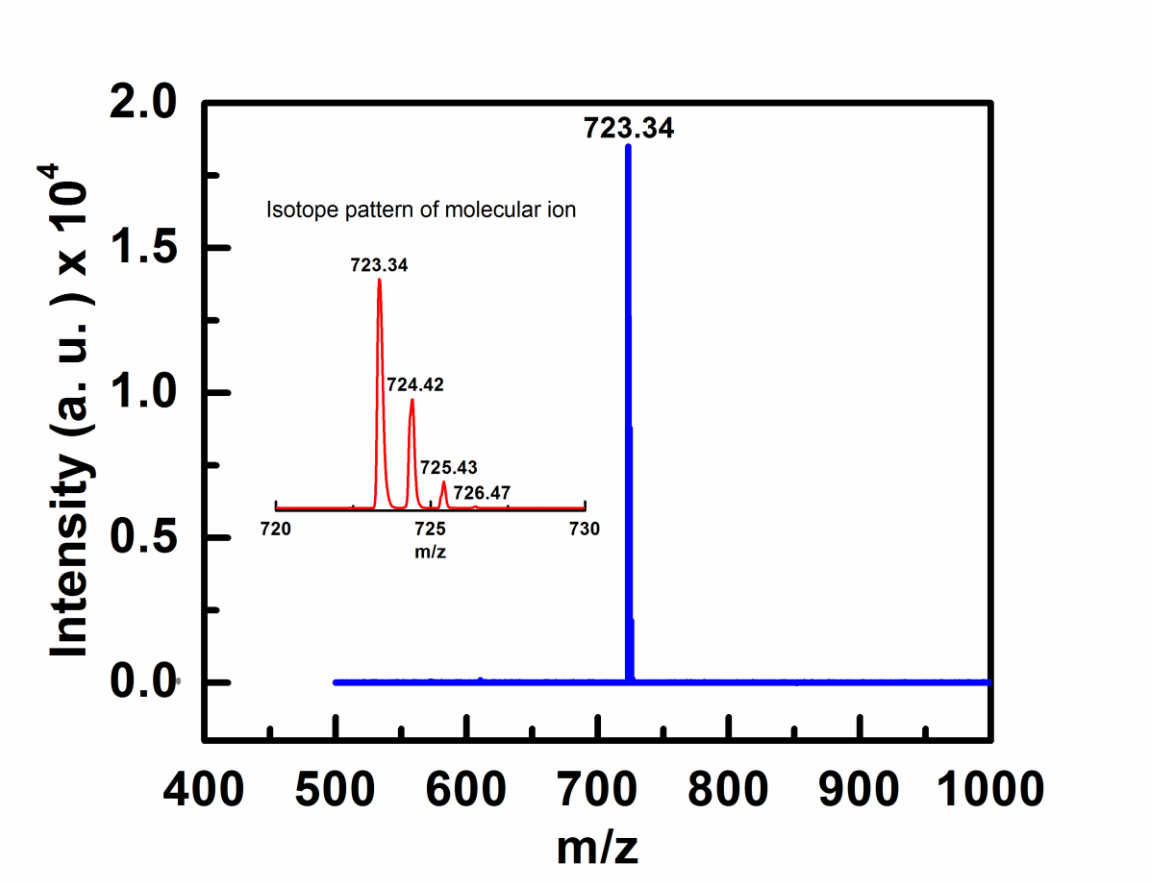


**Figure S14:** MALDI-TOF Mass Spectrum of **RF8b** (Insert: Isotope pattern of the molecular ion in reflective negative ion mode).

## UV-Visible emission spectra

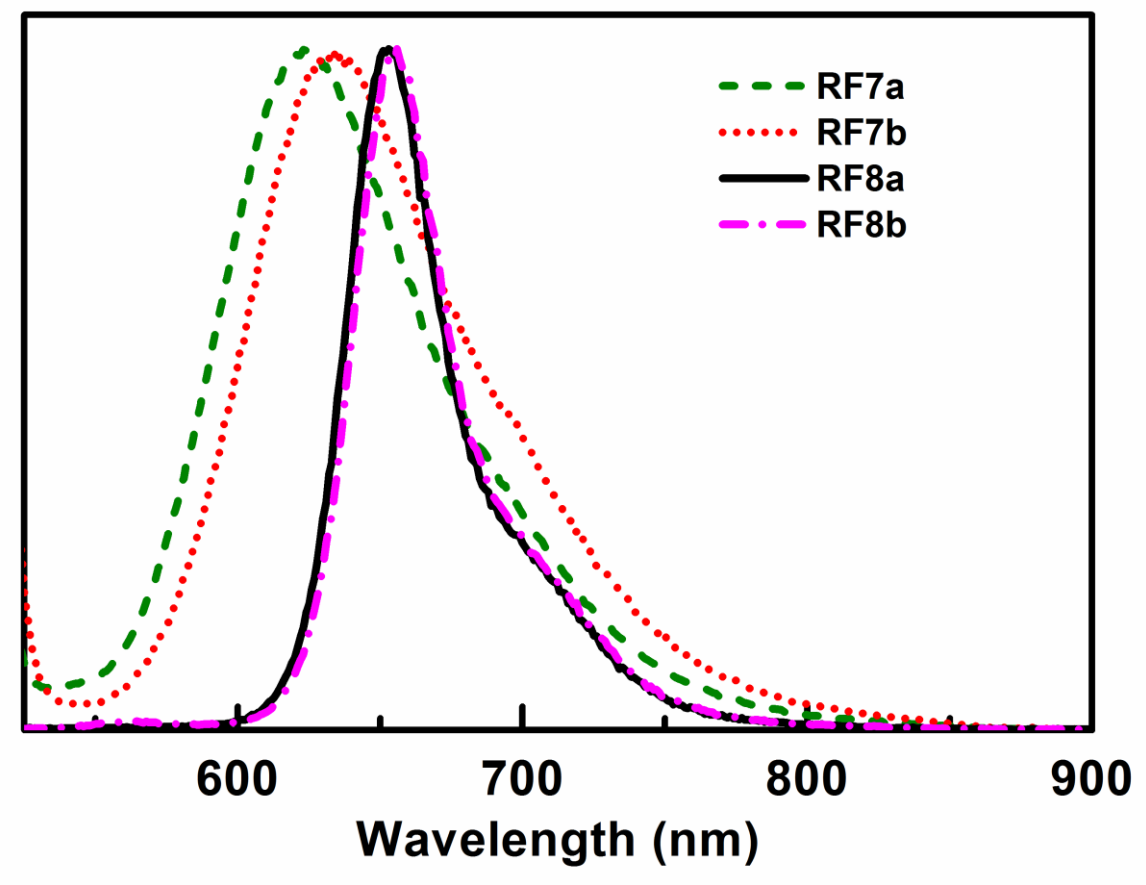


**Figure S15:** UV-Vis Emission Spectra of **RF7a, RF7b, RF8a** and **RF8b** in chloroform solution.

## Scattering correction for absorption spectra of films

Scattering corrections were done by using the scatter modeling method.[S1] In this method, a part of the uncorrected spectrum (raw data) where the absorbance is caused only due to scattering was selected. Then a polynomial (eq. 1 & 2) was fitted to this selected part using a least-squares fit to the logarithm of the absorbance.

$A = a\lambda^n$ eq. 1

$\log(A) = n\log(\lambda) + \log(a)$ eq. 2

Where: A is absorbance, λ is the wavelength, n is the scattering order and a is a coefficient.

Using the fit, the constants a and n were determined and then used to calculate the scattering contribution for the whole wavelength range (300 – 1000 nm). The corrected spectrum was obtained by subtracting the scattering contribution from the raw data.

Scatter contributions, raw data, and corrected spectra for the films of RF7a, RF7b, RF8a and RF8b are given below.

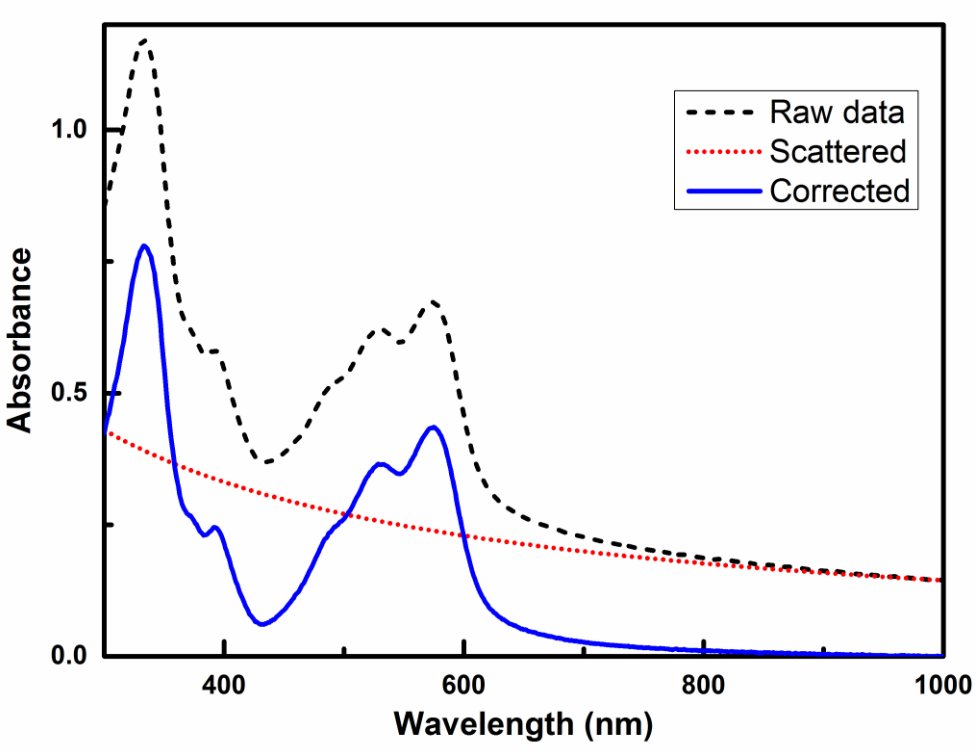


**Figure S16:** Scattering correction for absorption spectrum of **RF7a** in film.

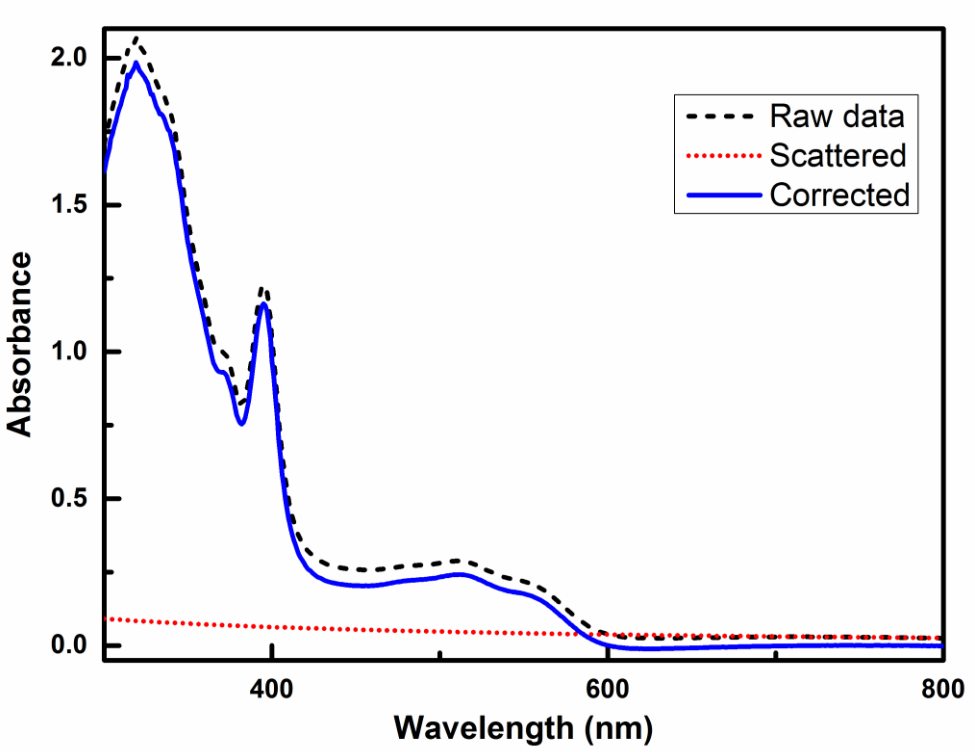


**Figure S17:** Scattering correction for absorption spectrum of **RF7b** in film.

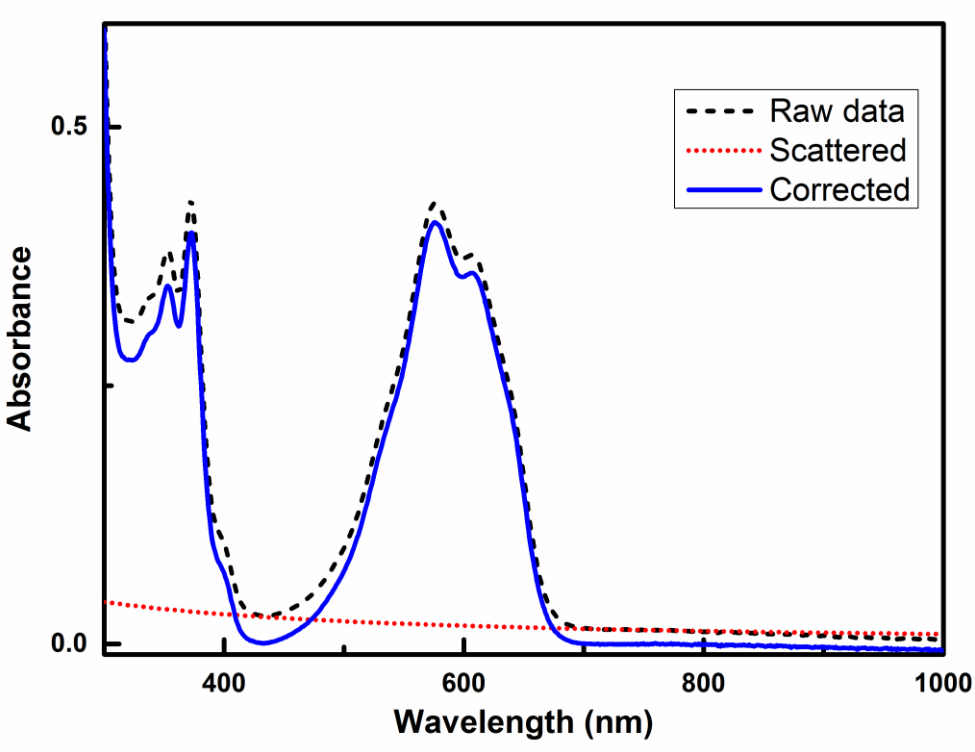


**Figure S18:** Scattering correction for absorption spectrum of **RF8a** in film.

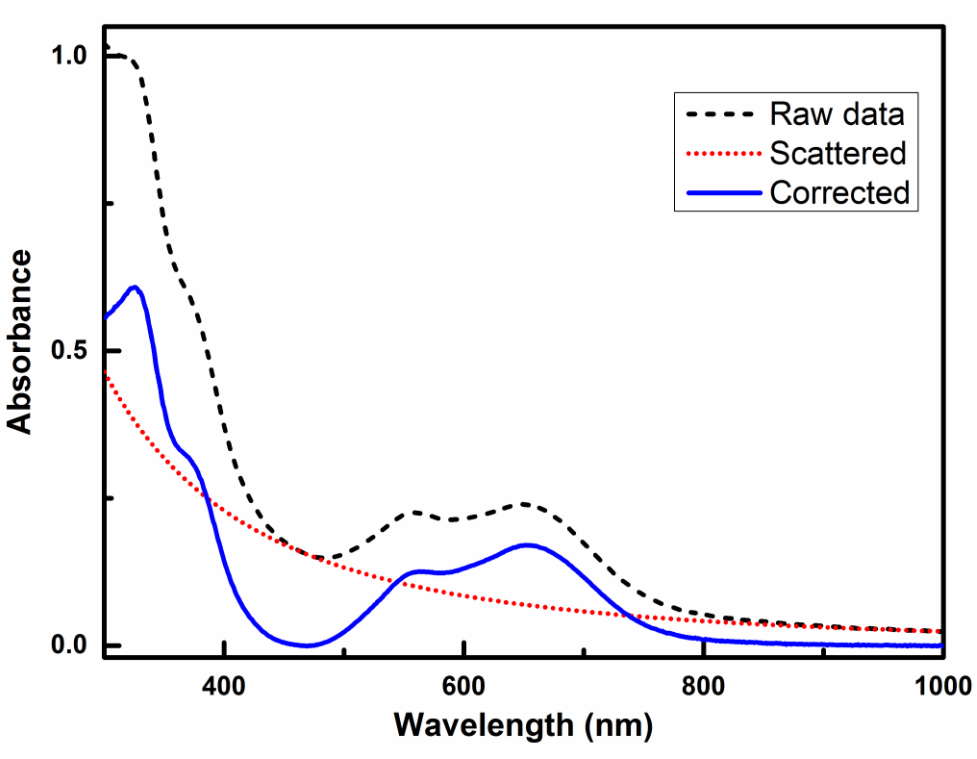


**Figure S19:** Scattering correction for absorption spectrum of **RF8b** in film.

## Computational data

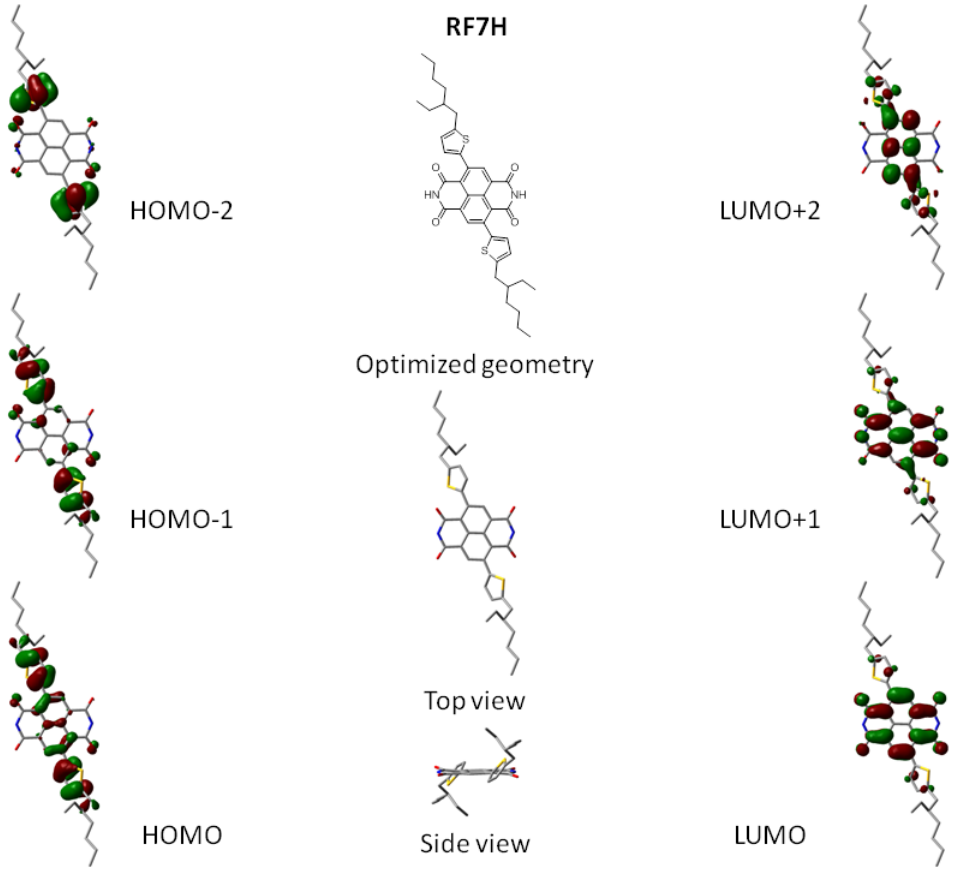


**Figure S20:** Optimized geometry and Kohn-Sham frontier molecular orbitals of local minima of **RF7H** at the B3LYP/6-31G(d,p) level of theory.

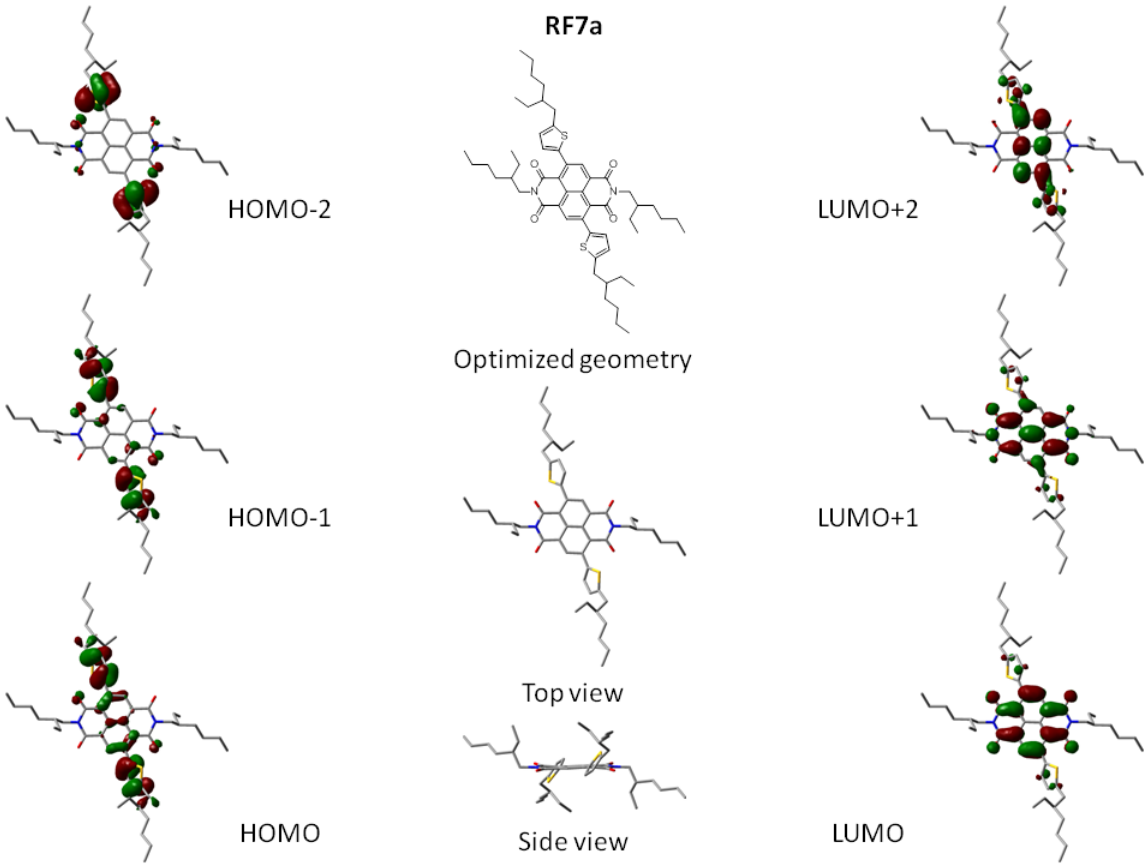


**Figure S21:** Optimized geometry and Kohn-Sham frontier molecular orbitals of local minima of **RF7a** at the B3LYP/6-31G(d,p) level of theory.

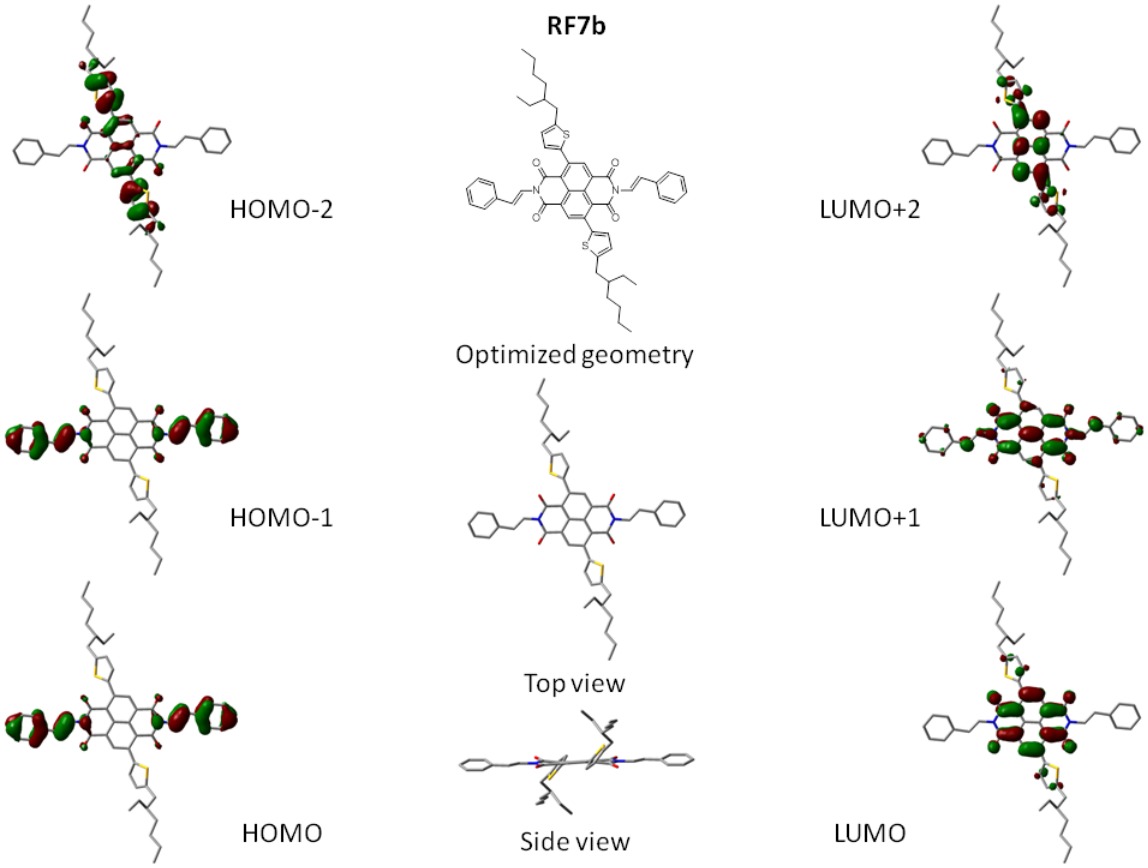


**Figure S22:** Optimized geometry and Kohn-Sham frontier molecular orbitals of local minima of **RF7b** at the B3LYP/6-31G(d,p) level of theory.

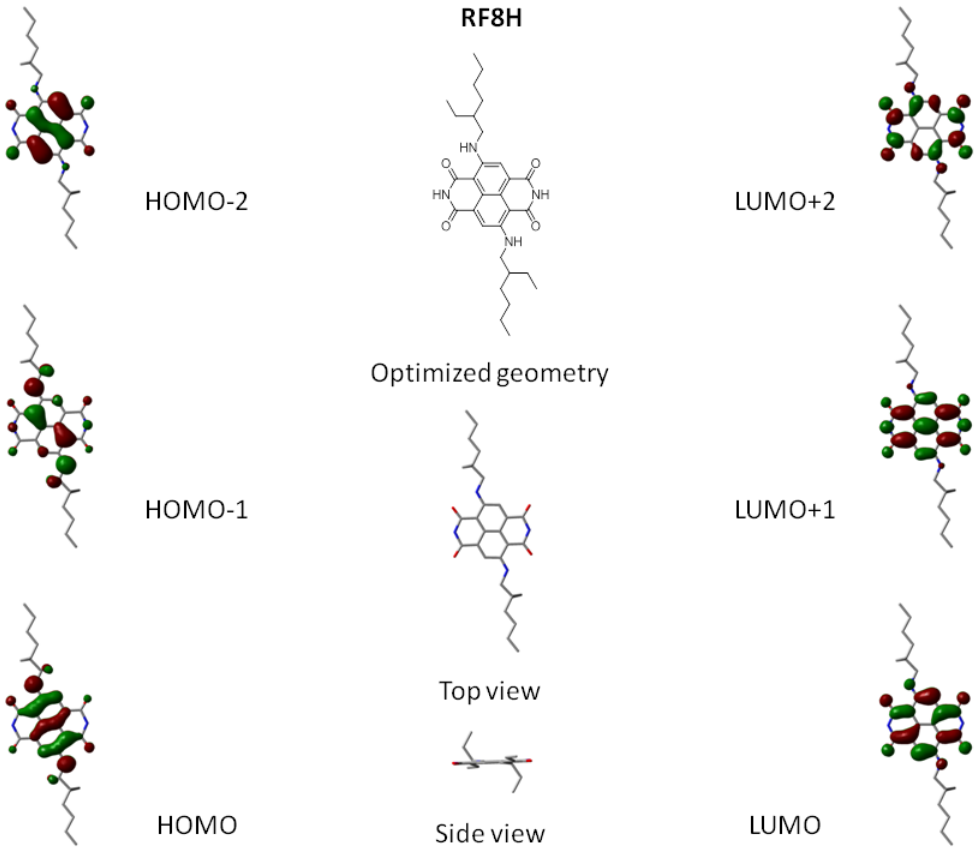


**Figure S23:** Optimized geometry and Kohn-Sham frontier molecular orbitals of local minima of **RF8H** at the B3LYP/6-31G(d,p) level of theory.

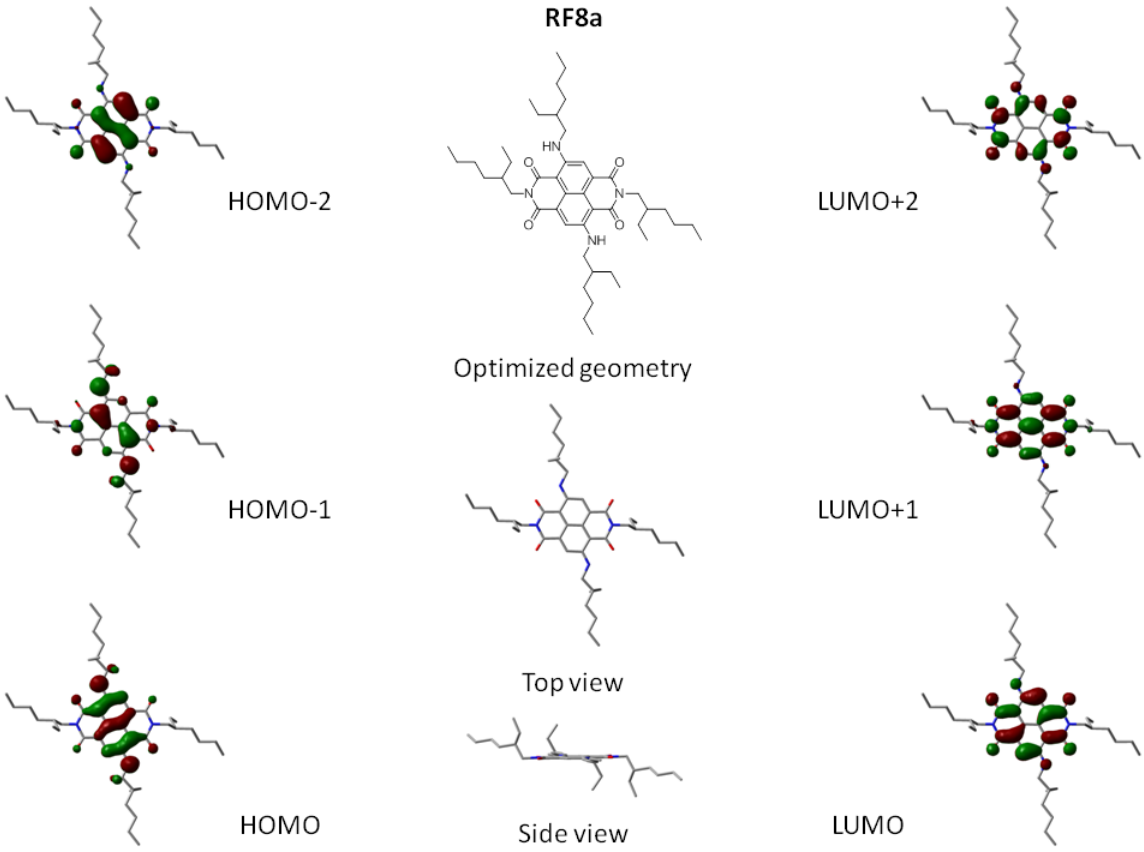


**Figure S24:** Optimized geometry and Kohn-Sham frontier molecular orbitals of local minima of **RF8a** at the B3LYP/6-31G(d,p) level of theory.

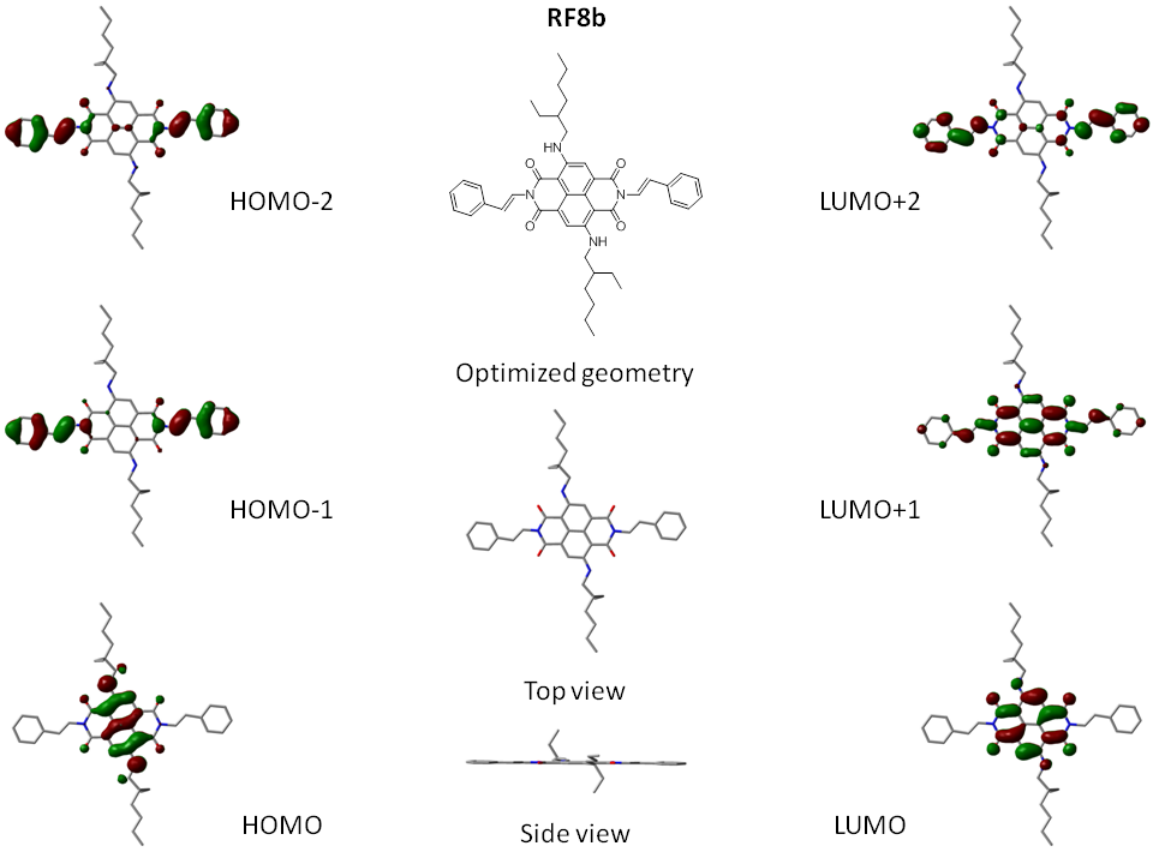


**Figure S25:** Optimized geometry and Kohn-Sham frontier molecular orbitals of local minima of **RF8b** at the B3LYP/6-31G(d,p) level of theory.

**Table S2:** Eigen values of frontier molecular orbitals (in eV) of molecules in gas phase and in chloroform polarizable continuum model (values in parenthesis), calculated for optimized geometries at B3LYP/6-31G(d,p) level of theory.

| | **RF7H** | **RF7a** | **RF7b** | **RF8H** | **RF8a** | **RF6** | **RF8b** |
|---|---|---|---|---|---|---|---|
| **LUMO+2** | -1.44 (-1.44) | -1.31 (-1.36) | -1.47 (-1.47) | -0.46 (-0.54) | -0.35 (-0.49) | -1.06 (-1.20) | -0.90 (-1.03) |
| **LUMO+1** | -1.66 (-1.69) | -1.52 (-1.61) | -1.96 (-2.04) | -1.25 (-1.31) | -1.14 (-1.25) | -1.20 (-1.36) | -1.71 (-1.82) |
| **LUMO** | -3.32 (-3.35) | -3.18 (-3.27) | -3.35 (-3.40) | -2.86 (-2.91) | -2.72 (-2.83) | -2.75 (-2.88) | -2.91 (-2.97) |
| **HOMO** | -5.82 (-5.85) | -5.74 (-5.82) | -5.69 (-5.82) | -5.31 (-5.31) | -5.17 (-5.22) | -5.20 (-5.28) | -5.33 (-5.36) |
| **HOMO-1** | -6.18 (-6.18) | -6.04 (-6.10) | -5.74 (-5.85) | -6.72 (-6.72) | -6.56 (-6.61) | -5.77 (-5.88) | -5.58 (-5.74) |
| **HOMO-2** | -6.78 (-6.83) | -6.67 (-6.78) | -5.85 (-5.90) | -6.86 (-6.91) | -6.69 (-6.80) | -5.77 (-5.88) | -5.69 (-5.85) |

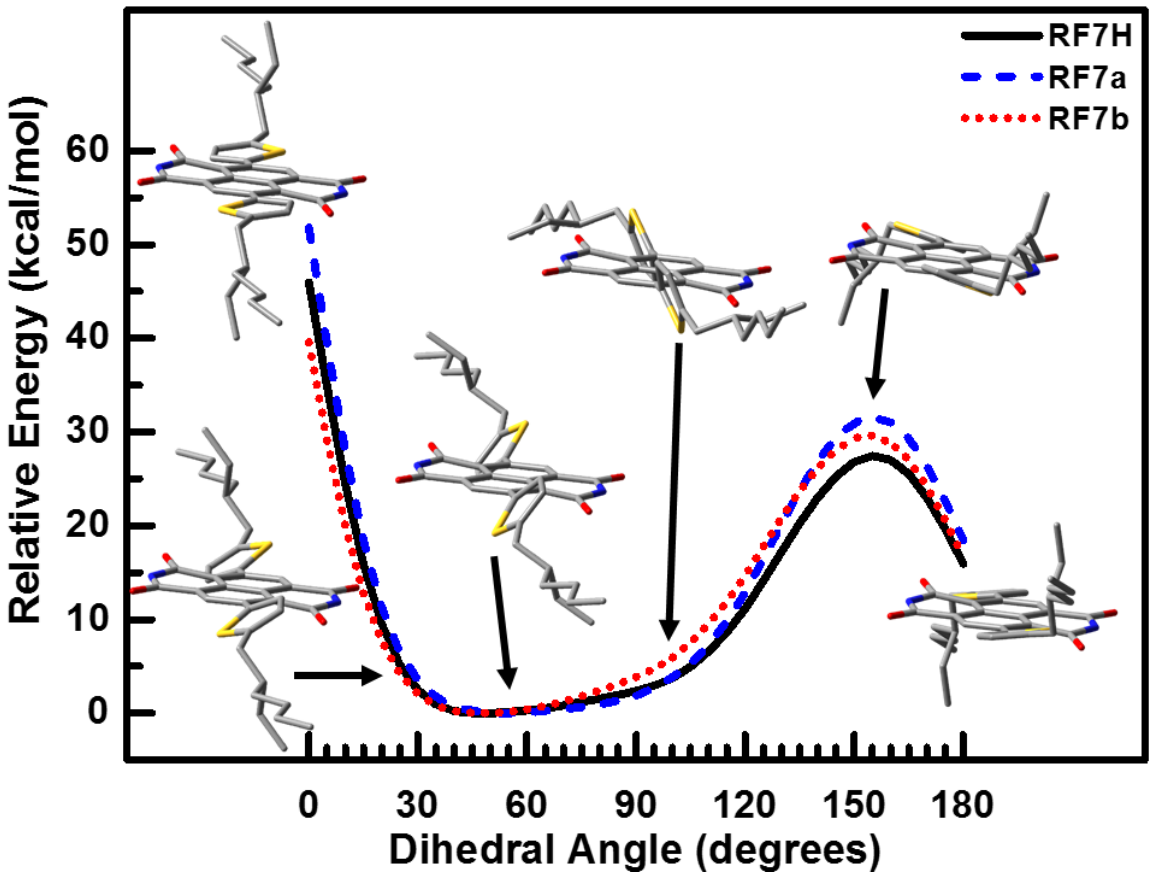


**Figure S26:** Potential energy scan over dihedral angle between core substituted thiophene units and NDI core of **RF7H, RF7a and RF7b** at the B3LYP/6-31G(d,p) level of theory.

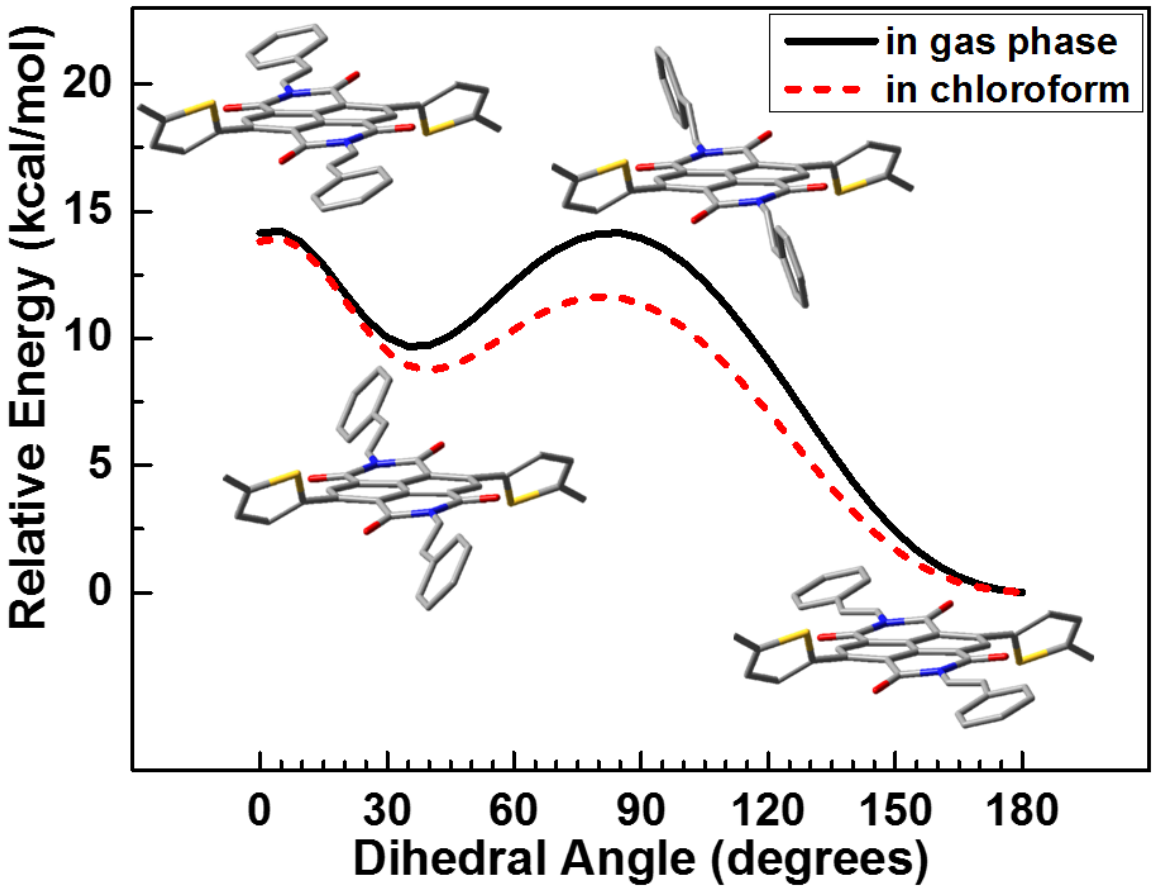


**Figure S27:** Potential energy scan over dihedral angle between styryl imide substitution and NDI core of **RF7b** at the B3LYP/6-31G(d,p) level of theory.

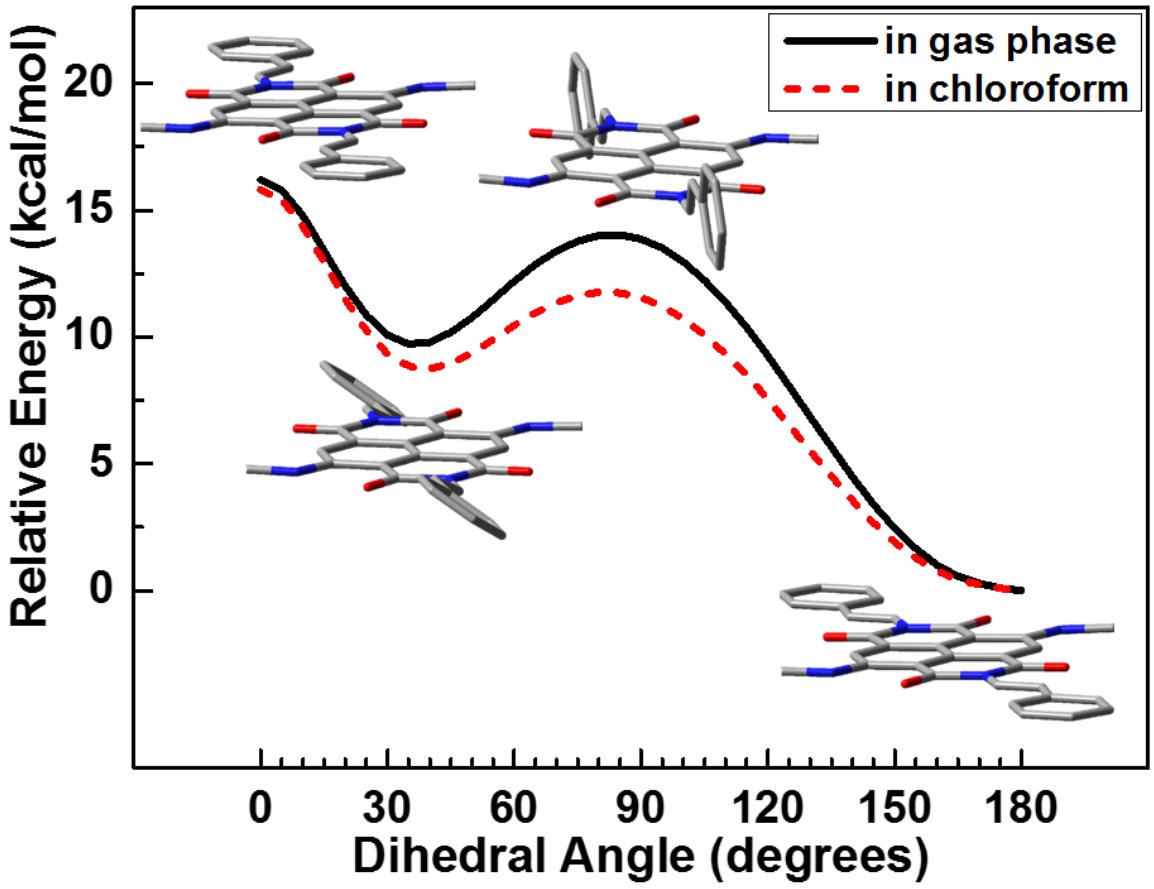


**Figure S28:** Potential energy scan over dihedral angle between styryl imide substitution and NDI core of **RF8b** at the B3LYP/6-31G(d,p) level of theory.

*Note:* The potential energy scans were done by scanning the respective dihedral angles of the optimized geometries in the gas phase or PCM model (chloroform).

**Cartesian coordinates, frequencies and energies of optimized geometries in gas phase**

Note: All molecules are neutral and were optimized using B3LYP/6-31G(d,p) level of theory at normal optimization criteria in Gaussian 09 software package.[S2]

**RF7H**

Cartesian coordinates

| | | | |
|---|---|---|---|
| C | 0.198827 | 0.180566 | -0.660617 |
| C | -0.198827 | -0.180566 | 0.660617 |
| C | 1.529120 | -0.059785 | -1.126102 |
| C | -1.529120 | 0.059785 | 1.126102 |
| C | -0.780381 | 0.796938 | -1.487470 |
| C | 0.780381 | -0.796938 | 1.487470 |
| C | 2.490883 | -0.617667 | -0.264829 |
| C | -2.490883 | 0.617667 | 0.264829 |
| C | -2.065013 | 0.997020 | -1.034919 |
| C | 2.065013 | -0.997020 | 1.034919 |
| C | 1.824730 | 0.201933 | -2.565747 |
| C | -1.824730 | -0.201933 | 2.565747 |
| C | -0.455904 | 1.200765 | -2.878841 |
| C | 0.455904 | -1.200765 | 2.878841 |
| N | 0.826256 | 0.865373 | -3.283936 |
| N | -0.826256 | -0.865373 | 3.283936 |
| O | 2.843131 | -0.134700 | -3.145258 |
| O | -2.843131 | 0.134700 | 3.145258 |
| O | -1.234304 | 1.763507 | -3.632239 |
| O | 1.234304 | -1.763507 | 3.632239 |
| H | -2.781036 | 1.430951 | -1.723168 |
| H | 2.781036 | -1.430951 | 1.723168 |
| C | 3.923189 | -0.818501 | -0.541587 |
| C | -3.923189 | 0.818501 | 0.541587 |
| C | 4.651732 | -1.944042 | -0.218092 |
| C | -4.651732 | 1.944042 | 0.218092 |
| S | 4.996784 | 0.437205 | -1.114719 |
| S | -4.996784 | -0.437205 | 1.114719 |
| C | 6.044573 | -1.811919 | -0.457808 |
| C | -6.044573 | 1.811919 | 0.457808 |
| C | 6.403354 | -0.570977 | -0.927862 |
| C | -6.403354 | 0.570977 | 0.927862 |
| H | 4.189307 | -2.850033 | 0.158078 |
| H | -4.189307 | 2.850033 | -0.158078 |
| H | 6.760872 | -2.608817 | -0.290339 |
| H | -6.760872 | 2.608817 | 0.290339 |
| C | 7.780859 | -0.066925 | -1.266096 |
| H | 8.252445 | -0.795082 | -1.937901 |
| H | 7.708074 | 0.867257 | -1.836806 |
| C | 8.722450 | 0.156095 | -0.050368 |
| H | 8.772205 | -0.798254 | 0.494643 |
| C | 10.150395 | 0.504662 | -0.548531 |
| H | 10.240048 | 0.248943 | -1.613064 |
| H | 10.300464 | 1.591980 | -0.495315 |
| C | 11.284809 | -0.207330 | 0.203318 |
| H | 11.156296 | -1.294013 | 0.095276 |
| H | 11.211338 | -0.002397 | 1.278696 |
| C | 12.681872 | 0.187058 | -0.291054 |
| H | 12.753541 | -0.009316 | -1.369660 |
| H | 12.813863 | 1.271229 | -0.172387 |
| C | 13.810940 | -0.547342 | 0.438096 |

| | | | |
|---|---|---|---|
| H | 13.730183 | -1.632026 | 0.303764 |
| H | 14.793988 | -0.239491 | 0.067435 |
| H | 13.783951 | -0.346307 | 1.515096 |
| C | 8.141567 | 1.215398 | 0.906975 |
| H | 8.046475 | 2.164507 | 0.359443 |
| H | 7.122233 | 0.919486 | 1.179814 |
| C | 8.943414 | 1.452226 | 2.190981 |
| H | 9.062957 | 0.525365 | 2.763492 |
| H | 9.942726 | 1.849365 | 1.986387 |
| H | 8.432116 | 2.173921 | 2.836321 |
| C | -7.780859 | 0.066925 | 1.266096 |
| H | -8.252445 | 0.795082 | 1.937901 |
| H | -7.708074 | -0.867257 | 1.836806 |
| C | -8.722450 | -0.156095 | 0.050368 |
| H | -8.772205 | 0.798254 | -0.494643 |
| C | -10.150395 | -0.504662 | 0.548531 |
| H | -10.240048 | -0.248943 | 1.613064 |
| H | -10.300464 | -1.591980 | 0.495315 |
| C | -11.284809 | 0.207330 | -0.203318 |
| H | -11.156296 | 1.294013 | -0.095276 |
| H | -11.211338 | 0.002397 | -1.278696 |
| C | -12.681872 | -0.187058 | 0.291054 |
| H | -12.753541 | 0.009316 | 1.369660 |
| H | -12.813863 | -1.271229 | 0.172387 |
| C | -13.810940 | 0.547342 | -0.438096 |
| H | -13.783951 | 0.346307 | -1.515096 |
| H | -14.793988 | 0.239491 | -0.067435 |
| H | -13.730183 | 1.632026 | -0.303764 |
| C | -8.141567 | -1.215398 | -0.906975 |
| H | -7.122233 | -0.919486 | -1.179814 |
| H | -8.046475 | -2.164507 | -0.359443 |
| C | -8.943414 | -1.452226 | -2.190981 |
| H | -9.942726 | -1.849365 | -1.986387 |
| H | -9.062957 | -0.525365 | -2.763492 |
| H | -8.432116 | -2.173921 | -2.836321 |
| H | -1.053511 | -1.055654 | 4.253940 |
| H | 1.053511 | 1.055654 | -4.253940 |

## Frequencies

| | | |
|---|---|---|
| 9.0658 | 12.1864 | 13.1320 |
| 13.8827 | 18.7688 | 23.2225 |
| 27.2303 | 35.2347 | 41.0823 |
| 46.3824 | 47.2425 | 51.5981 |
| 53.5619 | 71.4209 | 73.5960 |
| 79.8807 | 81.5212 | 90.5410 |
| 103.3961 | 116.8198 | 117.3225 |
| 128.3715 | 132.3126 | 133.2191 |
| 134.5289 | 139.4233 | 145.2478 |
| 160.7567 | 160.9432 | 168.2630 |
| 183.7272 | 207.5333 | 221.4537 |
| 223.5823 | 230.9533 | 241.6273 |
| 247.8022 | 253.8650 | 259.9828 |
| 262.2184 | 273.9884 | 276.9567 |
| 280.0852 | 290.2990 | 312.7572 |
| 315.1129 | 316.2903 | 327.0092 |
| 343.2715 | 357.6421 | 366.8036 |
| 367.5029 | 386.0764 | 386.4315 |
| 403.8330 | 428.7414 | 433.3285 |
| 457.4388 | 458.5594 | 465.5122 |
| 474.9596 | 482.9760 | 494.9783 |
| 509.2000 | 522.9052 | 544.3714 |
| 557.3968 | 567.8952 | 573.5907 |
| 584.7457 | 592.1249 | 617.1385 |
| 632.6109 | 643.0776 | 655.6089 |
| 666.9084 | 674.4007 | 679.8737 |

| | | |
|---|---|---|
| 689.2232 | 726.2216 | 726.3603 |
| 726.7507 | 734.7892 | 734.8583 |
| 743.1031 | 748.4367 | 748.6043 |
| 765.7312 | 767.2877 | 774.7518 |
| 781.0236 | 782.0736 | 782.2084 |
| 785.5244 | 785.7011 | 786.9209 |
| 789.7112 | 795.3548 | 816.8377 |
| 817.1860 | 825.6980 | 826.4351 |
| 887.2030 | 901.5216 | 902.1756 |
| 902.3911 | 904.6343 | 924.4504 |
| 924.4518 | 936.0231 | 945.3164 |
| 945.7741 | 967.9839 | 970.2271 |
| 982.8153 | 982.9299 | 1003.9883 |
| 1004.1052 | 1037.4553 | 1037.5079 |
| 1040.9847 | 1049.0068 | 1055.1690 |
| 1063.7137 | 1065.4312 | 1067.0829 |
| 1067.6748 | 1074.5878 | 1078.7047 |
| 1091.4360 | 1102.9461 | 1115.6168 |
| 1115.8838 | 1142.3784 | 1142.3926 |
| 1148.4896 | 1162.0479 | 1162.0639 |
| 1189.5343 | 1189.5804 | 1204.5770 |
| 1228.0255 | 1231.0971 | 1247.9072 |
| 1250.0922 | 1250.7707 | 1254.1557 |
| 1258.7852 | 1271.0466 | 1271.8231 |
| 1273.3256 | 1283.4685 | 1285.1315 |
| 1310.8471 | 1311.3027 | 1315.8773 |
| 1315.8798 | 1327.7306 | 1329.8358 |
| 1331.5202 | 1331.5576 | 1340.5750 |
| 1340.5863 | 1352.1217 | 1352.3289 |
| 1364.2868 | 1364.7830 | 1377.3245 |
| 1377.4739 | 1391.5069 | 1391.5108 |
| 1394.7637 | 1401.5842 | 1401.9238 |
| 1411.3237 | 1414.6809 | 1414.6841 |
| 1415.9522 | 1424.6785 | 1427.7515 |
| 1427.7581 | 1429.0311 | 1429.2744 |
| 1429.3132 | 1450.3339 | 1470.2439 |
| 1491.4765 | 1491.7115 | 1499.1301 |
| 1499.1740 | 1500.4799 | 1500.5712 |
| 1503.9282 | 1503.9952 | 1504.3308 |
| 1510.3718 | 1511.7359 | 1514.7200 |
| 1514.7202 | 1515.0802 | 1515.0807 |
| 1518.4203 | 1518.4209 | 1524.0652 |
| 1524.0665 | 1528.4254 | 1528.4254 |
| 1587.4509 | 1587.9518 | 1598.8435 |
| 1621.6712 | 1653.4446 | 1782.5559 |
| 1785.0652 | 1791.6048 | 1794.1801 |
| 3006.9495 | 3006.9499 | 3015.4406 |
| 3015.4448 | 3017.0431 | 3017.0433 |
| 3020.6451 | 3020.6506 | 3025.7328 |
| 3025.7363 | 3034.5552 | 3034.5798 |
| 3038.0457 | 3038.0495 | 3040.8115 |
| 3040.8306 | 3047.8824 | 3047.8826 |
| 3050.3953 | 3050.3958 | 3073.2009 |
| 3073.2112 | 3076.3704 | 3076.3767 |
| 3078.5531 | 3078.5598 | 3106.4199 |
| 3106.4244 | 3108.2649 | 3108.2684 |
| 3111.7167 | 3111.7211 | 3115.6692 |
| 3115.6810 | 3209.3364 | 3209.3625 |
| 3223.9546 | 3223.9629 | 3229.4078 |
| 3229.6284 | 3596.9731 | 3597.1597 |

## Energies

SCF Done: E(RB3LYP) = -2680.28543762 A.U. after 1 cycles
Zero-point correction= 0.727849 (Hartree/Particle)
Thermal correction to Energy= 0.773264

```
 Thermal correction to Enthalpy=                 0.774208
 Thermal correction to Gibbs Free Energy=        0.641208
 Sum of electronic and zero-point Energies=          -2679.557589
 Sum of electronic and thermal Energies=             -2679.512173
 Sum of electronic and thermal Enthalpies=           -2679.511229
 Sum of electronic and thermal Free Energies=        -2679.644230
```

**RF7a**

Cartesian coordinates

```
C       -0.304632   -0.611378    0.200390
C        0.304583    0.611295   -0.200258
C       -1.691185   -0.856253   -0.010787
C        1.691136    0.856171    0.010921
C        0.517361   -1.575720    0.833603
C       -0.517409    1.575633   -0.833478
C       -2.498416    0.141904   -0.587141
C        2.498364   -0.141977    0.587295
C        1.863869   -1.340023    1.009509
C       -1.863920    1.339944   -1.009367
C       -2.219859   -2.219924    0.289842
C        2.219821    2.219827   -0.289758
C       -0.036888   -2.875450    1.289223
C        0.036851    2.875340   -1.289151
N       -1.368409   -3.126239    0.948644
N        1.368386    3.126116   -0.948618
O       -3.343743   -2.581605   -0.024868
O        3.343725    2.581497    0.024896
O        0.635108   -3.691781    1.904932
O       -0.635144    3.691656   -1.904880
H        2.460296   -2.123172    1.462143
H       -2.460346    2.123093   -1.462001
C       -3.960433    0.109494   -0.771651
C        3.960377   -0.109553    0.771841
C       -4.634712    0.482932   -1.913872
C        4.634630   -0.482994    1.914077
S       -5.100822   -0.179613    0.522392
S        5.100799    0.179585   -0.522168
C       -6.047073    0.504412   -1.763087
C        6.046995   -0.504455    1.763329
C       -6.466725    0.188638   -0.493351
C        6.466679   -0.188658    0.493610
H       -4.124629    0.712353   -2.843045
H        4.124525   -0.712430    2.843233
H       -6.732666    0.746896   -2.567803
H        6.732569   -0.746936    2.568062
C       -7.874564    0.147524    0.038598
H       -8.473887   -0.482681   -0.630571
H       -7.891911   -0.348819    1.016866
C       -8.573125    1.529928    0.162410
H       -8.543562    1.992863   -0.835130
C      -10.060145    1.334830    0.561509
H      -10.352122    0.290286    0.386618
H      -10.171710    1.493091    1.643304
C      -11.052302    2.232315   -0.193307
H      -10.963700    2.032963   -1.271007
H      -10.783484    3.287784   -0.060777
C      -12.508816    2.024675    0.239322
H      -12.778072    0.967481    0.109269
H      -12.599016    2.228700    1.315039
C      -13.499431    2.902710   -0.531145
H      -13.458880    2.696394   -1.606728
H      -14.528583    2.731896   -0.199105
H      -13.277609    3.966886   -0.391696
```

| | | | |
|---|---|---|---|
| C | -7.802332 | 2.448172 | 1.131336 |
| H | -7.787666 | 1.973765 | 2.123473 |
| H | -6.757387 | 2.501353 | 0.805570 |
| C | -8.347458 | 3.874053 | 1.262490 |
| H | -8.384266 | 4.377964 | 0.289970 |
| H | -9.356224 | 3.893075 | 1.686885 |
| H | -7.706915 | 4.472026 | 1.918977 |
| C | 7.874531 | -0.147508 | -0.038299 |
| H | 8.473822 | 0.482701 | 0.630895 |
| H | 7.891895 | 0.348850 | -1.016560 |
| C | 8.573126 | -1.529895 | -0.162111 |
| H | 8.543543 | -1.992848 | 0.835419 |
| C | 10.060154 | -1.334753 | -0.561159 |
| H | 10.352103 | -0.290208 | -0.386231 |
| H | 10.171755 | -1.492983 | -1.642956 |
| C | 11.052309 | -2.232236 | 0.193663 |
| H | 10.963670 | -2.032914 | 1.271365 |
| H | 10.783519 | -3.287708 | 0.061097 |
| C | 12.508830 | -2.024552 | -0.238917 |
| H | 12.778058 | -0.967355 | -0.108829 |
| H | 12.599067 | -2.228547 | -1.314637 |
| C | 13.499443 | -2.902583 | 0.531556 |
| H | 13.277649 | -3.966761 | 0.392075 |
| H | 14.528601 | -2.731738 | 0.199550 |
| H | 13.458856 | -2.696295 | 1.607143 |
| C | 7.802385 | -2.448139 | -1.131079 |
| H | 6.757432 | -2.501351 | -0.805346 |
| H | 7.787739 | -1.973714 | -2.123208 |
| C | 8.347548 | -3.874006 | -1.262242 |
| H | 9.356327 | -3.892996 | -1.686607 |
| H | 8.384339 | -4.377933 | -0.289730 |
| H | 7.707038 | -4.471981 | -1.918760 |
| C | -1.945005 | -4.438830 | 1.309413 |
| H | -2.951478 | -4.246474 | 1.685298 |
| H | -1.325555 | -4.829919 | 2.117326 |
| C | 1.945021 | 4.438647 | -1.309539 |
| H | 2.951477 | 4.246214 | -1.685434 |
| H | 1.325561 | 4.829667 | -2.117478 |
| C | -2.025581 | -5.456437 | 0.150205 |
| H | -2.674602 | -5.014827 | -0.616150 |
| C | 2.025670 | 5.456404 | -0.150468 |
| H | 2.674770 | 5.014921 | 0.615892 |
| C | -2.709530 | -6.745203 | 0.682304 |
| H | -3.192209 | -6.535268 | 1.647071 |
| H | -1.944217 | -7.503388 | 0.898167 |
| C | -3.773168 | -7.336297 | -0.254645 |
| H | -4.552733 | -6.581379 | -0.428201 |
| H | -3.332938 | -7.544954 | -1.237960 |
| C | -4.419649 | -8.615506 | 0.290605 |
| H | -4.860195 | -8.407202 | 1.275353 |
| H | -3.640365 | -9.370689 | 0.462499 |
| C | -5.493364 | -9.191963 | -0.637153 |
| H | -5.936044 | -10.102941 | -0.221270 |
| H | -6.303985 | -8.472577 | -0.799658 |
| H | -5.075466 | -9.443704 | -1.618541 |
| C | -0.642775 | -5.721316 | -0.477049 |
| H | -0.206660 | -4.764599 | -0.788912 |
| H | 0.028907 | -6.120866 | 0.293744 |
| C | -0.653626 | -6.660325 | -1.688128 |
| H | -0.986534 | -7.668906 | -1.423359 |
| H | -1.316748 | -6.287051 | -2.476874 |
| H | 0.350522 | -6.750858 | -2.115205 |
| C | 2.709525 | 6.745110 | -0.682833 |
| H | 3.192145 | 6.535025 | -1.647597 |
| H | 1.944158 | 7.503217 | -0.898781 |
| C | 3.773206 | 7.336437 | 0.253922 |

| | | | |
|---|---|---|---|
| H | 4.552821 | 6.581592 | 0.427567 |
| H | 3.333042 | 7.545269 | 1.237230 |
| C | 4.419575 | 8.615567 | -0.291640 |
| H | 4.860043 | 8.407088 | -1.276386 |
| H | 3.640238 | 9.370677 | -0.463617 |
| C | 5.493344 | 9.192267 | 0.635904 |
| H | 6.304016 | 8.472955 | 0.798481 |
| H | 5.935941 | 10.103184 | 0.219799 |
| H | 5.075522 | 9.444184 | 1.617280 |
| C | 0.642912 | 5.721333 | 0.476870 |
| H | -0.028849 | 6.120757 | -0.293918 |
| H | 0.206855 | 4.764645 | 0.788905 |
| C | 0.653852 | 6.660510 | 1.687819 |
| H | 1.317059 | 6.287361 | 2.476553 |
| H | 0.986711 | 7.669062 | 1.422881 |
| H | -0.350257 | 6.751077 | 2.114980 |

## Frequencies

| | | |
|---|---|---|
| 3.9186 | 8.0668 | 11.9098 |
| 11.9284 | 14.9205 | 15.7848 |
| 17.5928 | 18.3374 | 20.9613 |
| 24.3653 | 24.9951 | 30.4642 |
| 34.4447 | 36.0366 | 36.1081 |
| 43.5636 | 47.6742 | 52.6428 |
| 53.2543 | 57.1577 | 58.0134 |
| 67.8629 | 68.1380 | 77.7040 |
| 80.3028 | 81.5964 | 82.7530 |
| 87.1684 | 101.5328 | 104.0529 |
| 111.4094 | 114.8766 | 115.4938 |
| 120.9799 | 121.5542 | 126.7693 |
| 127.5434 | 127.5551 | 130.0758 |
| 136.1910 | 138.2160 | 138.2343 |
| 147.0343 | 155.1108 | 162.9596 |
| 163.3316 | 179.7462 | 188.0282 |
| 197.1811 | 205.4047 | 210.3738 |
| 219.0526 | 228.7039 | 229.0976 |
| 236.0993 | 240.0915 | 240.4921 |
| 249.4248 | 250.9164 | 253.3985 |
| 256.1797 | 257.8323 | 260.7886 |
| 268.9040 | 271.5134 | 271.7000 |
| 275.5373 | 289.8159 | 307.1608 |
| 308.4626 | 313.1017 | 317.7106 |
| 325.0057 | 331.7829 | 345.1109 |
| 354.2872 | 356.1598 | 366.1950 |
| 367.8740 | 369.2128 | 374.2568 |
| 380.1318 | 386.2746 | 386.5690 |
| 406.7974 | 412.1589 | 431.6484 |
| 442.5288 | 447.1923 | 458.3088 |
| 461.9146 | 467.7222 | 475.3980 |
| 475.4722 | 486.5074 | 496.6646 |
| 498.4956 | 512.0840 | 513.7457 |
| 530.6429 | 554.8940 | 562.7345 |
| 564.3022 | 573.0431 | 574.6233 |
| 585.6940 | 597.4879 | 617.9067 |
| 631.6043 | 642.4799 | 648.1382 |
| 655.5330 | 678.7125 | 714.8977 |
| 725.7344 | 725.9020 | 734.0257 |
| 734.0597 | 734.2793 | 734.3386 |
| 740.0995 | 740.1973 | 747.5562 |
| 756.0149 | 757.0331 | 758.7853 |
| 770.8524 | 774.4873 | 778.3630 |
| 781.5788 | 781.9461 | 782.1244 |
| 782.8963 | 784.1504 | 784.1849 |
| 784.1937 | 785.6942 | 812.3448 |
| 815.7640 | 816.1616 | 824.1329 |

| | | |
|---|---|---|
| 824.8009 | 825.3272 | 864.1507 |
| 871.2979 | 898.8182 | 899.4282 |
| 902.6351 | 902.6482 | 904.4500 |
| 906.6030 | 923.9216 | 924.6989 |
| 924.8266 | 925.6711 | 941.6609 |
| 944.1799 | 945.4179 | 946.1367 |
| 964.8172 | 966.8909 | 969.0424 |
| 974.0709 | 983.2126 | 983.5765 |
| 988.4004 | 990.1562 | 1004.1814 |
| 1004.4790 | 1008.4980 | 1016.4215 |
| 1033.6596 | 1037.8778 | 1037.8936 |
| 1039.4108 | 1039.7462 | 1045.3121 |
| 1052.2996 | 1064.0671 | 1065.1688 |
| 1065.1852 | 1066.2687 | 1068.0842 |
| 1068.4468 | 1068.6349 | 1069.1641 |
| 1076.8139 | 1079.3511 | 1085.1640 |
| 1087.9946 | 1099.0203 | 1112.1574 |
| 1116.0136 | 1117.3538 | 1121.5848 |
| 1142.5937 | 1142.9283 | 1142.9305 |
| 1148.1039 | 1148.8944 | 1162.1587 |
| 1162.2086 | 1169.9521 | 1180.4935 |
| 1189.7255 | 1189.7695 | 1194.2238 |
| 1197.1009 | 1216.6932 | 1223.5217 |
| 1228.4480 | 1232.7222 | 1237.8153 |
| 1247.8537 | 1250.9286 | 1252.5310 |
| 1252.7148 | 1254.1881 | 1265.6849 |
| 1275.2168 | 1275.3110 | 1278.8129 |
| 1279.2409 | 1281.9042 | 1290.6592 |
| 1309.6008 | 1309.9437 | 1310.8400 |
| 1311.0450 | 1318.2760 | 1318.2776 |
| 1327.2012 | 1327.2958 | 1331.5018 |
| 1331.5103 | 1332.8548 | 1334.4014 |
| 1335.3547 | 1335.7055 | 1339.4538 |
| 1339.5404 | 1342.7842 | 1342.7939 |
| 1352.9937 | 1353.2581 | 1355.2530 |
| 1356.1079 | 1364.7849 | 1365.5857 |
| 1372.7739 | 1376.8779 | 1381.5026 |
| 1384.7039 | 1392.4009 | 1392.4657 |
| 1393.6345 | 1396.8119 | 1397.6202 |
| 1403.1196 | 1403.4386 | 1411.0361 |
| 1412.1935 | 1413.5500 | 1415.7265 |
| 1415.7576 | 1417.4186 | 1418.2984 |
| 1421.9930 | 1425.5486 | 1427.2335 |
| 1427.2344 | 1427.3983 | 1427.4732 |
| 1429.0334 | 1429.0336 | 1430.4376 |
| 1430.4544 | 1437.7455 | 1455.1326 |
| 1471.6846 | 1481.4665 | 1481.5711 |
| 1492.0639 | 1492.1965 | 1497.1206 |
| 1497.1704 | 1500.1215 | 1500.1479 |
| 1500.4887 | 1500.4902 | 1500.7628 |
| 1500.7928 | 1504.1548 | 1504.1577 |
| 1504.3516 | 1504.3549 | 1508.5137 |
| 1513.8819 | 1513.8822 | 1514.8080 |
| 1514.8269 | 1514.9216 | 1515.1096 |
| 1515.1115 | 1515.2377 | 1515.2421 |
| 1517.1584 | 1518.2673 | 1518.2690 |
| 1518.5783 | 1518.5826 | 1523.1529 |
| 1523.1562 | 1523.4070 | 1523.4088 |
| 1527.8871 | 1527.8877 | 1528.4714 |
| 1528.4730 | 1589.1126 | 1591.4865 |
| 1605.7419 | 1617.5202 | 1653.3510 |
| 1736.1240 | 1739.3222 | 1773.6000 |
| 1775.8516 | 3007.0869 | 3007.0873 |
| 3014.2173 | 3014.2230 | 3014.5442 |
| 3014.5479 | 3017.5764 | 3017.5766 |
| 3018.9270 | 3018.9293 | 3021.2648 |

| | | |
|---|---|---|
| 3021.2708 | 3025.7897 | 3025.7926 |
| 3027.8743 | 3027.8780 | 3033.9807 |
| 3034.0004 | 3035.5440 | 3035.5676 |
| 3037.6862 | 3037.6895 | 3037.9003 |
| 3037.9042 | 3040.2568 | 3040.2650 |
| 3040.3845 | 3040.4221 | 3044.2235 |
| 3044.2254 | 3046.8672 | 3046.8681 |
| 3048.1940 | 3048.1988 | 3050.1453 |
| 3050.1460 | 3052.6944 | 3052.6974 |
| 3073.0614 | 3073.0691 | 3074.2628 |
| 3074.2655 | 3076.0825 | 3076.0872 |
| 3076.9175 | 3076.9231 | 3077.5648 |
| 3077.5702 | 3097.9841 | 3098.0050 |
| 3105.6514 | 3105.6569 | 3106.1553 |
| 3106.1645 | 3107.9095 | 3107.9144 |
| 3108.2395 | 3108.2461 | 3110.6631 |
| 3110.6709 | 3111.2696 | 3111.2738 |
| 3115.7433 | 3115.7453 | 3115.8314 |
| 3115.8556 | 3158.9292 | 3158.9326 |
| 3208.3279 | 3208.3562 | 3223.2726 |
| 3223.2778 | 3232.9443 | 3233.1699 |

Energies

SCF Done: E(RB3LYP) = -3309.33274675 A.U. after 1 cycles
Zero-point correction= 1.182526 (Hartree/Particle)
Thermal correction to Energy= 1.250098
Thermal correction to Enthalpy= 1.251042
Thermal correction to Gibbs Free Energy= 1.064802
Sum of electronic and zero-point Energies= -3308.150220
Sum of electronic and thermal Energies= -3308.082648
Sum of electronic and thermal Enthalpies= -3308.081704
Sum of electronic and thermal Free Energies= -3308.267945

**RF7b**

Cartesian coordinates

| | | | |
|---|---|---|---|
| C | 0.293849 | 0.019488 | -0.646780 |
| C | -0.293849 | -0.019488 | 0.646780 |
| C | 1.650027 | -0.345080 | -0.858148 |
| C | -1.650027 | 0.345080 | 0.858148 |
| C | -0.514037 | 0.450633 | -1.724750 |
| C | 0.514037 | -0.450633 | 1.724750 |
| C | 2.459178 | -0.695856 | 0.240663 |
| C | -2.459178 | 0.695856 | -0.240663 |
| C | -1.841225 | 0.763377 | -1.517201 |
| C | 1.841225 | -0.763377 | 1.517201 |
| C | 2.133885 | -0.475042 | -2.258324 |
| C | -2.133885 | 0.475042 | 2.258324 |
| C | 0.026319 | 0.567254 | -3.102264 |
| C | -0.026319 | -0.567254 | 3.102264 |
| N | 1.330421 | 0.083791 | -3.308742 |
| N | -1.330421 | -0.083791 | 3.308742 |
| O | 3.171593 | -1.047621 | -2.539854 |
| O | -3.171593 | 1.047621 | 2.539854 |
| O | -0.643037 | 1.043390 | -4.007184 |
| O | 0.643037 | -1.043390 | 4.007184 |
| H | -2.436228 | 1.045528 | -2.377382 |
| H | 2.436228 | -1.045528 | 2.377382 |
| C | 3.907053 | -0.956797 | 0.225679 |
| C | -3.907053 | 0.956797 | -0.225679 |
| C | 4.554120 | -1.968751 | 0.902533 |
| C | -4.554120 | 1.968751 | -0.902533 |
| S | 5.081922 | 0.123222 | -0.490739 |

| | | | |
|---|---|---|---|
| S | -5.081922 | -0.123222 | 0.490739 |
| C | 5.969765 | -1.897327 | 0.819750 |
| C | -5.969765 | 1.897327 | -0.819750 |
| C | 6.423351 | -0.809796 | 0.112257 |
| C | -6.423351 | 0.809796 | -0.112257 |
| H | 4.020890 | -2.758147 | 1.420782 |
| H | -4.020890 | 2.758147 | -1.420782 |
| H | 6.634582 | -2.627363 | 1.268424 |
| H | -6.634582 | 2.627363 | -1.268424 |
| C | 1.929274 | 0.038255 | -4.599598 |
| C | -1.929274 | -0.038255 | 4.599598 |
| H | 2.896651 | -0.437902 | -4.539242 |
| H | -2.896651 | 0.437902 | 4.539242 |
| C | 1.449837 | 0.501252 | -5.767448 |
| C | -1.449837 | -0.501252 | 5.767448 |
| H | 0.490989 | 0.997101 | -5.803660 |
| H | -0.490989 | -0.997101 | 5.803660 |
| C | 2.171158 | 0.395878 | -7.044340 |
| C | -2.171158 | -0.395878 | 7.044340 |
| C | 1.666615 | 1.105508 | -8.149392 |
| C | -1.666615 | -1.105508 | 8.149392 |
| C | 3.332728 | -0.377599 | -7.234910 |
| C | -3.332728 | 0.377599 | 7.234910 |
| C | 2.300743 | 1.061185 | -9.389468 |
| C | -2.300743 | -1.061185 | 9.389468 |
| C | 3.966388 | -0.421461 | -8.472661 |
| C | -3.966388 | 0.421461 | 8.472661 |
| C | 3.456534 | 0.298649 | -9.557043 |
| C | -3.456534 | -0.298649 | 9.557043 |
| H | 0.766506 | 1.701753 | -8.024724 |
| H | -0.766506 | -1.701753 | 8.024724 |
| H | 3.738357 | -0.962281 | -6.415131 |
| H | -3.738357 | 0.962281 | 6.415131 |
| H | 1.890406 | 1.621640 | -10.224618 |
| H | -1.890406 | -1.621640 | 10.224618 |
| H | 4.859958 | -1.026932 | -8.595398 |
| H | -4.859958 | 1.026932 | 8.595398 |
| H | 3.952683 | 0.258747 | -10.522199 |
| H | -3.952683 | -0.258747 | 10.522199 |
| C | 7.847179 | -0.399336 | -0.152424 |
| H | 8.378409 | -1.266105 | -0.565327 |
| H | 7.876571 | 0.372147 | -0.931850 |
| C | 8.631924 | 0.107734 | 1.089248 |
| H | 8.585211 | -0.690903 | 1.844267 |
| C | 10.120969 | 0.332637 | 0.713792 |
| H | 10.338558 | -0.169810 | -0.238610 |
| H | 10.293141 | 1.401664 | 0.526406 |
| C | 11.129964 | -0.175217 | 1.754540 |
| H | 10.977267 | -1.254202 | 1.901378 |
| H | 10.934125 | 0.290513 | 2.728517 |
| C | 12.589595 | 0.077647 | 1.357795 |
| H | 12.783501 | -0.383043 | 0.379427 |
| H | 12.744935 | 1.156356 | 1.219391 |
| C | 13.595598 | -0.455540 | 2.382216 |
| H | 13.489909 | -1.538235 | 2.515278 |
| H | 14.626633 | -0.258569 | 2.071227 |
| H | 13.449081 | 0.012254 | 3.362402 |
| C | 7.963553 | 1.361408 | 1.686854 |
| H | 7.966531 | 2.154493 | 0.924955 |
| H | 6.909646 | 1.135772 | 1.885366 |
| C | 8.599790 | 1.896198 | 2.974230 |
| H | 8.619458 | 1.129795 | 3.757395 |
| H | 9.627530 | 2.238241 | 2.816286 |
| H | 8.029196 | 2.747047 | 3.360408 |
| C | -7.847179 | 0.399336 | 0.152424 |
| H | -8.378409 | 1.266105 | 0.565327 |

| | | | |
|---|---|---|---|
| H | -7.876571 | -0.372147 | 0.931850 |
| C | -8.631924 | -0.107734 | -1.089248 |
| H | -8.585211 | 0.690903 | -1.844267 |
| C | -10.120969 | -0.332637 | -0.713792 |
| H | -10.338558 | 0.169810 | 0.238610 |
| H | -10.293141 | -1.401664 | -0.526406 |
| C | -11.129964 | 0.175217 | -1.754540 |
| H | -10.977267 | 1.254202 | -1.901378 |
| H | -10.934125 | -0.290513 | -2.728517 |
| C | -12.589595 | -0.077647 | -1.357795 |
| H | -12.783501 | 0.383043 | -0.379427 |
| H | -12.744935 | -1.156356 | -1.219391 |
| C | -13.595598 | 0.455540 | -2.382216 |
| H | -13.449081 | -0.012254 | -3.362402 |
| H | -14.626633 | 0.258569 | -2.071227 |
| H | -13.489909 | 1.538235 | -2.515278 |
| C | -7.963553 | -1.361408 | -1.686854 |
| H | -6.909646 | -1.135772 | -1.885366 |
| H | -7.966531 | -2.154493 | -0.924955 |
| C | -8.599790 | -1.896198 | -2.974230 |
| H | -9.627530 | -2.238241 | -2.816286 |
| H | -8.619458 | -1.129795 | -3.757395 |
| H | -8.029196 | -2.747047 | -3.360408 |

## Frequencies

| | | |
|---|---|---|
| 7.2598 | 9.9485 | 10.7022 |
| 12.0085 | 12.3079 | 12.7184 |
| 18.0969 | 19.5175 | 19.7172 |
| 26.3042 | 28.3234 | 33.0347 |
| 33.4937 | 41.2984 | 41.6863 |
| 43.3743 | 50.4242 | 51.3573 |
| 55.9355 | 68.4473 | 69.4127 |
| 74.4477 | 76.4691 | 79.9326 |
| 86.7603 | 95.3183 | 101.0310 |
| 112.5163 | 112.7621 | 120.6840 |
| 124.6491 | 127.2010 | 129.6731 |
| 135.4969 | 139.2998 | 141.4656 |
| 143.6388 | 153.3416 | 155.8665 |
| 181.0293 | 186.0448 | 201.6209 |
| 201.8014 | 216.4904 | 219.0653 |
| 231.4237 | 232.3228 | 239.3216 |
| 243.6839 | 250.4944 | 256.4132 |
| 256.7608 | 262.3260 | 273.5417 |
| 273.9303 | 278.4591 | 280.5634 |
| 300.9586 | 320.7874 | 321.7053 |
| 335.8235 | 336.7498 | 350.8963 |
| 359.0939 | 366.6012 | 366.8769 |
| 374.6699 | 386.3147 | 386.6832 |
| 397.4050 | 413.9712 | 414.4735 |
| 426.3286 | 436.7755 | 445.3755 |
| 452.7766 | 462.0590 | 466.8838 |
| 474.9502 | 478.1327 | 488.0209 |
| 498.8768 | 500.3105 | 508.3368 |
| 514.1589 | 519.2262 | 527.9445 |
| 551.7200 | 555.5799 | 565.8302 |
| 574.7389 | 579.4093 | 584.1331 |
| 605.5174 | 611.6107 | 618.7916 |
| 633.0542 | 634.0304 | 634.0587 |
| 641.1360 | 663.2691 | 666.0893 |
| 675.0580 | 703.5362 | 705.4983 |
| 712.7366 | 726.0476 | 726.2221 |
| 734.0018 | 734.0051 | 738.8360 |
| 744.2784 | 747.4188 | 752.2786 |
| 758.2527 | 763.3022 | 766.5267 |
| 768.7768 | 773.6129 | 778.3066 |

| | | |
|---|---|---|
| 780.9059 | 781.9738 | 782.6947 |
| 784.1231 | 784.1909 | 816.1727 |
| 816.4137 | 825.2755 | 825.7219 |
| 846.3354 | 850.8658 | 850.9865 |
| 864.2837 | 878.4834 | 878.4857 |
| 884.5772 | 898.1917 | 901.8279 |
| 902.1524 | 902.4021 | 902.7844 |
| 924.6016 | 924.6020 | 925.3501 |
| 925.7495 | 945.8358 | 945.9387 |
| 962.0623 | 962.7732 | 969.5568 |
| 969.5886 | 973.5627 | 975.3230 |
| 983.2580 | 983.5332 | 993.6567 |
| 993.7067 | 1004.2123 | 1004.3055 |
| 1013.5291 | 1013.5575 | 1020.5425 |
| 1020.5888 | 1037.5197 | 1037.5325 |
| 1044.7992 | 1048.2761 | 1057.4149 |
| 1057.4450 | 1062.6044 | 1065.1904 |
| 1068.0496 | 1068.5085 | 1069.5441 |
| 1078.5272 | 1083.9850 | 1097.4416 |
| 1110.0606 | 1111.3744 | 1114.4377 |
| 1114.6229 | 1130.8620 | 1131.6124 |
| 1142.8303 | 1142.8374 | 1162.7379 |
| 1162.7697 | 1169.4822 | 1187.7676 |
| 1187.7775 | 1189.8200 | 1189.9882 |
| 1197.1164 | 1208.9136 | 1212.7805 |
| 1214.8663 | 1228.8084 | 1228.9515 |
| 1232.8065 | 1247.6753 | 1249.6390 |
| 1251.4468 | 1251.8506 | 1254.4419 |
| 1265.8111 | 1272.2100 | 1272.4172 |
| 1283.7811 | 1302.1009 | 1310.4003 |
| 1310.8604 | 1316.6871 | 1316.7210 |
| 1329.4567 | 1330.0553 | 1331.2874 |
| 1331.2930 | 1334.3766 | 1338.3706 |
| 1339.9173 | 1339.9615 | 1351.6717 |
| 1352.9465 | 1362.5720 | 1363.2320 |
| 1364.7015 | 1365.2188 | 1370.7392 |
| 1370.8493 | 1371.9956 | 1374.8584 |
| 1382.1633 | 1392.3267 | 1392.3600 |
| 1400.2955 | 1402.4037 | 1402.7335 |
| 1407.0797 | 1412.7356 | 1415.4251 |
| 1415.4841 | 1426.8939 | 1426.8985 |
| 1428.6882 | 1428.6885 | 1443.4467 |
| 1451.3120 | 1472.0398 | 1491.2941 |
| 1491.3118 | 1493.5643 | 1493.7564 |
| 1499.2213 | 1499.2582 | 1500.3999 |
| 1500.4595 | 1503.9245 | 1503.9319 |
| 1507.5253 | 1512.9623 | 1513.7461 |
| 1513.7462 | 1515.2495 | 1515.2506 |
| 1518.1922 | 1518.1928 | 1518.9515 |
| 1522.8063 | 1522.8077 | 1528.5467 |
| 1528.5468 | 1541.1485 | 1541.1554 |
| 1587.3318 | 1590.7356 | 1605.5060 |
| 1613.7091 | 1630.6459 | 1630.6505 |
| 1652.1688 | 1657.5938 | 1657.7622 |
| 1701.3488 | 1701.6820 | 1741.6973 |
| 1745.3523 | 1779.1166 | 1780.3317 |
| 3008.7189 | 3008.7193 | 3015.5145 |
| 3015.5183 | 3017.5330 | 3017.5332 |
| 3021.5163 | 3021.5218 | 3026.3006 |
| 3026.3043 | 3034.8373 | 3034.8577 |
| 3037.8008 | 3037.8041 | 3040.7850 |
| 3040.8025 | 3048.3990 | 3048.3998 |
| 3050.4163 | 3050.4167 | 3073.3838 |
| 3073.3948 | 3076.7932 | 3076.7970 |
| 3079.4852 | 3079.4919 | 3105.9950 |
| 3105.9995 | 3108.6108 | 3108.6144 |

| | | |
|---|---|---|
| 3111.5863 | 3111.5904 | 3115.8270 |
| 3115.8376 | 3175.8998 | 3175.9054 |
| 3181.7494 | 3181.7518 | 3191.3388 |
| 3191.3388 | 3199.2343 | 3199.2354 |
| 3207.7844 | 3207.8074 | 3208.8398 |
| 3208.8652 | 3223.5449 | 3223.5513 |
| 3234.3539 | 3234.5720 | 3259.3787 |
| 3259.4449 | 3268.0974 | 3268.1053 |

Energies

SCF Done: E(RB3LYP) = -3297.19265572 A.U. after 1 cycles
Zero-point correction= 0.955502 (Hartree/Particle)
Thermal correction to Energy= 1.015155
Thermal correction to Enthalpy= 1.016099
Thermal correction to Gibbs Free Energy= 0.846913
Sum of electronic and zero-point Energies= -3296.237154
Sum of electronic and thermal Energies= -3296.177501
Sum of electronic and thermal Enthalpies= -3296.176556
Sum of electronic and thermal Free Energies= -3296.345743

**RF8H**

Cartesian coordinates

| | | | |
|---|---|---|---|
| C | -1.834360 | -2.527391 | -0.244909 |
| C | -1.532346 | -1.102318 | -0.123924 |
| C | -0.172944 | -0.685883 | -0.059466 |
| C | 0.898336 | -1.626156 | -0.109057 |
| C | 0.610071 | -3.077644 | -0.227798 |
| C | -2.582106 | -0.142041 | -0.070771 |
| C | 0.172922 | 0.685900 | 0.059318 |
| C | -0.898358 | 1.626174 | 0.108901 |
| C | -2.214645 | 1.230215 | 0.046309 |
| C | -0.610091 | 3.077663 | 0.227618 |
| C | 1.834339 | 2.527409 | 0.244740 |
| C | 1.532324 | 1.102335 | 0.123778 |
| C | 2.582082 | 0.142057 | 0.070646 |
| C | 2.214623 | -1.230199 | -0.046452 |
| H | 2.971252 | -2.004012 | -0.084595 |
| H | -2.971274 | 2.004030 | 0.084441 |
| O | -1.462702 | 3.952230 | 0.275315 |
| O | 2.970736 | 3.013211 | 0.314140 |
| O | -2.970756 | -3.013195 | -0.314299 |
| O | 1.462683 | -3.952207 | -0.275536 |
| N | 0.741785 | 3.391737 | 0.283796 |
| N | -0.741805 | -3.391717 | -0.283981 |
| N | -3.884106 | -0.508188 | -0.127326 |
| H | -4.037164 | -1.505199 | -0.260496 |
| N | 3.884081 | 0.508195 | 0.127252 |
| H | 4.037142 | 1.505212 | 0.260377 |
| C | -5.016813 | 0.403166 | -0.095867 |
| H | -4.950972 | 1.050727 | 0.788872 |
| H | -4.995119 | 1.067187 | -0.972613 |
| C | 5.016785 | -0.403161 | 0.095765 |
| H | 4.950990 | -1.050646 | -0.789036 |
| H | 4.995032 | -1.067261 | 0.972449 |
| C | -6.352165 | -0.362919 | -0.082307 |
| H | -6.354735 | -1.010007 | -0.973000 |
| C | 6.352145 | 0.362913 | 0.082371 |
| H | 6.354612 | 1.009985 | 0.973076 |
| C | -7.511905 | 0.641591 | -0.246998 |
| H | -7.523588 | 1.336733 | 0.603503 |
| H | -7.308212 | 1.258735 | -1.132838 |
| C | -8.900815 | 0.009259 | -0.404424 |

| | | | |
|---|---|---|---|
| H | -8.874739 | -0.728666 | -1.219121 |
| H | -9.168042 | -0.548692 | 0.502309 |
| C | -9.999461 | 1.040876 | -0.692692 |
| H | -10.019765 | 1.782630 | 0.117215 |
| H | -9.743756 | 1.596446 | -1.605127 |
| C | -11.388586 | 0.415022 | -0.847596 |
| H | -11.689758 | -0.113560 | 0.063950 |
| H | -12.148578 | 1.174513 | -1.057268 |
| H | -11.407056 | -0.309528 | -1.669631 |
| C | 7.511858 | -0.641608 | 0.247183 |
| H | 7.308088 | -1.258727 | 1.133022 |
| H | 7.523602 | -1.336774 | -0.603298 |
| C | 8.900762 | -0.009288 | 0.404712 |
| H | 8.874634 | 0.728625 | 1.219418 |
| H | 9.168061 | 0.548673 | -0.501993 |
| C | 9.999379 | -1.040921 | 0.693037 |
| H | 10.019721 | -1.782666 | -0.116876 |
| H | 9.743614 | -1.596496 | 1.605453 |
| C | 11.388503 | -0.415086 | 0.848029 |
| H | 11.406936 | 0.309447 | 1.670079 |
| H | 12.148475 | -1.174590 | 1.057726 |
| H | 11.689730 | 0.113512 | -0.063490 |
| C | 6.498079 | 1.292965 | -1.146393 |
| H | 5.662479 | 2.002327 | -1.155518 |
| H | 7.397248 | 1.904039 | -1.009256 |
| C | 6.568232 | 0.594045 | -2.509685 |
| H | 5.668627 | 0.005100 | -2.716400 |
| H | 6.660004 | 1.334096 | -3.310793 |
| H | 7.430031 | -0.076761 | -2.585096 |
| C | -6.497947 | -1.292960 | 1.146484 |
| H | -7.397152 | -1.904011 | 1.009472 |
| H | -5.662361 | -2.002340 | 1.155494 |
| C | -6.567885 | -0.594042 | 2.509788 |
| H | -6.659537 | -1.334099 | 3.310904 |
| H | -5.668240 | -0.005110 | 2.716367 |
| H | -7.429667 | 0.076770 | 2.585342 |
| H | 0.969414 | 4.376225 | 0.367172 |
| H | -0.969433 | -4.376204 | -0.367377 |

## Frequencies

| | | |
|---|---|---|
| 10.4534 | 17.1085 | 18.7871 |
| 22.6181 | 33.0127 | 42.5132 |
| 44.2178 | 48.4679 | 51.1059 |
| 64.4426 | 66.0869 | 73.3770 |
| 74.5096 | 85.8871 | 103.4520 |
| 105.7680 | 116.0384 | 121.4442 |
| 130.4604 | 141.3913 | 141.7628 |
| 159.1400 | 162.7683 | 169.1785 |
| 175.1760 | 189.5499 | 202.9487 |
| 218.3413 | 229.2486 | 243.7515 |
| 244.0985 | 251.0073 | 255.0059 |
| 260.3971 | 263.8834 | 277.3932 |
| 283.3725 | 285.7626 | 312.8656 |
| 317.8468 | 320.5294 | 357.8332 |
| 365.4464 | 369.8413 | 412.0489 |
| 412.4682 | 421.8307 | 433.8738 |
| 446.5362 | 451.8194 | 462.6042 |
| 478.7050 | 521.0012 | 522.1123 |
| 534.8784 | 537.7200 | 553.2621 |
| 569.3272 | 582.9353 | 617.2126 |
| 621.6126 | 642.9647 | 643.8491 |
| 649.2990 | 662.8535 | 672.5763 |
| 685.9395 | 687.3070 | 715.7188 |
| 730.4689 | 739.8573 | 740.0609 |
| 750.7442 | 757.7458 | 762.5187 |

| | | |
|---|---|---|
| 767.2531 | 770.8716 | 773.0883 |
| 773.2111 | 781.1658 | 781.6778 |
| 782.9084 | 807.5996 | 819.0668 |
| 830.0934 | 904.3336 | 904.3894 |
| 915.8871 | 918.4453 | 930.3110 |
| 934.8896 | 934.9036 | 976.3681 |
| 977.6512 | 977.6969 | 981.9234 |
| 999.5541 | 1001.1325 | 1015.8962 |
| 1035.8964 | 1037.3648 | 1050.8619 |
| 1052.2806 | 1054.0265 | 1065.9160 |
| 1070.1343 | 1072.3329 | 1101.4950 |
| 1101.8607 | 1119.0792 | 1139.6317 |
| 1151.6848 | 1154.6243 | 1155.0506 |
| 1173.6000 | 1176.0990 | 1187.0916 |
| 1187.4742 | 1206.1331 | 1239.5606 |
| 1245.3028 | 1247.7988 | 1259.8255 |
| 1260.0191 | 1273.0275 | 1280.5527 |
| 1285.4388 | 1287.7810 | 1310.6573 |
| 1312.2041 | 1322.1997 | 1322.4236 |
| 1327.5733 | 1336.9277 | 1337.8672 |
| 1339.9265 | 1340.7312 | 1349.8580 |
| 1367.3950 | 1375.7445 | 1381.2007 |
| 1389.4844 | 1391.2308 | 1400.2356 |
| 1400.9249 | 1403.4572 | 1403.9308 |
| 1406.2401 | 1415.0062 | 1416.8306 |
| 1419.3890 | 1420.5032 | 1428.9426 |
| 1428.9610 | 1431.9629 | 1432.3536 |
| 1445.4196 | 1451.7342 | 1468.7575 |
| 1474.0792 | 1498.6991 | 1498.8997 |
| 1501.2926 | 1501.3382 | 1509.2507 |
| 1509.3952 | 1511.7586 | 1511.9932 |
| 1513.9627 | 1513.9634 | 1519.4972 |
| 1520.3085 | 1522.8764 | 1522.9950 |
| 1527.1654 | 1528.7313 | 1528.9252 |
| 1535.7563 | 1536.3804 | 1553.8772 |
| 1578.3872 | 1624.2204 | 1647.4975 |
| 1676.7156 | 1727.5339 | 1731.8990 |
| 1785.0402 | 1787.6254 | 3001.4965 |
| 3001.7105 | 3003.2499 | 3003.2852 |
| 3015.7089 | 3015.7160 | 3019.6874 |
| 3019.6903 | 3028.1464 | 3028.1613 |
| 3038.1492 | 3038.1567 | 3039.5171 |
| 3039.5299 | 3044.4798 | 3044.4817 |
| 3049.1169 | 3049.1235 | 3053.5811 |
| 3053.5833 | 3056.3811 | 3056.4008 |
| 3075.0864 | 3075.1094 | 3082.4538 |
| 3082.5039 | 3106.3660 | 3106.3735 |
| 3112.5132 | 3112.5165 | 3115.8343 |
| 3115.8599 | 3119.8363 | 3119.8801 |
| 3236.8599 | 3237.0872 | 3479.6438 |
| 3482.3198 | 3601.1490 | 3601.3548 |

## Energies

SCF Done: E(RB3LYP) = -1687.40759017 A.U. after 1 cycles
Zero-point correction= 0.669154 (Hartree/Particle)
Thermal correction to Energy= 0.707541
Thermal correction to Enthalpy= 0.708486
Thermal correction to Gibbs Free Energy= 0.594161
Sum of electronic and zero-point Energies= -1686.738436
Sum of electronic and thermal Energies= -1686.700049
Sum of electronic and thermal Enthalpies= -1686.699105
Sum of electronic and thermal Free Energies= -1686.813430

**RF8a**

Cartesian coordinates

| | | | |
|---|---|---|---|
| C | -2.830735 | -1.169398 | -0.656169 |
| C | -1.856990 | -0.129076 | -0.324239 |
| C | -0.493168 | -0.483027 | -0.161853 |
| C | -0.066073 | -1.829589 | -0.312917 |
| C | -1.043280 | -2.896978 | -0.641580 |
| C | -2.262660 | 1.228172 | -0.161759 |
| C | 0.493173 | 0.483018 | 0.161806 |
| C | 0.066077 | 1.829579 | 0.312875 |
| C | -1.254881 | 2.185536 | 0.154992 |
| C | 1.043283 | 2.896967 | 0.641545 |
| C | 2.830740 | 1.169389 | 0.656126 |
| C | 1.856995 | 0.129068 | 0.324193 |
| C | 2.262664 | -1.228181 | 0.161718 |
| C | 1.254886 | -2.185546 | -0.155030 |
| H | 1.506962 | -3.231637 | -0.273912 |
| H | -1.506958 | 3.231625 | 0.273876 |
| O | 0.714128 | 4.068455 | 0.785590 |
| O | 4.037538 | 0.941471 | 0.834333 |
| O | -4.037543 | -0.941488 | -0.834325 |
| O | -0.714130 | -4.068471 | -0.785596 |
| N | 2.377165 | 2.492743 | 0.780226 |
| N | -2.377164 | -2.492755 | -0.780252 |
| N | -3.556009 | 1.606751 | -0.297496 |
| H | -4.181246 | 0.857232 | -0.585309 |
| N | 3.556015 | -1.606760 | 0.297451 |
| H | 4.181254 | -0.857238 | 0.585253 |
| C | -4.066921 | 2.959178 | -0.148837 |
| H | -3.684384 | 3.401919 | 0.779742 |
| H | -3.710759 | 3.598608 | -0.970782 |
| C | 4.066925 | -2.959188 | 0.148798 |
| H | 3.684380 | -3.401936 | -0.779775 |
| H | 3.710770 | -3.598612 | 0.970750 |
| C | -5.606705 | 2.970497 | -0.132084 |
| H | -5.937187 | 2.488823 | -1.065531 |
| C | 5.606709 | -2.970507 | 0.132031 |
| H | 5.937199 | -2.488824 | 1.065471 |
| C | -6.107109 | 4.429216 | -0.174402 |
| H | -5.764114 | 4.966003 | 0.720577 |
| H | -5.627212 | 4.932600 | -1.025077 |
| C | -7.626927 | 4.588781 | -0.309097 |
| H | -7.980694 | 3.997606 | -1.166097 |
| H | -8.130614 | 4.174569 | 0.573860 |
| C | -8.063921 | 6.048664 | -0.488479 |
| H | -7.701036 | 6.641836 | 0.361925 |
| H | -7.574393 | 6.466118 | -1.378790 |
| C | -9.581275 | 6.212523 | -0.615020 |
| H | -10.096449 | 5.838041 | 0.276877 |
| H | -9.861218 | 7.263028 | -0.743428 |
| H | -9.969157 | 5.657410 | -1.476676 |
| C | 6.107114 | -4.429225 | 0.174357 |
| H | 5.627223 | -4.932602 | 1.025042 |
| H | 5.764111 | -4.966021 | -0.720613 |
| C | 7.626933 | -4.588789 | 0.309042 |
| H | 7.980706 | -3.997605 | 1.166033 |
| H | 8.130612 | -4.174586 | -0.573924 |
| C | 8.063928 | -6.048670 | 0.488434 |
| H | 7.701036 | -6.641850 | -0.361961 |
| H | 7.574407 | -6.466115 | 1.378753 |
| C | 9.581283 | -6.212528 | 0.614964 |
| H | 9.969173 | -5.657406 | 1.476611 |
| H | 9.861227 | -7.263031 | 0.743381 |
| H | 10.096449 | -5.838055 | -0.276941 |

| | | | |
|---|---|---|---|
| C | 6.194513 | -2.137707 | -1.032464 |
| H | 5.824457 | -1.109255 | -0.950042 |
| H | 7.279717 | -2.071037 | -0.895168 |
| C | 5.897077 | -2.659227 | -2.443755 |
| H | 4.822222 | -2.700373 | -2.648613 |
| H | 6.343114 | -1.998783 | -3.193987 |
| H | 6.305330 | -3.661732 | -2.608171 |
| C | -6.194520 | 2.137688 | 1.032398 |
| H | -7.279724 | 2.071022 | 0.895094 |
| H | -5.824467 | 1.109235 | 0.949968 |
| C | -5.897092 | 2.659192 | 2.443696 |
| H | -6.343136 | 1.998740 | 3.193919 |
| H | -4.822238 | 2.700332 | 2.648563 |
| H | -6.305344 | 3.661696 | 2.608120 |
| C | 3.377841 | 3.515978 | 1.145944 |
| H | 4.006619 | 3.078706 | 1.923504 |
| H | 2.816236 | 4.353046 | 1.561956 |
| C | -3.377847 | -3.515997 | -1.145931 |
| H | -4.006632 | -3.078741 | -1.923496 |
| H | -2.816250 | -4.353077 | -1.561928 |
| C | 4.274362 | 3.996215 | -0.015670 |
| H | 4.821178 | 3.117659 | -0.381007 |
| C | 5.305269 | 5.009116 | 0.552298 |
| H | 5.317049 | 4.946060 | 1.649416 |
| H | 4.977842 | 6.032511 | 0.322785 |
| C | 6.744097 | 4.804346 | 0.056092 |
| H | 7.074306 | 3.792765 | 0.331289 |
| H | 6.772884 | 4.841774 | -1.040393 |
| C | 7.732760 | 5.830822 | 0.622267 |
| H | 7.700395 | 5.796990 | 1.719943 |
| H | 7.405573 | 6.841514 | 0.342067 |
| C | 9.172007 | 5.610523 | 0.147133 |
| H | 9.852210 | 6.358335 | 0.567699 |
| H | 9.540334 | 4.621930 | 0.444095 |
| H | 9.243236 | 5.673504 | -0.944753 |
| C | 3.442859 | 4.568926 | -1.180397 |
| H | 2.712121 | 3.815085 | -1.496839 |
| H | 2.855603 | 5.421077 | -0.814584 |
| C | 4.259059 | 4.993774 | -2.405909 |
| H | 4.943448 | 5.817069 | -2.177971 |
| H | 4.857264 | 4.161966 | -2.795493 |
| H | 3.599408 | 5.332584 | -3.211546 |
| C | -4.274360 | -3.996197 | 0.015706 |
| H | -4.821161 | -3.117627 | 0.381029 |
| C | -5.305285 | -5.009101 | -0.552223 |
| H | -5.317093 | -4.946061 | -1.649342 |
| H | -4.977856 | -6.032494 | -0.322704 |
| C | -6.744098 | -4.804319 | -0.055979 |
| H | -7.074311 | -3.792740 | -0.331179 |
| H | -6.772852 | -4.841732 | 1.040508 |
| C | -7.732781 | -5.830799 | -0.622110 |
| H | -7.700449 | -5.796982 | -1.719788 |
| H | -7.405590 | -6.841488 | -0.341907 |
| C | -9.172013 | -5.610489 | -0.146937 |
| H | -9.540346 | -4.621898 | -0.443901 |
| H | -9.852231 | -6.358305 | -0.567472 |
| H | -9.243210 | -5.673455 | 0.944952 |
| C | -3.442851 | -4.568890 | 1.180438 |
| H | -2.855605 | -5.421053 | 0.814638 |
| H | -2.712105 | -3.815049 | 1.496860 |
| C | -4.259049 | -4.993708 | 2.405962 |
| H | -4.857236 | -4.161884 | 2.795540 |
| H | -4.943455 | -5.816994 | 2.178040 |
| H | -3.599397 | -5.332519 | 3.211598 |

Frequencies

| | | |
|---|---|---|
| 7.2379 | 10.5628 | 13.7320 |
| 15.5415 | 16.3986 | 18.1360 |
| 24.1025 | 25.1647 | 26.1056 |
| 27.4933 | 28.0888 | 42.0014 |
| 44.5113 | 49.9168 | 52.5454 |
| 56.5041 | 56.9371 | 72.8594 |
| 74.5160 | 75.7766 | 76.8527 |
| 78.1260 | 79.6903 | 86.3621 |
| 102.5460 | 105.3802 | 105.5098 |
| 111.9501 | 114.0791 | 121.7344 |
| 123.2917 | 125.0056 | 128.8258 |
| 130.1873 | 130.1894 | 142.5663 |
| 143.7402 | 145.7157 | 146.9386 |
| 169.7595 | 172.2770 | 183.2990 |
| 184.5468 | 199.3481 | 203.3772 |
| 217.9927 | 224.3277 | 228.3427 |
| 236.9338 | 242.9214 | 243.6771 |
| 248.8462 | 249.8683 | 253.9715 |
| 256.1017 | 258.9463 | 260.9664 |
| 262.8088 | 274.8714 | 276.7998 |
| 278.8956 | 280.3498 | 312.0987 |
| 314.9817 | 318.6507 | 323.3473 |
| 332.2310 | 349.2119 | 357.1245 |
| 366.4395 | 368.1457 | 370.7693 |
| 375.4424 | 387.2201 | 405.1541 |
| 410.3272 | 421.4141 | 433.5423 |
| 441.5122 | 446.3141 | 451.8172 |
| 457.4294 | 461.0047 | 470.0636 |
| 481.7768 | 501.9189 | 511.7043 |
| 525.0707 | 525.2976 | 536.4161 |
| 552.5928 | 560.3906 | 561.1240 |
| 572.4879 | 582.0066 | 619.0598 |
| 622.1661 | 652.2794 | 653.2589 |
| 656.6739 | 664.8671 | 666.8974 |
| 687.3867 | 729.8624 | 731.0486 |
| 734.4103 | 734.4594 | 740.4187 |
| 740.6607 | 744.3551 | 758.9337 |
| 760.3458 | 765.4261 | 771.7965 |
| 772.1089 | 780.9518 | 781.2776 |
| 781.9779 | 782.0937 | 782.3675 |
| 785.1143 | 799.7936 | 809.2755 |
| 818.3786 | 821.6439 | 826.5967 |
| 849.3891 | 903.8692 | 905.1368 |
| 905.3338 | 906.2232 | 915.1517 |
| 915.6217 | 918.5019 | 921.3625 |
| 934.1782 | 934.4732 | 937.1204 |
| 940.3698 | 961.5572 | 963.6849 |
| 973.3942 | 974.1421 | 977.4099 |
| 980.2731 | 986.2413 | 986.6150 |
| 1000.8781 | 1001.1545 | 1009.2071 |
| 1015.4482 | 1034.5785 | 1035.3241 |
| 1036.9334 | 1040.3213 | 1040.8396 |
| 1047.9903 | 1052.3955 | 1053.1609 |
| 1063.2198 | 1066.3036 | 1066.7393 |
| 1067.2973 | 1069.0401 | 1069.4472 |
| 1074.6472 | 1085.6898 | 1099.3107 |
| 1100.8937 | 1101.1496 | 1121.2390 |
| 1134.3547 | 1136.0561 | 1147.8989 |
| 1148.2652 | 1151.1477 | 1152.7095 |
| 1156.3452 | 1166.8718 | 1168.5507 |
| 1178.3745 | 1181.8444 | 1185.8235 |
| 1186.4564 | 1196.9691 | 1197.3007 |
| 1215.9900 | 1225.6922 | 1236.9949 |
| 1243.8229 | 1245.4298 | 1252.7740 |

| | | |
|---|---|---|
| 1253.0453 | 1257.2159 | 1257.5730 |
| 1278.5175 | 1279.1757 | 1279.5228 |
| 1282.9383 | 1286.4266 | 1308.6015 |
| 1309.0640 | 1310.6201 | 1312.6735 |
| 1322.2776 | 1322.4644 | 1325.2939 |
| 1325.6288 | 1326.0907 | 1332.9176 |
| 1333.4152 | 1336.0943 | 1337.6554 |
| 1339.9563 | 1340.1715 | 1341.7983 |
| 1342.0881 | 1352.2706 | 1353.8385 |
| 1357.5386 | 1363.5718 | 1376.6964 |
| 1376.9340 | 1384.4298 | 1384.8671 |
| 1389.0358 | 1389.0524 | 1394.7100 |
| 1395.1850 | 1398.7413 | 1400.5265 |
| 1403.1472 | 1403.8095 | 1410.3047 |
| 1410.8656 | 1415.1789 | 1415.4664 |
| 1416.6512 | 1416.7891 | 1419.6447 |
| 1419.8666 | 1424.6317 | 1427.3596 |
| 1427.3981 | 1429.9030 | 1429.9207 |
| 1430.2729 | 1430.2853 | 1434.7553 |
| 1434.9267 | 1439.6435 | 1450.4122 |
| 1470.6102 | 1473.2495 | 1480.4328 |
| 1485.1439 | 1496.3952 | 1496.4257 |
| 1498.3379 | 1498.5554 | 1500.3335 |
| 1500.3377 | 1501.5877 | 1501.6196 |
| 1503.7394 | 1503.7413 | 1507.2000 |
| 1507.3232 | 1511.7050 | 1511.8680 |
| 1514.7399 | 1514.7409 | 1515.0785 |
| 1515.0793 | 1515.8161 | 1515.8167 |
| 1519.0857 | 1519.0872 | 1519.1171 |
| 1519.9538 | 1522.1543 | 1522.2070 |
| 1523.6838 | 1523.6851 | 1527.1750 |
| 1528.1978 | 1528.3300 | 1528.3356 |
| 1528.4519 | 1532.8839 | 1533.5814 |
| 1549.7018 | 1585.9531 | 1622.3054 |
| 1643.2909 | 1667.2666 | 1690.8503 |
| 1703.1859 | 1755.6321 | 1757.5790 |
| 2996.7655 | 2996.9391 | 3000.4865 |
| 3000.5441 | 3014.0975 | 3014.1014 |
| 3015.4291 | 3015.4340 | 3018.7369 |
| 3018.7386 | 3019.4010 | 3019.4042 |
| 3027.0456 | 3027.0531 | 3027.4563 |
| 3027.4685 | 3036.0511 | 3036.0691 |
| 3037.2858 | 3037.2878 | 3038.3534 |
| 3038.3636 | 3039.8832 | 3039.9178 |
| 3042.3130 | 3042.3176 | 3042.6036 |
| 3042.6049 | 3045.2703 | 3045.2721 |
| 3047.5815 | 3047.5840 | 3048.6476 |
| 3048.6552 | 3050.3244 | 3050.3319 |
| 3053.0911 | 3053.0924 | 3056.6467 |
| 3056.6683 | 3074.6849 | 3074.6902 |
| 3074.9694 | 3074.9971 | 3075.9589 |
| 3075.9596 | 3081.9213 | 3081.9652 |
| 3097.7353 | 3097.7716 | 3105.3787 |
| 3105.3885 | 3106.4807 | 3106.4886 |
| 3107.1964 | 3107.2034 | 3110.2112 |
| 3110.2192 | 3112.4405 | 3112.4445 |
| 3115.0411 | 3115.0555 | 3116.4410 |
| 3116.4470 | 3117.8196 | 3117.8753 |
| 3159.2024 | 3159.2035 | 3240.4471 |
| 3240.6792 | 3474.0433 | 3476.8117 |

## Energies

SCF Done: E(RB3LYP) = -2316.45413317 A.U. after 1 cycles
Zero-point correction= 1.123729 (Hartree/Particle)
Thermal correction to Energy= 1.184144

```
 Thermal correction to Enthalpy=                 1.185089
 Thermal correction to Gibbs Free Energy=        1.018206
 Sum of electronic and zero-point Energies=          -2315.330405
 Sum of electronic and thermal Energies=             -2315.269989
 Sum of electronic and thermal Enthalpies=           -2315.269045
 Sum of electronic and thermal Free Energies=        -2315.435927
```

**RF8b**

Cartesian coordinates

```
C       -2.795807   -1.398083   -0.157619
C       -1.867967   -0.274647   -0.138313
C       -0.472178   -0.517085   -0.090313
C        0.028051   -1.843773   -0.058142
C       -0.889430   -3.009255   -0.074749
C       -2.349941    1.069938   -0.156475
C        0.470321    0.539095   -0.064843
C       -0.030154    1.865970   -0.093302
C       -1.383377    2.117866   -0.137456
C        0.887841    3.031249   -0.080608
C        2.793959    1.419827    0.010834
C        1.865976    0.296506   -0.012221
C        2.347444   -1.047800    0.021336
C        1.380823   -2.095484   -0.002730
H        1.694401   -3.130727    0.027259
H       -1.697825    3.153016   -0.165123
O        0.461973    4.177957   -0.110236
O        4.021180    1.272837    0.064670
O       -4.023666   -1.251548   -0.203414
O       -0.463278   -4.155958   -0.048614
C        3.249041    3.782919   -0.019681
C       -3.250486   -3.761356   -0.135580
H       -4.238113   -3.327082   -0.170734
H        4.236496    3.348440    0.018233
C       -3.075124   -5.094663   -0.112403
C        3.074131    5.116202   -0.047182
H       -2.078812   -5.509685   -0.083132
H        2.077968    5.531465   -0.078240
N        2.268147    2.751977   -0.032209
N       -2.269821   -2.730178   -0.121132
N       -3.670534    1.361665   -0.188330
H       -4.278621    0.550287   -0.254584
N        3.667238   -1.342103    0.073163
H        4.277104   -0.532365    0.142866
C       -4.247114    2.696793   -0.168710
H       -3.808559    3.279456    0.652060
H       -4.005182    3.232124   -1.098794
C        4.229135   -2.681403    0.155614
H        3.853063   -3.296360   -0.672814
H        3.902668   -3.172677    1.084074
C       -5.777329    2.638578   -0.004582
H       -6.163274    2.034286   -0.840173
C        5.767770   -2.644960    0.122110
H        6.086057   -1.981566    0.941168
C       -4.177430   -6.067663   -0.127764
C       -3.847509   -7.435457   -0.139407
C       -5.543667   -5.724151   -0.129706
C       -4.833331   -8.420268   -0.155426
H       -2.799219   -7.722359   -0.136606
C       -6.528227   -6.706737   -0.145950
H       -5.844612   -4.681230   -0.115677
C       -6.180821   -8.060917   -0.159271
H       -4.547442   -9.468243   -0.164635
H       -7.574852   -6.415367   -0.146797
```

| | | | |
|---|---|---|---|
| H | -6.953168 | -8.824208 | -0.171178 |
| C | 4.176760 | 6.088865 | -0.033982 |
| C | 5.542880 | 5.744890 | -0.034627 |
| C | 3.847319 | 7.456771 | -0.021963 |
| C | 6.527802 | 6.727144 | -0.020042 |
| H | 5.843421 | 4.701868 | -0.049789 |
| C | 4.833501 | 8.441247 | -0.007643 |
| H | 2.799123 | 7.744030 | -0.023028 |
| C | 6.180876 | 8.081440 | -0.006047 |
| H | 7.574329 | 6.435423 | -0.021255 |
| H | 4.547985 | 9.489320 | 0.001941 |
| H | 6.953500 | 8.844472 | 0.004447 |
| C | -6.359546 | 4.058397 | -0.165846 |
| H | -5.962242 | 4.715006 | 0.620214 |
| H | -5.992595 | 4.474756 | -1.114121 |
| C | -7.891847 | 4.133627 | -0.161796 |
| H | -8.293067 | 3.430022 | -0.905429 |
| H | -8.283295 | 3.804700 | 0.809574 |
| C | -8.425681 | 5.541073 | -0.458779 |
| H | -8.013382 | 6.246483 | 0.275490 |
| H | -8.052546 | 5.871226 | -1.437740 |
| C | -9.954852 | 5.621840 | -0.441138 |
| H | -10.356143 | 5.336523 | 0.537951 |
| H | -10.304142 | 6.635942 | -0.660078 |
| H | -10.396021 | 4.950302 | -1.186376 |
| C | 6.312772 | -4.052544 | 0.441130 |
| H | 5.859779 | -4.389776 | 1.383598 |
| H | 5.972153 | -4.763778 | -0.323609 |
| C | 7.838362 | -4.143818 | 0.575075 |
| H | 8.187785 | -3.383439 | 1.288352 |
| H | 8.317648 | -3.904863 | -0.382997 |
| C | 8.316616 | -5.526562 | 1.037431 |
| H | 7.958729 | -6.287662 | 0.330776 |
| H | 7.849481 | -5.766210 | 2.002167 |
| C | 9.839241 | -5.626088 | 1.167471 |
| H | 10.223544 | -4.900204 | 1.893031 |
| H | 10.147986 | -6.622489 | 1.499427 |
| H | 10.333126 | -5.427196 | 0.209605 |
| C | 6.325234 | -2.037914 | -1.187788 |
| H | 5.919064 | -1.027056 | -1.311108 |
| H | 7.406811 | -1.905397 | -1.071285 |
| C | 6.052650 | -2.839285 | -2.466722 |
| H | 4.981052 | -2.955235 | -2.659417 |
| H | 6.481777 | -2.326828 | -3.333344 |
| H | 6.494239 | -3.840376 | -2.427906 |
| C | -6.211427 | 1.926453 | 1.299357 |
| H | -7.300471 | 1.807429 | 1.278837 |
| H | -5.806849 | 0.907615 | 1.298981 |
| C | -5.804857 | 2.618256 | 2.606206 |
| H | -6.159545 | 2.042137 | 3.466490 |
| H | -4.717857 | 2.705902 | 2.703265 |
| H | -6.228750 | 3.624116 | 2.689920 |

## Frequencies

| | | |
|---|---|---|
| 6.5534 | 9.8686 | 11.5779 |
| 17.6193 | 20.8526 | 23.4110 |
| 24.1613 | 24.2123 | 25.9780 |
| 30.3185 | 35.2066 | 39.7534 |
| 46.7795 | 50.6077 | 58.1802 |
| 59.6635 | 62.1500 | 66.9698 |
| 68.4305 | 69.6999 | 71.1207 |
| 93.5708 | 97.8644 | 104.6293 |
| 112.1315 | 118.4172 | 127.9592 |
| 128.8524 | 130.2415 | 136.2103 |
| 138.0630 | 146.7390 | 151.2957 |

| | | |
|---|---|---|
| 165.7722 | 183.8248 | 191.6538 |
| 199.2887 | 212.2588 | 218.4735 |
| 226.9866 | 233.4209 | 237.0107 |
| 239.6448 | 243.5184 | 250.9074 |
| 253.8629 | 256.9314 | 258.1280 |
| 275.1317 | 279.0736 | 282.6481 |
| 315.1105 | 315.6696 | 324.6928 |
| 347.3833 | 357.1638 | 368.6010 |
| 374.2234 | 383.7123 | 386.1253 |
| 413.4603 | 413.8962 | 419.3261 |
| 423.4163 | 431.5514 | 444.4631 |
| 446.5099 | 451.0380 | 460.3096 |
| 471.7327 | 504.8123 | 516.2867 |
| 517.0684 | 518.5737 | 527.9616 |
| 528.7299 | 529.1070 | 549.9425 |
| 550.5689 | 570.3086 | 570.6501 |
| 575.5915 | 611.1092 | 614.0069 |
| 633.1899 | 634.5099 | 634.5417 |
| 645.0932 | 653.6668 | 654.1070 |
| 663.3434 | 672.2432 | 685.3022 |
| 704.0363 | 704.5478 | 723.1371 |
| 733.3052 | 735.0366 | 738.8016 |
| 739.6688 | 748.6050 | 754.8912 |
| 767.9079 | 769.4823 | 769.5414 |
| 770.0782 | 772.4830 | 778.3824 |
| 783.2118 | 806.9343 | 818.2256 |
| 825.5582 | 838.4462 | 849.0005 |
| 849.0166 | 876.1309 | 880.1383 |
| 880.1593 | 899.2124 | 904.4303 |
| 905.7460 | 916.9237 | 919.9035 |
| 923.3903 | 923.4180 | 934.7353 |
| 934.9854 | 937.6775 | 943.4339 |
| 968.2764 | 968.2771 | 976.5224 |
| 976.8908 | 982.6901 | 983.7923 |
| 992.8408 | 992.8464 | 1001.5935 |
| 1001.9762 | 1013.4825 | 1013.5822 |
| 1023.3968 | 1023.4848 | 1036.7701 |
| 1037.1626 | 1043.9665 | 1052.1052 |
| 1053.4878 | 1057.7332 | 1058.9782 |
| 1059.9627 | 1070.6373 | 1073.9026 |
| 1101.7958 | 1102.0572 | 1103.4442 |
| 1111.5687 | 1118.8473 | 1119.3580 |
| 1140.2539 | 1148.9869 | 1154.7676 |
| 1156.4391 | 1162.9117 | 1170.9681 |
| 1175.1457 | 1185.2514 | 1185.7304 |
| 1187.7063 | 1187.7294 | 1206.7675 |
| 1211.9484 | 1213.1339 | 1215.1815 |
| 1228.0868 | 1244.9155 | 1245.9180 |
| 1253.4213 | 1259.4364 | 1261.2902 |
| 1263.4319 | 1280.0330 | 1285.8889 |
| 1288.4675 | 1310.1207 | 1312.2899 |
| 1322.1928 | 1323.1233 | 1324.0444 |
| 1331.3373 | 1331.5816 | 1337.5942 |
| 1338.1351 | 1340.5777 | 1341.3015 |
| 1354.6877 | 1358.1636 | 1364.2558 |
| 1366.2341 | 1370.9053 | 1371.0245 |
| 1376.0716 | 1378.2964 | 1388.7930 |
| 1391.3561 | 1396.4592 | 1397.9714 |
| 1401.2081 | 1401.9190 | 1402.7521 |
| 1405.5617 | 1416.1184 | 1418.7251 |
| 1419.6819 | 1427.9711 | 1430.0022 |
| 1430.6980 | 1433.0895 | 1435.4633 |
| 1447.9674 | 1474.4731 | 1476.1782 |
| 1491.8901 | 1491.9013 | 1497.4667 |
| 1498.0217 | 1500.7836 | 1500.9980 |
| 1507.1712 | 1508.2147 | 1510.8291 |

```
1511.1150              1513.0934              1515.7668
1517.7761              1519.0036              1521.6216
1521.7053              1526.7189              1527.2090
1527.7292              1534.4105              1535.4020
1541.3217              1541.3321              1552.4318
1587.4046              1618.7758              1630.8973
1630.9346              1640.3742              1657.6266
1657.7328              1669.3754              1698.6194
1701.5772              1701.7991              1710.2995
1757.0005              1757.5193              3000.6092
3000.8347              3002.8511              3003.2989
3015.4507              3015.5889              3019.3824
3019.8491              3027.6107              3028.1999
3037.9425              3038.8142              3041.4198
3042.1037              3044.9431              3045.1013
3048.6110              3049.1725              3052.1985
3053.3945              3056.1083              3056.2657
3074.6971              3075.0896              3080.5556
3082.6052              3106.1863              3106.9530
3112.5833              3113.0495              3116.3781
3116.4484              3118.7760              3118.8486
3174.5251              3174.5344              3180.0335
3180.0399              3190.1159              3190.1202
3197.6740              3197.6804              3206.8166
3206.8449              3244.5313              3245.5008
3263.2457              3263.4487              3272.0965
3272.2008              3499.3338              3502.2298
```

Energies

```
SCF Done:  E(RB3LYP) =  -2304.31399777     A.U. after    1 cycles
Zero-point correction=                           0.896659 (Hartree/Particle)
Thermal correction to Energy=                    0.949361
Thermal correction to Enthalpy=                  0.950305
Thermal correction to Gibbs Free Energy=         0.799203
Sum of electronic and zero-point Energies=          -2303.417339
Sum of electronic and thermal Energies=             -2303.364637
Sum of electronic and thermal Enthalpies=           -2303.363693
Sum of electronic and thermal Free Energies=        -2303.514795
```

# Reference


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