ELECTRONIC SUPPORTING INFORMATION

Bridgehead Enolate or Bridgehead Organolithium?: DFT Calculations Provide Insights into a Difficult Bridgehead Substitution Reaction in the Synthesis of the Polycyclic Polyprenylated Acylphloroglucinol (PPAP) Nemorosone

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25
Structure_9.xyz
H          -2.21900       -1.12000        1.59700
C          -2.06300       -0.36500        0.81700
C          -0.65600        1.71200        0.20500
C          -1.17800       -0.00500       -1.40100
C          -0.05100        0.86700       -0.96600
C          -1.52800       -1.10600       -0.46700
C          -1.15400        0.77100        1.33100
H          -0.28400        0.33700        1.83900
H          -3.05000        0.04200        0.55900
H          -2.30400       -1.77100       -0.85500
H          -1.70100        1.34200        2.09300
O          -1.83800        0.28600       -2.42700
C           1.08300        0.05100       -0.50700
C          -0.27000       -1.96000       -0.15300
O          -0.42100       -3.13300        0.17600
C           1.01500       -1.29400       -0.23400
H           1.88300       -1.90000       -0.00300
O           2.21400        0.78600       -0.36200
C           3.36900        0.16200        0.19400
H           3.14500       -0.29700        1.16400
H           4.10600        0.95800        0.32000
H           3.77100       -0.60300       -0.48100
Li         -0.47100        1.50700       -2.86900
H          -1.49200        2.32200       -0.16600
H           0.09300        2.41000        0.59400


This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -620.8724174 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -620.89177897 au
E(B3LYP/6-311+G**) = -621.0453805 au
Zero point vibrational energy: 123.317 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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25
Structure_10.xyz
H           1.57500       -0.66000        2.07500
C           1.69500       -0.77200        0.99000
C           0.44700       -1.71400       -1.05900
C           1.26600        0.66100       -1.10600
C           0.10800       -0.24900       -1.29000
C           1.67000        0.62300        0.32600
C           0.70700       -1.84100        0.46000
H          -0.25900       -1.73200        0.96600
H           2.71900       -1.14100        0.83800
H           2.59500        1.15900        0.55400
H           1.08900       -2.83600        0.72600
C          -0.99500        0.28100       -0.65400
C           0.50500        1.71600        0.60600
O           0.96800        2.87800        0.89300
C          -0.79700        1.44100        0.18000
H          -1.56500        2.18400        0.37700
O          -2.15400       -0.44300       -0.66500
C          -3.19800       -0.04700        0.21900
H          -2.83400        0.07300        1.24600
H          -3.94200       -0.84600        0.18200
H          -3.66300        0.89100       -0.10900
O           1.63800        1.58000       -1.88100
Li          1.48100        3.18100       -0.87400
H           1.32300       -2.02000       -1.64400
H          -0.38000       -2.36400       -1.36100

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -620.8619449 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -620.87749023 au
E(B3LYP/6-311+G**) = -621.0322197 au
Zero point vibrational energy: 122.903 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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25
Structure_11.xyz
H           2.11100         1.21200        -1.39300
C           1.48100         1.35100        -0.50500
C          -1.02900         1.43300         0.21600
C           0.67100         0.36000         1.56300
C          -0.66300         0.12200         0.91200
C           1.75700         0.19400         0.52300
C           0.00300         1.55100        -0.94500
H          -0.25200         0.78100        -1.68400
H           1.82800         2.27000        -0.01400
H           2.75500         0.33500         0.95400
H          -0.07600         2.52100        -1.45800
O           0.84100         0.78300         2.69200
C          -0.72500        -1.07600         0.24600
C           1.67000        -1.25000        -0.00000
O          -1.83000        -1.56500        -0.39300
C          -3.09900        -0.99600        -0.09200
H          -3.12200        -0.64800         0.94700
H          -3.83900        -1.78500        -0.25200
H          -3.32800        -0.15400        -0.75700
C           0.45500        -1.88400         0.00800
H           0.35900        -2.91600        -0.31300
O           2.79500        -1.81500        -0.34800
Li          4.22000        -2.57100        -0.63000
H          -0.93600         2.27700         0.91200
H          -2.04600         1.46800        -0.18800

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -620.8505352 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -620.87861253 au
E(B3LYP/6-311+G**) = -621.0297443 au
Zero point vibrational energy:  123.068 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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34
Structure_13.xyz
H           3.54300        2.18900        0.01200
C           2.50400        2.02000       -0.29400
C           0.99000        0.48600       -1.71300
C           0.33500        1.26500        0.47000
C           0.32000        0.03800       -0.37400
C           1.67500        1.65100        0.99400
C           2.43100        0.97700       -1.42900
H           3.04900        0.11300       -1.15900
H           2.11600        2.98200       -0.65600
H           1.64400        2.51200        1.66700
H           2.87900        1.40900       -2.33400
O          -0.69600        1.96200        0.59500
C           1.07300       -1.03900        0.27000
C           2.30500        0.45900        1.76500
O           3.11700        0.69500        2.65600
C           1.91000       -0.87100        1.35100
H           2.36200       -1.69500        1.89200
O           0.87200       -2.24100       -0.33500
C           1.64600       -3.35900        0.08900
H           2.72000       -3.14000        0.04500
H           1.40400       -4.16900       -0.60100
H           1.38400       -3.66100        1.11100
Li         -1.70500        0.48200       -0.11800
O          -3.56400        0.15100       -0.02600
C          -4.20300       -1.03300       -0.50300
H          -4.98300       -0.78200       -1.23300
H          -4.64700       -1.59200        0.33100
H          -3.43400       -1.64200       -0.98300
C          -4.45200        1.04500        0.64900
H          -3.85300        1.89000        0.99400
H          -4.91600        0.54600        1.50900
H          -5.23300        1.39900       -0.03500
H           0.40500        1.29400       -2.17500
H           1.00300       -0.34200       -2.43000

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -775.9327938 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -775.95272165 au
E(B3LYP/6-311+G**) = -776.1527105 au
Zero point vibrational energy:  174.927 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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34
Structure_14.xyz
H          -2.47600       -1.53800        2.08300
C          -2.30400       -1.75700        1.02100
C          -2.91000       -0.85100       -1.31700
C          -0.49700       -1.24300       -0.74000
C          -1.50200       -0.27700       -1.25700
C          -0.81100       -1.53200        0.68800
C          -3.35200       -1.01300        0.15700
H          -3.50600       -0.00500        0.56000
H          -2.46500       -2.83800        0.90700
H          -0.20800       -2.32900        1.13100
H          -4.31500       -1.53500        0.24200
C          -1.31800        0.94300       -0.64100
C          -0.02700       -0.17600        1.09000
O           1.06300       -0.38900        1.72400
C          -0.38200        1.01900        0.45200
H           0.15500        1.92400        0.72500
O          -2.18900        1.95400       -0.94600
C          -2.20300        3.10000       -0.10200
H          -2.27600        2.82200        0.95600
H          -3.08100        3.68000       -0.39500
H          -1.30400        3.71400       -0.24700
O           0.61800       -1.51300       -1.24400
Li          1.92300       -0.89800        0.06100
O           3.70900       -0.30000       -0.09600
C           4.61900       -0.46500       -1.18000
H           4.81800        0.49900       -1.66700
H           4.15000       -1.14400       -1.89600
H           5.56500       -0.89600       -0.82700
C           4.17700        0.59200        0.92100
H           4.39000        1.57900        0.49000
H           5.08600        0.19300        1.38900
H           3.37300        0.66900        1.65600
H          -2.93000       -1.81000       -1.85000
H          -3.59100       -0.17800       -1.84700

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -775.9223089 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -775.93795937 au
E(B3LYP/6-311+G**) = -776.1391021 au
Zero point vibrational energy:  174.656 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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34
Structure_15.xyz
H          -0.71000       -2.14300        1.38600
C          -1.41400       -2.00700        0.55500
C          -3.67000       -0.82000       -0.01700
C          -1.81800       -0.89300       -1.57100
C          -2.76400        0.05300       -0.88500
C          -0.69800       -1.24500       -0.61800
C          -2.72800       -1.37500        1.09200
H          -2.47200       -0.53300        1.74700
H          -1.64000       -3.00900        0.16700
H           0.03300       -1.91600       -1.08300
H          -3.23800       -2.12000        1.72000
O          -2.00800       -1.42100       -2.65200
C          -2.12600        1.14900       -0.35400
C           0.02900        0.06400       -0.25600
O          -2.75500        2.19000        0.27600
C          -4.15400        2.35600        0.08200
H          -4.44600        1.99900       -0.91300
H          -4.35800        3.42600        0.18300
H          -4.73200        1.81400        0.84000
C          -0.68600        1.23700       -0.27000
H          -0.20400        2.18700       -0.05800
O           1.30500       -0.02200       -0.02900
Li          2.96700       -0.03800        0.09400
O           4.84100        0.19600        0.13000
C           5.80500       -0.84800       -0.03100
H           5.25800       -1.79100       -0.08100
H           6.49300       -0.86800        0.82400
H           6.37400       -0.70400       -0.95800
C           5.42900        1.50000        0.19800
H           5.98900        1.71400       -0.72000
H           6.09800        1.57200        1.06500
H           4.61400        2.21900        0.30600
H          -4.10300       -1.63500       -0.61300
H          -4.51000       -0.28900        0.44500

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -775.9158333 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -775.94280417 au
E(B3LYP/6-311+G**) = -776.1412299 au
Zero point vibrational energy:  174.538 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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34
Structure_16.xyz
H          -2.49400       -1.88900        1.84100
C          -2.38400       -1.85000        0.75000
C          -2.97900       -0.42000       -1.30200
C          -0.61000       -1.22800       -0.99200
C          -1.48900       -0.09500       -1.32800
C          -0.88700       -1.69600        0.39800
C          -3.32900       -0.77900        0.16100
H          -3.25400        0.13900        0.75700
H          -2.69000       -2.83700        0.37700
H          -0.33500       -2.59900        0.67300
H          -4.36600       -1.12900        0.25300
C          -1.04200        1.00000       -0.61100
C          -0.06900       -0.49100        1.11700
O           0.64000       -0.78600        2.08700
C          -0.06900        0.78200        0.43500
H           0.43200        1.60100        0.94400
O          -1.73200        2.17200       -0.75000
C          -1.52600        3.20800        0.20500
H          -1.66900        2.85000        1.23100
H          -2.26900        3.97500       -0.02500
H          -0.52300        3.64500        0.11300
O           0.46700       -1.49500       -1.58000
Li          1.55900       -0.21400       -0.78100
O           3.38000       -0.04500       -0.31200
C           4.50400       -0.16300       -1.18000
H           4.12900       -0.16000       -2.20600
H           5.04100       -1.10100       -0.99000
H           5.18900        0.68400       -1.03900
C           3.72900       -0.06100        1.08100
H           2.79500       -0.07200        1.64900
H           4.32300        0.82900        1.32700
H           4.30800       -0.96400        1.31000
H          -3.21500       -1.25100       -1.97800
H          -3.56700        0.44000       -1.63600

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -775.9192983 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -775.93599352 au
E(B3LYP/6-311+G**) = -776.1363092 au
Zero point vibrational energy:  174.587 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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43
Structure_17.xyz
H           3.51200        2.48200        1.23400
C           2.48500        2.29500        0.89900
C           1.08600        1.54800       -1.14800
C           0.60400        0.79500        1.08100
C           0.70100        0.28800       -0.31200
C           1.91300        1.08600        1.73400
C           2.43800        2.10900       -0.63500
H           3.23700        1.42000       -0.93600
H           1.89200        3.17700        1.17700
H           1.81900        1.38400        2.78200
H           2.66700        3.07200       -1.11200
O          -0.50300        1.08200        1.58100
C           1.70900       -0.75800       -0.41400
C           2.83500       -0.15800        1.67000
O           3.70100       -0.30000        2.53300
C           2.62600       -1.06900        0.56600
H           3.27400       -1.93800        0.53000
O           1.65900       -1.41600       -1.61200
C           2.70600       -2.32700       -1.93200
H           3.69000       -1.85900       -1.81800
H           2.54700       -2.61000       -2.97500
H           2.66400       -3.22600       -1.30400
Li         -1.39100        0.01900        0.15300
O          -3.02600        0.97800       -0.39000
O          -2.03100       -1.80800        0.51100
C          -3.74400        0.64600       -1.57300
H          -3.38100        1.23200       -2.42900
H          -4.81900        0.83000       -1.44000
H          -3.57800       -0.41700       -1.76100
C          -3.17600        2.34500       -0.00900
H          -2.84400        3.01200       -0.81600
H          -2.55200        2.49600        0.87300
H          -4.22700        2.56200        0.22900
C          -2.87400       -2.02500        1.63900
H          -3.48900       -2.92400        1.49400
H          -3.52100       -1.15000        1.72700
H          -2.28000       -2.13800        2.55600
C          -1.12400       -2.88800        0.27900
H          -1.68200       -3.81500        0.08600
H          -0.46400       -3.03200        1.14500
H          -0.52400       -2.61700       -0.59000
H           0.30400        2.31600       -1.05800
H           1.15900        1.30000       -2.21300

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -930.9807108 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -931.00063912 au
E(B3LYP/6-311+G**) = -931.2473497 au
Zero point vibrational energy:  226.260 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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43
Structure_18.xyz
H          -2.07700        2.71400       -1.34900
C          -1.92800        2.46400       -0.29000
C          -3.07700        1.17200        1.62300
C          -0.67700        0.68400        1.07800
C          -2.03800        0.11100        1.28000
C          -0.70300        1.52900       -0.15000
C          -3.26800        1.99400        0.32600
H          -3.79100        1.34800       -0.38900
H          -1.63300        3.40300        0.20100
H           0.21300        2.10300       -0.31700
H          -3.91100        2.87100        0.48600
C          -2.32500       -0.76500        0.25500
C          -0.52100        0.20500       -1.05000
O           0.59900        0.14400       -1.65800
C          -1.41500       -0.85400       -0.85800
H          -1.29200       -1.74700       -1.46500
O          -3.56900       -1.34500        0.24500
C          -3.98900       -2.00300       -0.94400
H          -3.81000       -1.38700       -1.83300
H          -5.06100       -2.18300       -0.82600
H          -3.47800       -2.96700       -1.07100
O           0.39000        0.31100        1.60500
H          -2.74500        1.80600        2.45500
H          -4.02500        0.71900        1.92800
Li          1.67100       -0.04300        0.04100
O           3.19900        1.16400       -0.21100
O           2.16900       -1.92200        0.33700
C           2.13600       -2.48200        1.64700
H           2.42000       -1.69300        2.34500
H           2.84500       -3.31800        1.72400
H           1.12500       -2.82900        1.89600
C           1.77500       -2.85300       -0.67200
H           2.51600       -3.65900       -0.75800
H           1.70700       -2.29500       -1.60700
H           0.79200       -3.27900       -0.43700
C           4.28700        1.36800        0.67900
H           4.48100        2.44000        0.81600
H           5.20000        0.88200        0.30400
H           4.00700        0.92800        1.63900
C           3.41700        1.71400       -1.51100
H           3.60900        2.79300       -1.44200
H           2.50300        1.52800       -2.07600
H           4.27300        1.22600       -1.99800

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -930.9703516 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -930.98725507 au
E(B3LYP/6-311+G**) = -931.2342246 au
Zero point vibrational energy:  226.068 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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43
Structure_19.xyz
H           1.35900        1.22200       -2.46100
C           1.72200        0.23000       -2.16400
C           3.79900       -0.91800       -1.08600
C           1.50700       -1.52400       -0.41300
C           2.84300       -1.06500        0.09000
C           0.81300       -0.33400       -1.02200
C           3.24900        0.29800       -1.88300
H           3.46000        1.19300       -1.28600
H           1.55600       -0.43000       -3.02700
H          -0.16100       -0.59800       -1.45300
H           3.77100        0.42900       -2.84300
O           1.04900       -2.65700       -0.34800
C           2.73700       -0.04200        0.99100
C           0.52000        0.56300        0.22600
O           3.91100        0.50400        1.45800
C           3.85400        1.72500        2.18100
H           3.30500        2.50100        1.63300
H           4.89100        2.03900        2.31900
H           3.39000        1.59200        3.16700
C           1.45600        0.58900        1.24500
H           1.23500        1.15700        2.14300
O          -0.64500        1.12300        0.26900
Li         -2.17200        0.22600        0.36800
O          -3.68700        1.26800       -0.17100
O          -2.33700       -1.64700        0.79900
C          -3.37500        2.59100       -0.62500
H          -3.79900        3.33700        0.06000
H          -3.77900        2.75000       -1.63400
H          -2.28700        2.66100       -0.63300
C          -5.08200        1.00300       -0.09900
H          -5.57600        1.69400        0.59800
H          -5.19800       -0.02200        0.26100
H          -5.54700        1.09900       -1.09000
C          -2.36000       -2.63000       -0.24800
H          -2.90600       -2.19200       -1.08700
H          -2.88900       -3.53000        0.09400
H          -1.33600       -2.88100       -0.54700
C          -1.61600       -2.11400        1.95000
H          -0.60900       -2.43700        1.66800
H          -2.15900       -2.94600        2.41700
H          -1.55400       -1.27900        2.65200
H           4.82700       -0.72200       -0.76400
H           3.81900       -1.82500       -1.70500

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -930.9728475 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -930.99323731 au
E(B3LYP/6-311+G**) = -931.2415307 au
Zero point vibrational energy:  226.305 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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43
Structure_20.xyz
H          -3.41200       -2.65000        0.10600
C          -3.03900       -1.94600       -0.64900
C          -3.02300        0.55200       -1.27000
C          -0.86900       -0.76600       -1.29400
C          -1.54300        0.49500       -0.90100
C          -1.49400       -1.92500       -0.59600
C          -3.73000       -0.57500       -0.47900
H          -3.71800       -0.29600        0.58300
H          -3.31800       -2.36700       -1.62500
H          -1.08800       -2.89100       -0.91200
H          -4.78600       -0.66800       -0.76800
C          -1.18700        0.74900        0.41400
C          -0.82900       -1.65700        0.85100
O          -0.51700       -2.63900        1.52800
C          -0.52700       -0.27800        1.17200
H          -0.10900       -0.09300        2.15800
O          -1.67900        1.89900        0.98600
C          -1.74000        1.98300        2.40700
H          -2.22000        1.10000        2.84500
H          -2.33500        2.87300        2.62700
H          -0.74400        2.10300        2.85000
O           0.26500       -0.82800       -1.81800
Li          1.31500       -0.17200       -0.32000
O           1.98700        1.64200       -0.72400
O           2.85600       -1.18400        0.31400
C           4.09200       -1.06400       -0.38300
H           4.08700       -0.09100       -0.87800
H           4.19400       -1.86200       -1.13200
H           4.93700       -1.11600        0.31600
C           2.74600       -2.41400        1.04100
H           2.87100       -3.26800        0.36100
H           1.75000       -2.45000        1.48600
H           3.51800       -2.45600        1.82200
C           1.56000        2.19100       -1.97700
H           1.55700        1.37200       -2.69600
H           2.25600        2.97900       -2.29400
H           0.54300        2.59000       -1.89300
C           1.99100        2.61500        0.31900
H           2.34400        2.11600        1.22500
H           0.98000        3.01100        0.48500
H           2.67200        3.44000        0.07100
H          -3.16900        0.42300       -2.35000
H          -3.44900        1.52500       -1.00700

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -930.9698002 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -930.98676701 au
E(B3LYP/6-311+G**) = -931.2345388 au
Zero point vibrational energy:  226.372 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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52
Structure_21.xyz
H          -3.72400       -2.20500       -1.42200
C          -2.66400       -1.92600       -1.43600
C          -1.04700       -0.02200       -2.12800
C          -0.79200       -1.24400       -0.08600
C          -0.76400        0.14400       -0.60400
C          -2.16400       -1.81900        0.05700
C          -2.45100       -0.66200       -2.30000
H          -3.20500        0.08600       -2.02800
H          -2.11800       -2.76800       -1.88500
H          -2.17400       -2.81500        0.51000
H          -2.63900       -0.92200       -3.35200
O           0.25500       -1.90400        0.04300
C          -1.75400        0.97700        0.04600
C          -3.05500       -0.89200        0.92600
O          -3.97700       -1.38800        1.57300
C          -2.74200        0.51900        0.89600
H          -3.37300        1.17000        1.49100
O          -1.63300        2.30200       -0.29200
C          -2.66200        3.20300        0.10500
H          -3.64900        2.83600       -0.19700
H          -2.44400        4.14700       -0.39900
H          -2.65800        3.36400        1.19100
O           2.19300        1.87000       -0.21500
O           1.76100       -0.24000        2.10100
C           1.86000        2.78300        0.82800
H           0.78700        3.01200        0.81000
H           2.43600        3.71400        0.72200
H           2.11800        2.29500        1.76900
C           1.83600        2.38700       -1.49600
H           2.38000        3.32200       -1.69500
H           0.75600        2.55800       -1.55200
H           2.12300        1.63600       -2.23600
C           2.81300       -1.10300        2.51100
H           3.14100       -0.85800        3.53100
H           3.64100       -0.95500        1.81600
H           2.49400       -2.15400        2.47800
C           0.61300       -0.36000        2.94100
H           0.85200       -0.03500        3.96400
H           0.25400       -1.39700        2.96300
H          -0.16700        0.27800        2.52200
H          -0.28200       -0.66300       -2.58900
H          -1.00700        0.94100       -2.65100
Li          1.40400       -0.11900        0.04300
O           3.05700       -0.94400       -0.91700
C           4.30600       -0.30600       -1.15100
H           5.12400       -0.85900       -0.66500
H           4.23100        0.69800       -0.73100
H           4.51800       -0.24200       -2.22800
C           3.01900       -2.27300       -1.43100
H           2.03300       -2.67000       -1.19500
H           3.79700       -2.89100       -0.96100
H           3.17700       -2.26900       -2.51900

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -1086.0160984846 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -1086.03489331 au
E(B3LYP/6-311+G**) = -1086.3312003507 au
Zero point vibrational energy: 277.859 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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52
Structure_23.xyz
H           1.84700         1.35100         2.56100
C           2.28500         1.60700         1.58700
C           4.31600         0.99500         0.06700
C           2.05200         1.28400        -0.85300
C           3.21800         0.34400        -0.76500
C           1.29100         1.19800         0.44700
C           3.73000         1.04000         1.50800
H           3.72400         0.00800         1.87900
H           2.34000         2.70400         1.55200
H           0.43600         1.88300         0.46900
H           4.36700         1.61800         2.19300
O           1.77800         2.02300        -1.78600
C           2.84200        -0.93900        -0.47600
C           0.70700        -0.24900         0.44700
O           3.85300        -1.86100        -0.30900
C           3.53500        -3.12900         0.24100
H           2.99900        -3.04300         1.19400
H           4.49200        -3.63200         0.40500
H           2.93300        -3.73500        -0.45000
C           1.47000        -1.25400        -0.13000
H           1.05800        -2.25700        -0.19200
O          -0.49600        -0.38700         0.89000
H           5.24700         0.41800         0.05800
H           4.55300         2.00300        -0.29900
Li         -2.10000        -0.08500         0.10500
O          -2.17500         0.63000        -1.74500
O          -3.21900         1.18900         1.20800
O          -3.11000        -1.82100         0.09200
C          -1.09300         0.33000        -2.63800
C          -2.96800         1.71900        -2.19800
C          -2.51800         2.39900         1.49600
C          -3.76800         0.60200         2.38600
C          -4.22300        -2.16800        -0.71600
C          -2.47100        -2.94900         0.69100
H          -0.53100        -0.49400        -2.19500
H          -0.42600         1.19300        -2.74400
H          -1.48900         0.03400        -3.61900
H          -3.75200         1.87900        -1.45600
H          -3.42400         1.48800        -3.17200
H          -2.36300         2.63000        -2.30000
H          -2.13200         2.78200         0.54900
H          -1.67900         2.20800         2.17600
H          -3.19800         3.13900         1.94100
H          -4.24800        -0.33000         2.08400
H          -4.51000         1.27300         2.84100
H          -2.97600         0.38600         3.11600
H          -4.61300        -1.24200        -1.14500
H          -5.00700        -2.65400        -0.11800
H          -3.92300        -2.84500        -1.52700
H          -1.58000        -2.56400         1.18900
H          -2.17900        -3.67800        -0.07800
H          -3.14500        -3.43700         1.40900

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -1086.0145619626 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -1086.03781819 au
E(B3LYP/6-311+G**) = -1086.332252 au
Zero point vibrational energy: 277.833 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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52
Structure_24.xyz
H          -3.33700       -1.99500        1.82200
C          -3.16900       -1.79600        0.75500
C          -3.55700        0.02500       -1.05100
C          -1.36900       -1.15200       -0.87900
C          -2.04200        0.18700       -0.95800
C          -1.63400       -1.74600        0.48000
C          -3.99700       -0.56200        0.31600
H          -3.87600        0.23300        1.06200
H          -3.54500       -2.67800        0.21800
H          -1.22000       -2.75300        0.58900
H          -5.06200       -0.83600        0.31800
C          -1.53700        1.03300        0.00000
C          -0.75900       -0.81600        1.41600
O          -0.15000       -1.34800        2.36800
O          -2.08100        2.30200        0.06200
C          -1.97200        3.03300        1.27800
H          -2.28400        2.43700        2.14200
H          -2.63700        3.89400        1.16700
H          -0.95000        3.39700        1.44800
O          -0.62500       -1.64100       -1.72400
O           1.50700        1.44000       -1.55900
O           2.73400        0.76300        1.26500
C           4.04400        1.12700        0.85300
H           3.97600        1.47000       -0.18200
H           4.72500        0.26600        0.90700
H           4.44000        1.93600        1.48300
C           2.70000        0.25600        2.60500
H           3.43400       -0.55300        2.72100
H           1.69500       -0.13700        2.78100
H           2.93600        1.05800        3.31800
C           0.86600        1.20400       -2.82300
H           1.04200        0.16200       -3.08800
H           1.29600        1.86700       -3.58600
H          -0.21300        1.36100       -2.73200
C           1.30200        2.78500       -1.11900
H           1.78100        2.88000       -0.14300
H           0.23100        3.00200       -1.02800
H           1.76300        3.48900       -1.82600
H          -3.83700       -0.64300       -1.87600
H          -4.05700        0.98200       -1.23000
C          -0.62300        0.54800        1.00400
H          -0.10100        1.22400        1.67500
Li          1.37700        0.08300       -0.07600
O           2.25100       -1.65300       -0.53400
C           2.70000       -1.91200       -1.86100
H           3.02200       -0.95900       -2.28800
H           1.88800       -2.33500       -2.46500
H           3.55200       -2.60600       -1.84700
C           1.85700       -2.85600        0.13700
H           1.44400       -2.57100        1.10600
H           2.72800       -3.51200        0.27100
H           1.08600       -3.37300       -0.44700

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -1086.0031361933 au
E(B3LYP/6-31G*)cPCM (dielectric constant 7.4257)  = -1086.02147140 au
E(B3LYP/6-311+G**) = -1086.3171349407 au
Zero point vibrational energy: 278.357 kcal/mol
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ELECTRONIC SUPPORTING INFORMATION

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9
dimethylether
O           0.00000         0.00000         0.83200
C          -1.17100         0.00000         0.04700
H          -1.23200        -0.89300        -0.59800
H          -1.23200         0.89300        -0.59800
H          -2.02200         0.00000         0.73300
C           1.17100         0.00000         0.04700
H           1.23200        -0.89300        -0.59800
H           2.02200         0.00000         0.73300
H           1.23200         0.89300        -0.59800

This Molecule has 0 Imaginary Frequencies
E(B3LYP/6-31G*) = -155.0250548 au
E(B3LYP/6-311+G**) = -155.0769894 au
Zero point vibrational energy:  50.442 kcal/mol
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