Alkynyl Crown Ethers as a Scaffold for Hyperconjugative Assistance in Non-catalyzed Azide-Alkyne Click Reactions: Ion Sensing through Enhanced Transition State Stabilization

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Supporting Information

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1. Kinetic data

Kinetic studies were conducted by ^{1}H NMR using benzyl phenyl ether as an internal standard to monitor the consumption of starting materials.

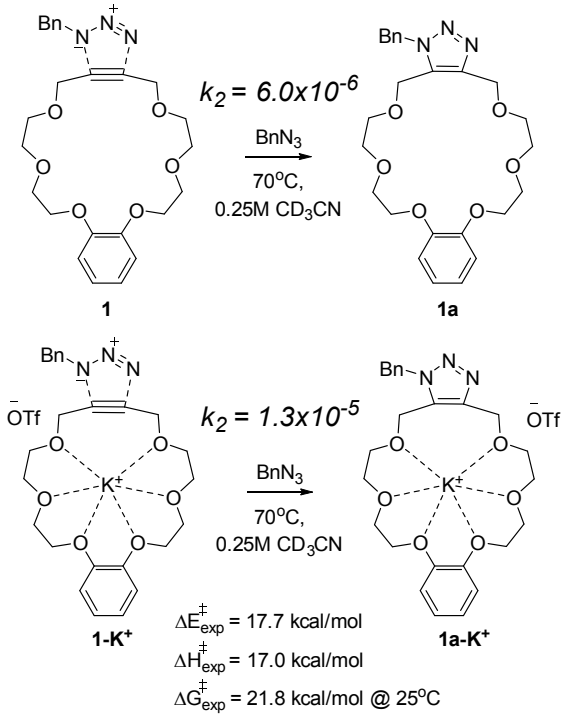

Figure S1. Rate constants (70°C) for the cycloaddition of alkynyl crown ether accelerated by potassium ion coordination. Experimental activation parameters for the potassium "catalyzed" reaction.

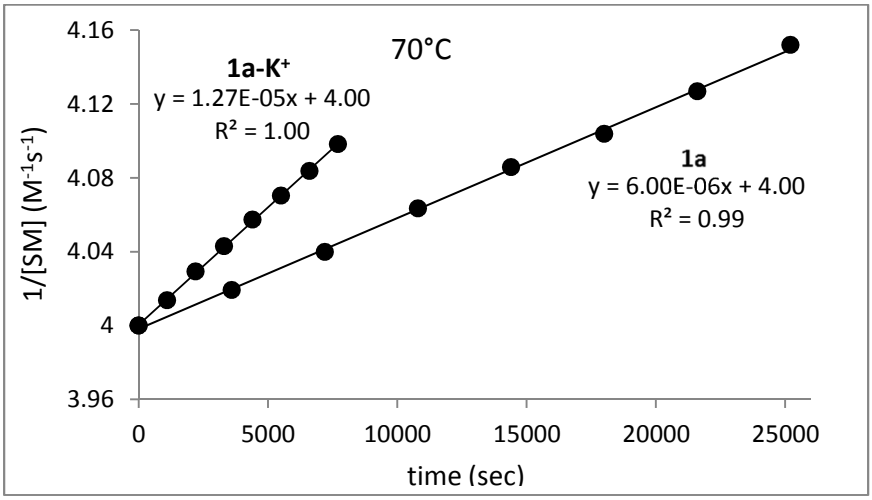

Figure S2. Rate constant determination (70°C) for the cycloaddition of alkynyl crown ether accelerated by potassium ion coordination. Plot given is the average of three kinetic runs.

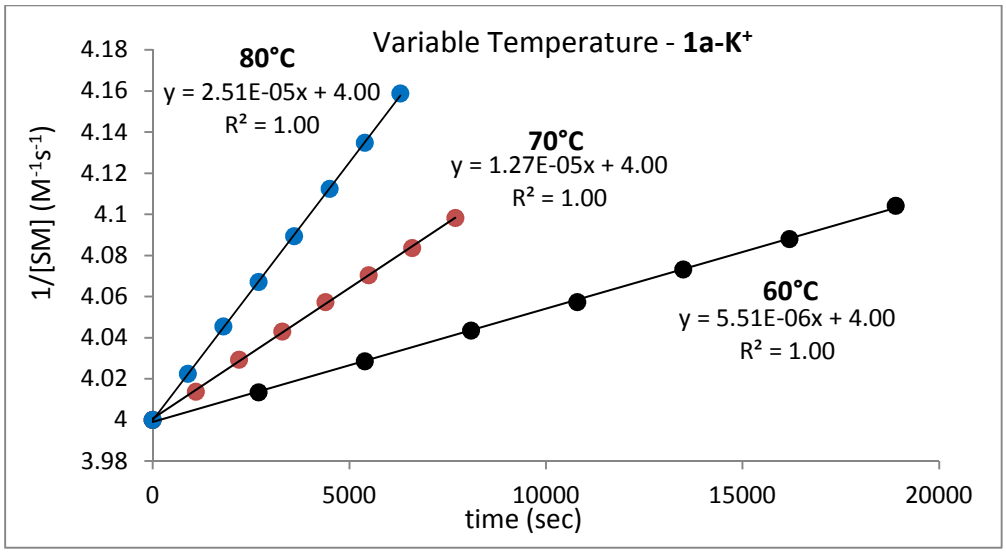

Figure S3. Rate constant determination at various temperatures for the cycloaddition of alkynyl crown ether with potassium ion. Plot given is the average of three kinetic runs.

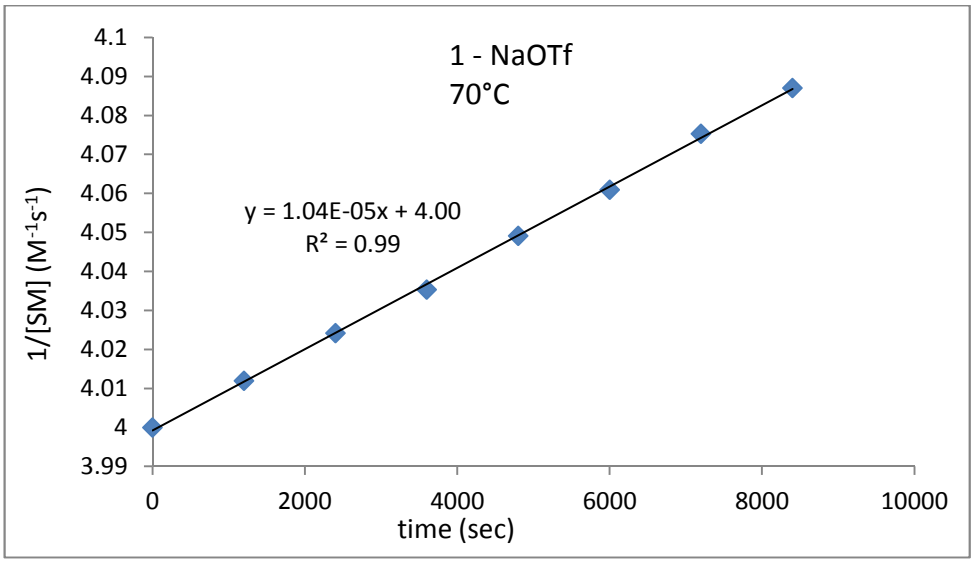

Figure S4. Rate constant determination (70°C) for the cycloaddition of alkynyl crown ether accelerated by sodium ion coordination.

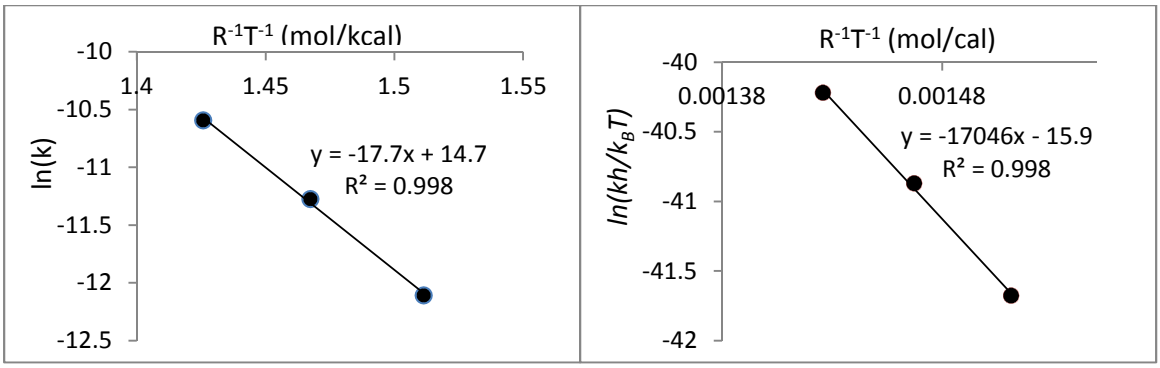

Figure S5. Arrhenius and Eyring plots for **1-K**$^+$ to **1a-K**$^+$.

2. NBO analysis

$\pi + (\pi^*) \rightarrow \sigma^*_{CO}$, kcal/mol	SM - F_{ij}	TS - F_{ij} $\pi + (\pi^*)$
1	0.063/0.063	0.064/0.056 (0.080/0.078)
1-K$^+$	0.061/0.060	0.064/0.056 (0.079.0.079)

Table S1. NBO analysis factors leading to increased/decreased interaction energies for the (sum of) two propargylic CO acceptor in alkynyl crown ether upon ion coordination. Values given for M06-2x/6-31G(d) in the gas phase.

3. B3LYP/6-31G(d) activation barriers

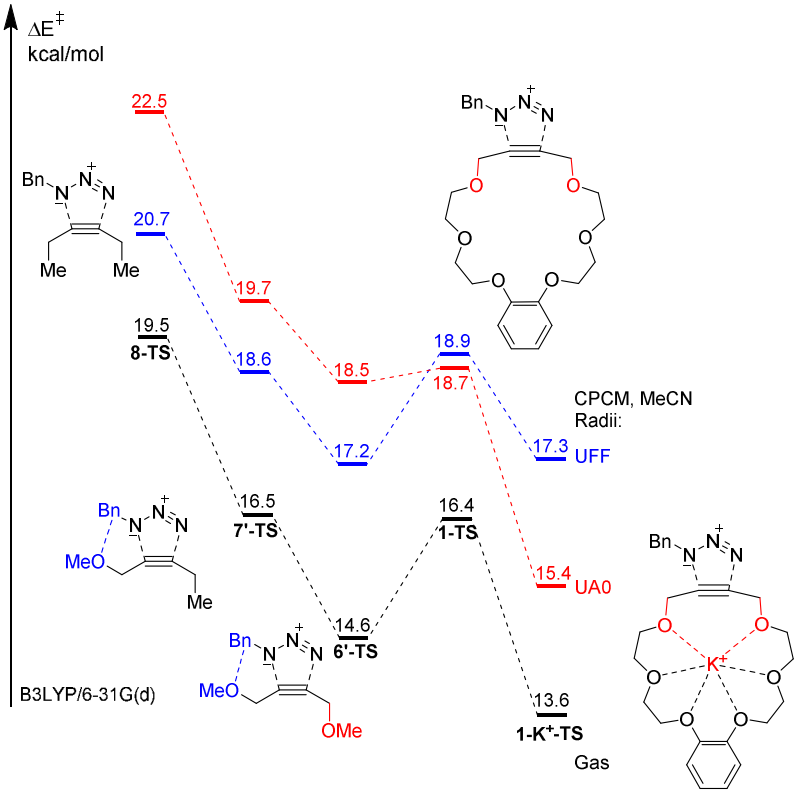

Figure S6. Activation barriers for the cycloadditions of benzyl azide with various alkynes calculated at the B3LYP/6-31G(d) level of theory with CPCM (acetonitrile, radii are color coded) solvation corrections (single point on gas phase geometries). Lowest energy TSs are shown.

4. B3LYP/6-31G(d) – Conformation analysis

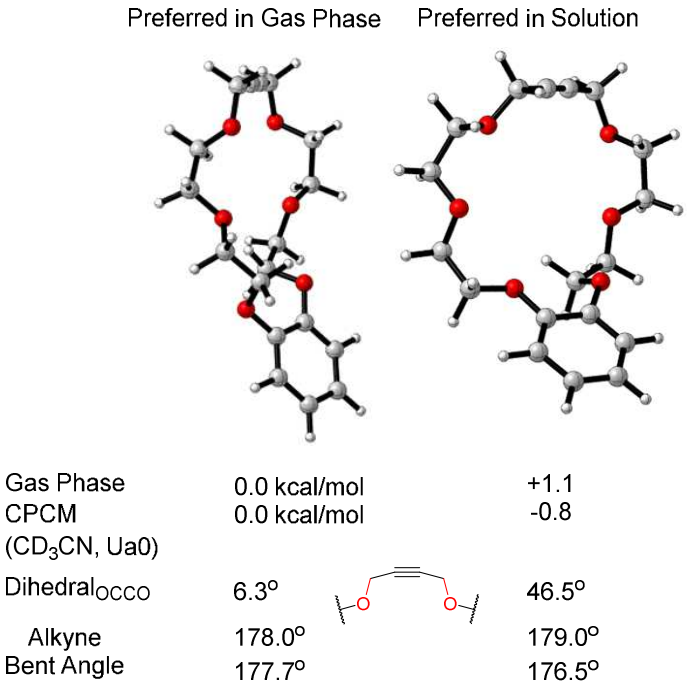

Figure S7. Geometries of the lowest energy alkynyl crown ether-potassium complex 1-K^+ optimized at the B3LYP/6-31G(d) and M062X/6-31G(d) levels of theory. Dihedral angles given for the OCCO bonds in red.

5. Cartesian Coordinates and Energies

All stationary points have been shown to be either minima (zero imaginary frequencies) or first-order saddle points (one imaginary frequency). Since solvation corrections consisted of single point energy calculations on gas phase geometries, these are not true transition states and may be higher order saddle points.

M06-2X/6-31G(d)

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H	-1.25585800	-1.35348000	-0.88225700
C	0.39435300	-0.30252600	0.00039600
C	0.77220600	1.03742600	0.00062200
C	1.38071400	-1.29151700	-0.00017300
C	2.12300300	1.38242300	0.00031500

H	0.00648000	1.80554600	0.00095100
C	2.72689100	-0.94712200	-0.00044000
H	1.09034800	-2.34028400	-0.00043300
C	3.10212600	0.39535100	-0.00018700
H	2.40778000	2.43027800	0.00046200
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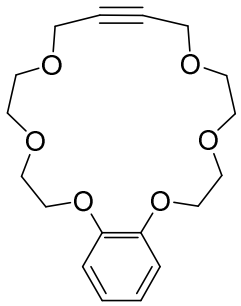

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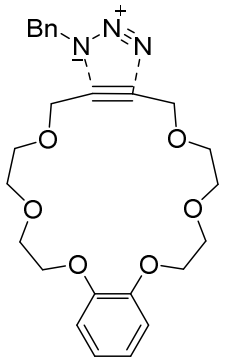

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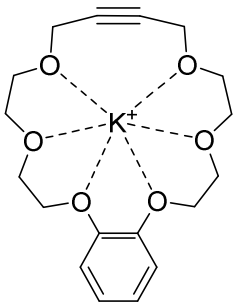

"Aligned"

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"Misalgined"

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H	2.73690000	-0.93180700	2.77425700
H	1.00486700	-0.62149200	2.99908900
C	-4.28356900	0.56043200	0.04500200
H	-5.10516100	1.07906600	-0.46624300
H	-4.61546800	0.31304200	1.06345400
C	-2.58760200	-2.62583900	-1.91832200

H	-2.31449500	-2.35568700	-2.94148100
H	-3.14925000	-3.56847400	-1.95278300
O	1.35451900	1.70988200	-0.75685100
C	-3.88684500	-0.64747100	-0.68149600
C	-3.38591100	-1.55650700	-1.29700800
H	-1.94329600	-4.50032900	-0.19079200
H	-2.29329400	-2.97020600	0.65616800
H	-0.32700800	-4.26723300	1.58037800
H	0.51662500	-3.99479900	0.03116100
H	-3.12167200	2.26901100	1.94062600
H	-4.21080800	3.01273000	0.73703900
H	-2.33122800	3.77947100	-0.60935300
H	-2.13911600	4.37433000	1.06237300
O	1.70190800	0.01176600	1.23295500
C	2.71008100	0.04043400	0.30099900
C	2.50825600	0.94775400	-0.74996300
C	3.87410100	-0.72264200	0.33028400
C	3.44223600	1.07643100	-1.76465200
C	4.81159300	-0.58666500	-0.69539000
H	4.06959400	-1.41853500	1.13780700
C	4.59967800	0.29921300	-1.74437600
H	3.24805900	1.78951300	-2.55954700
H	5.71424900	-1.18767800	-0.66505800
H	5.33202700	0.39532700	-2.53806200
K	-0.72183800	0.02247400	-0.16128700

Gas
HF=-1750.8942236
UA0
HF=-1750.9522265
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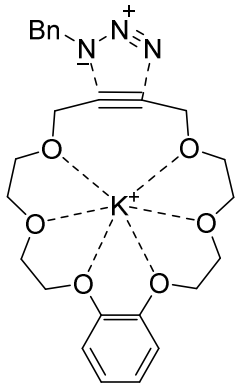
Sum of electronic and thermal Enthalpies= -1750.514458
Sum of electronic and thermal Free Energies= -1750.595565



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C	0.19079300	-2.90860900	-0.60996500
C	-1.07085500	-3.22691300	-1.37845000
O	1.09036700	0.94752200	-1.00737300
O	-1.16238700	2.58996000	-0.79274500
O	-1.79264400	-2.02300600	-1.57077800
O	-0.19481500	-2.49229000	0.68957100
C	-2.04257600	3.47430700	-0.12452400

H	-2.16055800	4.40503200	-0.69731300
H	-1.64470400	3.72595800	0.87001800
C	-3.38403100	2.79543300	0.00501200
H	-4.11184800	3.47673600	0.46134100
H	-3.74440800	2.48605900	-0.98246700
C	-3.12236100	-2.23336100	-2.00279000
H	-3.68916500	-2.75440800	-1.21748400
H	-3.14496300	-2.85036500	-2.91270900
C	-3.71764500	-0.87295600	-2.31079200
H	-4.75387500	-0.95896900	-2.65387000
H	-3.13163100	-0.39190600	-3.09741500
C	2.20553300	1.01595600	-0.12750700
H	2.20616100	1.96560800	0.42576000
H	3.14056000	0.95810400	-0.70331000
C	0.88974900	-2.35865000	1.59272600
H	0.45071900	-2.31322700	2.59282600
H	1.52971700	-3.25033200	1.55495600
O	-3.21409300	1.64542200	0.83883500
C	2.12542300	-0.10616100	0.82532800
C	1.71067600	-1.15072400	1.34924200
H	0.81957900	-3.80756300	-0.54866200
H	0.76443100	-2.11689500	-1.11625600
H	-0.82189600	-3.67964100	-2.34816600
H	-1.67414200	-3.93968100	-0.79920900
H	0.39178000	1.80254200	-2.70050200
H	1.89694900	2.52837500	-2.09249800
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C	-4.53841900	-0.07659800	-0.18443900
C	-4.32327100	0.81991400	0.87648600
C	-5.62744900	-0.94174400	-0.13656600
C	-5.18342900	0.85083500	1.96135000
C	-6.49033000	-0.90286900	0.96053300
H	-5.81829600	-1.64607700	-0.93826200
C	-6.27411200	-0.01664200	2.00795600
H	-4.98187200	1.55667900	2.76110300
H	-7.33742300	-1.58002100	0.98702600
H	-6.94732300	0.00390300	2.85751300
K	-1.17756300	0.00331400	0.11032500
N	3.00887500	-1.44906900	3.00506400
N	3.70432900	0.50973600	2.10828300
N	3.67101500	-0.51751300	2.82058900
C	5.00123800	1.07349800	1.69924900
H	4.85053200	2.15060500	1.58911700
H	5.71692800	0.93158100	2.51553500
C	5.52538900	0.48671900	0.40552900
C	5.42212300	-0.88027200	0.13728400
C	6.13229000	1.32247000	-0.53254700
C	5.92717500	-1.40064300	-1.05036500
H	4.94649000	-1.54448100	0.85420600
C	6.64246100	0.80072600	-1.71889300
H	6.21211900	2.38835400	-0.33126400
C	6.53896800	-0.56236100	-1.98035700
H	5.84805300	-2.46510400	-1.24788900
H	7.11690700	1.46057500	-2.43838900
H	6.93475700	-0.97105800	-2.90446000

Gas
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 Sum of electronic and thermal Energies=   -2185.252570
 Sum of electronic and thermal Enthalpies=   -2185.251626
 Sum of electronic and thermal Free Energies=   -2185.353674
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 Sum of electronic and thermal Enthalpies=   -2185.310833
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UFF
HF=-2185.8929065
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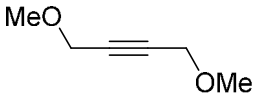

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C	-4.08819900	-0.42603800	0.06819600
O	2.72165900	-0.39349000	-0.39308700
O	-2.72167900	-0.39337000	0.39319000
C	2.01063600	0.45659200	0.47408700
H	2.40063600	1.48581100	0.40857000
H	2.13501800	0.13159200	1.52022200
C	-2.01061800	0.45646400	-0.47419600
H	-2.13490200	0.13112800	-1.52023800
H	-2.40066100	1.48569000	-0.40903300
C	0.58779000	0.44624800	0.13151000
C	-0.58779700	0.44627000	-0.13151300
H	-4.25012500	-0.80034400	-0.95376900
H	-4.54648400	0.57103900	0.15023100
H	4.57103600	-1.10104300	-0.77627700
H	4.25017900	-0.80007000	0.95390600
H	4.54646500	0.57100900	-0.15048800
H	-4.57106700	-1.10084100	0.77648000

Gas
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 Sum of electronic and thermal Enthalpies=   -384.651300
 Sum of electronic and thermal Free Energies=   -384.697847
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HF=-384.8234982
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 Sum of electronic and thermal Energies=   -384.659214
 Sum of electronic and thermal Enthalpies=   -384.658270
 Sum of electronic and thermal Free Energies=   -384.705284
UFF
HF=-384.8250159
Sum of electronic and zero-point Energies=   -384.670633

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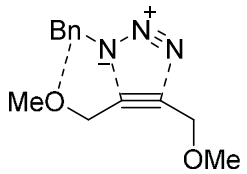


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 O                -4.12090200   -0.68616900   -0.67032200
 C                -1.24132700    2.24035300    0.08170000
 H                -2.06457800    2.59929300   -0.55550500
 H                -1.26236500    2.81809500    1.01882500
 C                -3.10937400   -1.25671200    0.12633900
 H                -3.52715500   -1.62889000    1.07579600
 H                -2.65616300   -2.12413200   -0.38032900
 C                -1.45648900    0.81346000    0.36788000
 C                -2.06343000   -0.26168200    0.40156900
 H                -5.60844800   -1.99628200   -0.04681600
 H                -4.72796400   -2.48239800   -1.52029500
 H                 1.16489100    3.84246500   -1.42045600
 H                 0.18755900    4.43035500   -0.04546900
 N                -0.82318600   -1.55380500    1.58669000
 N                 0.28381300    0.42901000    1.61632500
 N                 0.01894100   -0.78600300    1.77975800
 C                 1.69116000    0.78515600    1.37883500
 H                 1.64636400    1.82163200    1.03987400
 H                 2.23525900    0.76183900    2.33063700
 H                -0.58590300    4.12610700   -1.62529600
 H                -5.87364300   -1.11411200   -1.57625100
 C                 2.37900000   -0.08734500    0.35439300
 C                 3.57394500   -0.73444300    0.66334600
 C                 1.81047400   -0.26517200   -0.91080600
 C                 4.20560600   -1.54340700   -0.27924300
 H                 4.01328300   -0.60732100    1.65011300
 C                 2.43906900   -1.07550700   -1.84938700
 H                 0.87845300    0.24068400   -1.14870500
 C                 3.63794000   -1.71548200   -1.53749100
 H                 5.13560600   -2.04371400   -0.02653300
 H                 1.99207300   -1.20942100   -2.82998500
 H                 4.12462200   -2.34924500   -2.27273300
Gas
Frequencies --  -447.1512
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 Sum of electronic and thermal Enthalpies=          -819.442867
 Sum of electronic and thermal Free Energies=       -819.511547
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UFF
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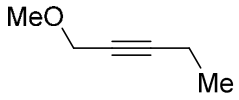


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 H                  2.73299200   -1.43789500    0.69932400
 H                  2.86525500   -1.15593200   -1.02885500
 C                 -1.32792300    0.58826500   -0.17348500
 H                 -1.55668500    0.99461100   -1.17273800
 H                 -1.46016400    1.41362000    0.54572000
 C                  1.20596100   -0.25151000   -0.11161200
 C                  0.05889900    0.11986800   -0.13626900
 H                 -3.82973700    0.33300900   -0.88167300
 H                 -3.72727600    0.74822200    0.85115600
 H                 -4.16041100   -0.91139200    0.35549900
 C                  3.56064800    0.49765200    0.18711000
 H                  3.46003500    1.25785400   -0.59154100
 H                  3.33643800    0.96565400    1.14888800
 H                  4.59775500    0.15200200    0.20247900
Gas
HF=-309.6474144
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 Sum of electronic and thermal Energies=             -309.490103
 Sum of electronic and thermal Enthalpies=           -309.489159
 Sum of electronic and thermal Free Energies=        -309.530764
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HF=-309.652266
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 Sum of electronic and thermal Enthalpies=           -309.494073
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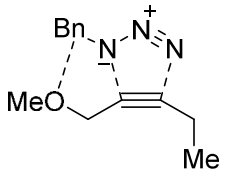


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 O                  0.46730900    2.17179800    0.41606800
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H	1.86301500	2.34319000	-1.09938400
C	3.43235100	-1.68524300	0.39315200
H	3.88049700	-2.18632300	-0.47231300
H	2.89693700	-2.46655100	0.94388400
C	1.92318300	0.42101500	-0.21709400
C	2.44947000	-0.69040000	-0.08413400
H	-0.73520500	3.69801500	0.96120600
H	0.34085100	4.07095300	-0.41629900
N	1.18151300	-2.00820400	-1.18084800
N	0.23935100	0.01829400	-1.55128200
N	0.40899400	-1.22517800	-1.54140500
C	-1.13283600	0.52742100	-1.55656400
H	-1.01664400	1.60491800	-1.41897500
H	-1.58019700	0.36698400	-2.54526400
C	-2.02711100	-0.04541400	-0.47889700
C	-3.38297600	-0.24545300	-0.73789800
C	-1.51887200	-0.36193500	0.78279000
C	-4.22729200	-0.74511700	0.25000400
H	-3.78094300	-0.01334400	-1.72340300
C	-2.36193800	-0.86752700	1.76787600
H	-0.46322300	-0.20424800	0.98585100
C	-3.71700200	-1.05868400	1.50615800
H	-5.28051600	-0.89889900	0.03459200
H	-1.95809500	-1.11362800	2.74551500
H	-4.37147900	-1.45522800	2.27647400
H	1.00151700	4.00207300	1.24051200
C	4.51475900	-1.05428800	1.27030900
H	5.06549500	-0.29083300	0.71359100
H	4.06824300	-0.57700300	2.14710300
H	5.22672000	-1.81033100	1.61409900

Gas

Frequencies -- -455.8694

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Sum of electronic and thermal Free Energies= -744.341935

UA0

HF=-744.5866849

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UFF

HF=-744.5874788

Sum of electronic and zero-point Energies= -744.302671

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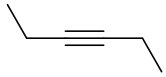

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H	2.11562100	1.33485300	-0.87418200
H	2.10905000	1.32970900	0.88084600
C	-1.95055200	-0.69570100	0.00044900
H	-2.11508600	-1.33286100	-0.87638800
H	-2.11257100	-1.33164100	0.87864900
C	2.96385100	-0.45466600	0.00116800
H	2.83540200	-1.07987700	-0.88608200
H	3.98594200	-0.06584300	0.00727100
H	2.82722600	-1.08638100	0.88256600
C	-2.96308600	0.45578000	0.00113800
H	-2.83128800	1.08322900	-0.88403600
H	-3.98568900	0.06825900	0.00333200
H	-2.82813900	1.08492300	0.88463800

Gas

HF=-234.4780998

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UA0

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UFF

HF=-234.4808651

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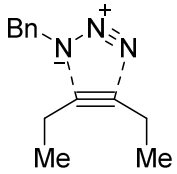

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C	3.21478200	-1.58098900	0.21066800
H	3.65797700	-2.00620600	-0.69684000
H	2.68032600	-2.40619400	0.69471000
C	1.71688500	0.58393700	-0.20182900
C	2.23966100	-0.53778000	-0.17126300
N	0.98173800	-1.74673700	-1.44869700
N	0.08371500	0.32477100	-1.63190500
N	0.22832100	-0.91999200	-1.74200700
C	-1.26635200	0.86629100	-1.53616500
H	-1.11398700	1.93958200	-1.37450600
H	-1.77952200	0.77062700	-2.50126300
C	-2.12519000	0.29068700	-0.42793800
C	-3.51464800	0.39407300	-0.51722700
C	-1.55808600	-0.31398000	0.69488600
C	-4.32791400	-0.08938400	0.50205000

H	-3.96274000	0.85431600	-1.39520300
C	-2.37379000	-0.80241400	1.71331900
H	-0.47727400	-0.40930700	0.76931100
C	-3.75772500	-0.69042800	1.62206500
H	-5.40724800	-0.00428400	0.41840800
H	-1.92264100	-1.27494700	2.58061100
H	-4.39093400	-1.07377900	2.41622200
C	4.30730600	-1.03655300	1.13280800
H	4.85414500	-0.22653600	0.64184000
H	3.87083500	-0.63829100	2.05328000
H	5.01992700	-1.82260700	1.40007100
C	2.54710300	2.55853900	1.05956700
H	2.54463800	2.00041400	1.99996200
H	3.54201600	2.46641300	0.61529300
H	2.36193400	3.61327900	1.28238000

Gas

Frequencies -- -450.1831

HF=-669.4064847

Sum of electronic and zero-point Energies= -669.126665

Sum of electronic and thermal Energies= -669.110350

Sum of electronic and thermal Enthalpies= -669.109406

Sum of electronic and thermal Free Energies= -669.172121

UA0

HF=-669.4122632

Sum of electronic and zero-point Energies= -669.132903

Sum of electronic and thermal Energies= -669.116493

Sum of electronic and thermal Enthalpies= -669.115549

Sum of electronic and thermal Free Energies= -669.179226

UFF

HF=-669.4124547

Sum of electronic and zero-point Energies= -669.132976

Sum of electronic and thermal Energies= -669.116603

Sum of electronic and thermal Enthalpies= -669.115658

Sum of electronic and thermal Free Energies= -669.178894

B3LYP/6-31G(d)

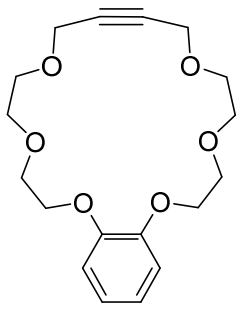
BnN_3

N	-1.95004400	0.42561100	-0.00134800
N	-3.15598200	0.16853300	-0.00082000
N	-4.29391700	0.06129500	0.00042800
C	-1.04871000	-0.74732700	0.00111200
H	-1.25143400	-1.36822700	0.88629600
H	-1.25113100	-1.37217900	-0.88124000
C	0.40108100	-0.30805500	-0.00003200
C	0.77663500	1.03756100	0.00054600
C	1.39759500	-1.29312900	-0.00020300
C	2.12811300	1.39134700	0.00037400
H	0.00823900	1.80307500	0.00116300
C	2.74573000	-0.94008300	-0.00030500
H	1.11716000	-2.34502400	-0.00005800
C	3.11583200	0.40696800	-0.00036800
H	2.40648200	2.44195500	0.00057600
H	3.50633200	-1.71638000	-0.00062300
H	4.16629300	0.68501200	-0.00068000

Gas

HF=-435.1435284
Sum of electronic and zero-point Energies= -435.011354
Sum of electronic and thermal Energies= -435.003625
Sum of electronic and thermal Enthalpies= -435.002681
Sum of electronic and thermal Free Energies= -435.045214
UA0
HF=-435.1517379
Sum of electronic and zero-point Energies= -435.020102
Sum of electronic and thermal Energies= -435.012383
Sum of electronic and thermal Enthalpies= -435.011439
Sum of electronic and thermal Free Energies= -435.053610
UFF
HF=-435.1487546
Sum of electronic and zero-point Energies= -435.016513
Sum of electronic and thermal Energies= -435.008825
Sum of electronic and thermal Enthalpies= -435.007880
Sum of electronic and thermal Free Energies= -435.050052

K^+
Gas
HF=-599.7249892
Sum of electronic and zero-point Energies= -599.724989
Sum of electronic and thermal Energies= -599.723573
Sum of electronic and thermal Enthalpies= -599.722629
Sum of electronic and thermal Free Energies= -599.740165
UA0
HF=-599.8607192
Sum of electronic and zero-point Energies= -599.860719
Sum of electronic and thermal Energies= -599.859303
Sum of electronic and thermal Enthalpies= -599.858359
Sum of electronic and thermal Free Energies= -599.875895
UFF
HF=-599.8479295
Sum of electronic and zero-point Energies= -599.847929
Sum of electronic and thermal Energies= -599.846513
Sum of electronic and thermal Enthalpies= -599.845569
Sum of electronic and thermal Free Energies= -599.863105



Gas Phase Minimum

C	-1.10756100	3.14956800	0.84397000
C	-2.46262200	2.49049800	0.67603200
O	-2.83765100	2.58230200	-0.69143700
O	-0.10364800	2.32954000	0.27512100
C	1.08986700	3.03093500	-0.01489700
C	2.12375300	2.06767400	-0.55915300

C	-4.18277900	2.21805300	-0.94955500
O	2.72193800	1.35680000	0.53507500
C	-4.50477900	0.81918900	-0.62864900
C	-4.76435000	-0.32091400	-0.31758700
C	3.19431100	-0.88216700	-0.24897400
C	3.63342700	0.39834300	0.13718500
C	-5.04040000	-1.70645200	0.09332300
O	-3.87514500	-2.40817300	0.49240500
C	-3.03947000	-2.80158700	-0.59025800
C	-1.69182900	-3.21083500	-0.02747400
O	-0.92772200	-2.04521100	0.21023700
C	0.16921400	-2.24908200	1.07843300
C	1.12912200	-1.08144400	0.95710600
O	1.86935100	-1.22614100	-0.27374900
C	4.13543900	-1.82828700	-0.66599700
C	4.99645300	0.69756400	0.13602700
C	5.49506700	-1.51639800	-0.68488400
C	5.93067800	-0.25650100	-0.27011500
H	-1.13141400	4.13264800	0.34792500
H	-0.90879900	3.31682600	1.91624700
H	-2.42146200	1.44202900	1.00060300
H	-3.19511900	3.01896200	1.31038700
H	0.89356800	3.81051500	-0.77022800
H	1.49390100	3.52616900	0.88318200
H	1.64700200	1.36846300	-1.25669900
H	2.90278800	2.62768600	-1.09643200
H	-4.33570300	2.40898700	-2.01752400
H	-4.87158400	2.87948400	-0.39417800
H	-5.56486700	-2.24201000	-0.71610300
H	-5.70219200	-1.71141700	0.96706000
H	-3.49881000	-3.64691200	-1.12940900
H	-2.89410700	-1.97410900	-1.29785500
H	-1.17133900	-3.87151300	-0.74141600
H	-1.85523200	-3.78039700	0.90118700
H	-0.18145900	-2.32781700	2.12254100
H	0.70555000	-3.17931600	0.83217500
H	0.58534600	-0.13271900	0.95576900
H	1.82324900	-1.09213900	1.80564600
H	3.77519100	-2.80686500	-0.96899100
H	5.30424000	1.68939200	0.45533300
H	6.21358100	-2.26451400	-1.00852100
H	6.98942900	-0.01330300	-0.26912600

Gas
HF=-1151.5484606
Sum of electronic and zero-point Energies= -1151.144818
Sum of electronic and thermal Energies= -1151.120995
Sum of electronic and thermal Enthalpies= -1151.120051
Sum of electronic and thermal Free Energies= -1151.201325
UA0
HF=-1151.5660615
Sum of electronic and zero-point Energies= -1151.163347
Sum of electronic and thermal Energies= -1151.140273
Sum of electronic and thermal Enthalpies= -1151.139329
Sum of electronic and thermal Free Energies= -1151.218872
UFF
HF=-1151.5638884
Sum of electronic and zero-point Energies= -1151.160327

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 Sum of electronic and thermal Energies=            -1151.137330
 Sum of electronic and thermal Enthalpies=          -1151.136386
 Sum of electronic and thermal Free Energies=       -1151.215309
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Solvation Correction Minimum

```
C                 -2.27992300   -3.32312900    0.22385400
 C                 -3.49787300   -2.70988000   -0.44030400
 C                 -1.53225300    3.83119100   -0.55561600
 C                 -0.43149500    3.99394600    0.47500300
 O                 -4.27358000   -2.04839600    0.55110900
 O                 -1.32360400   -2.30521700    0.43366700
 O                  0.62001500    3.09759400    0.16888500
 O                 -2.25460500    2.65545000   -0.24733800
 C                 -0.21970000   -2.71320200    1.21281100
 C                  0.86745600   -1.65976200    1.12103300
 C                  1.55431200    2.95693400    1.21551200
 C                  2.73645100    2.14252000    0.73049000
 C                 -5.18201200   -1.09122600    0.03093400
 C                 -3.17777200    2.29031900   -1.26083000
 O                  1.44515300   -1.72746500   -0.19062100
 C                 -4.51841300    0.12276200   -0.46643000
 C                 -3.91293200    1.10108500   -0.83751300
 O                  2.32160800    0.80227300    0.50575400
 C                  3.23522300   -0.07182300   -0.01760700
 C                  2.75779500   -1.36378900   -0.33902600
 C                  4.57995400    0.23635300   -0.25085500
 C                  3.62862300   -2.29483700   -0.90220200
 C                  5.43942100   -0.71166000   -0.81536500
 C                  4.96601500   -1.97650000   -1.14965600
 H                 -2.58353400   -3.79106700    1.17486900
 H                 -1.86462600   -4.11487600   -0.42354400
 H                 -3.15898000   -2.00453700   -1.21080200
 H                 -4.09964300   -3.49646900   -0.92566900
 H                 -2.19581300    4.71356400   -0.53328900
 H                 -1.08259700    3.77143600   -1.55983500
 H                 -0.06377800    5.03497300    0.46845300
 H                 -0.84858700    3.78889800    1.47314900
 H                  0.18167100   -3.67678600    0.85805100
 H                 -0.51666800   -2.83936800    2.26919500
 H                  0.44860000   -0.66509100    1.29891200
 H                  1.63484300   -1.86489800    1.87966800
 H                  1.09345300    2.47211300    2.09135000
 H                  1.93587800    3.94150300    1.54055400
 H                  3.53059400    2.17565500    1.49145500
 H                  3.12549200    2.58017100   -0.19861600
 H                 -5.84993000   -0.83936100    0.86235000
 H                 -5.80562200   -1.53055400   -0.76632200
 H                 -3.88634100    3.11515200   -1.45784900
 H                 -2.64682500    2.09489500   -2.20827400
 H                  4.96491500    1.21975200   -0.00644900
 H                  3.22492900   -3.27220400   -1.14901800
 H                  6.47799900   -0.44675300   -0.99338300
 H                  5.62740400   -2.71587000   -1.59199100
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Gas

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HF=-1151.5467553
Sum of electronic and zero-point Energies=          -1151.143423
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 Sum of electronic and thermal Energies=            -1151.119536
 Sum of electronic and thermal Enthalpies=          -1151.118591
 Sum of electronic and thermal Free Energies=       -1151.199605
UA0
HF=-1151.567397
Sum of electronic and zero-point Energies=         -1151.164945
 Sum of electronic and thermal Energies=           -1151.142672
 Sum of electronic and thermal Enthalpies=         -1151.141728
 Sum of electronic and thermal Free Energies=      -1151.217700
UFF
HF=-1151.5659064
Sum of electronic and zero-point Energies=         -1151.162490
 Sum of electronic and thermal Energies=           -1151.138483
 Sum of electronic and thermal Enthalpies=         -1151.137539
 Sum of electronic and thermal Free Energies=      -1151.220430
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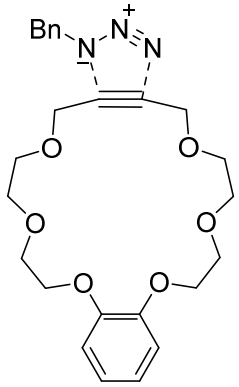


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C                  0.52509900   -1.97382200   -0.80589200
 C                -0.37697500    -0.77157900   -0.59084800
 O                -0.70932300    -0.67031300    0.79706000
 O                 1.79058600    -1.71888300   -0.22799600
 C                 2.57931700    -2.87697100   -0.04801200
 C                 3.92024500    -2.46983700    0.52614400
 C                -2.08308100    -0.47924900    1.07343200
 O                 4.73373100    -1.93279600   -0.52656800
 C                -2.58660800     0.83349700    0.61865800
 C                -2.64775300     1.94940200    0.08465200
 C                 5.81389500     0.08797600    0.24267800
 C                 5.86696800    -1.28180600   -0.07917200
 C                -2.12971900     3.11407300   -0.67504000
 O                -0.74270600     3.04808600   -0.94540400
 C                 0.07880800     3.29869000    0.18879500
 C                 1.51654100     3.42842000   -0.27459500
 O                 2.05955000     2.14372800   -0.51037700
 C                 3.26836600     2.18007700   -1.24693900
 C                 3.99068500     0.85376700   -1.11557900
 O                 4.66289200     0.82447500    0.16082700
 C                 6.97055000     0.72151900    0.70857900
 C                 7.07058900    -1.97914600    0.03534600
 C                 8.16506300     0.01390600    0.84215800
 C                 8.22179400    -1.33663300    0.49279100
 H                 0.06028700    -2.85896900   -0.34130300
 H                 0.62666400    -2.17426600   -1.88702000
 H                 0.12370000     0.14854400   -0.91284300
 H                -1.28332700    -0.90339700   -1.19866800
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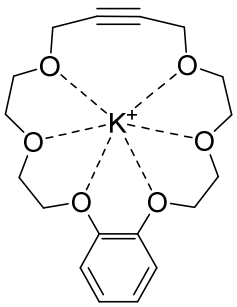
H	2.08306400	-3.57077700	0.65195400
H	2.73371200	-3.41186700	-0.99963800
H	3.76645000	-1.72014500	1.31135000
H	4.42049200	-3.34512100	0.96603700
H	-2.18362800	-0.56826700	2.16004400
H	-2.69076400	-1.27841000	0.61657000
H	-2.37880300	4.04365800	-0.13975200
H	-2.62820500	3.15824600	-1.64921300
H	-0.23083300	4.23990800	0.67330800
H	-0.00471600	2.48613700	0.92334600
H	2.10640100	3.95277800	0.49633500
H	1.53546400	4.04238700	-1.18933900
H	3.05508200	2.37556800	-2.31227500
H	3.92778500	2.98374100	-0.88331300
H	3.28465400	0.02378400	-1.18798900
H	4.73440300	0.76633700	-1.91790000
H	6.90723900	1.77629000	0.95892500
H	7.08279200	-3.03049800	-0.23864200
H	9.05404900	0.52349000	1.20372500
H	9.15295400	-1.88925300	0.58032400
N	-4.71365900	0.62120600	1.40856400
N	-5.09737200	1.71373600	0.91321400
N	-4.62786100	2.62712000	0.34318100
C	-5.71332200	-0.38461400	1.81499100
H	-5.15249700	-1.11401500	2.40599100
H	-6.44563100	0.08069500	2.48637200
C	-6.40837200	-1.07276400	0.65600100
C	-5.91965300	-2.28107100	0.14560700
C	-7.53660600	-0.49518400	0.05983800
C	-6.53938900	-2.89836200	-0.94192300
H	-5.05032100	-2.74527900	0.60688800
C	-8.15843200	-1.10870400	-1.02752900
H	-7.92988100	0.44132900	0.44920100
C	-7.66009100	-2.31194800	-1.53189400
H	-6.14970300	-3.83777500	-1.32509200
H	-9.03419700	-0.64980400	-1.47858300
H	-8.14579100	-2.79168600	-2.37733200

Gas
Frequencies -- -340.4683
HF=-1586.6658305
Sum of electronic and zero-point Energies= -1586.128856
Sum of electronic and thermal Energies= -1586.095907
Sum of electronic and thermal Enthalpies= -1586.094963
Sum of electronic and thermal Free Energies= -1586.199979

UA0
HF=-1586.6845923
Sum of electronic and zero-point Energies= -1586.147891
Sum of electronic and thermal Energies= -1586.117516
Sum of electronic and thermal Enthalpies= -1586.116571
Sum of electronic and thermal Free Energies= -1586.212448

UFF
HF=-1586.6892887
Sum of electronic and zero-point Energies= -1586.153725
Sum of electronic and thermal Energies= -1586.123376
Sum of electronic and thermal Enthalpies= -1586.122432
Sum of electronic and thermal Free Energies= -1586.217742



"Aligned"

C	-2.40989700	-3.25556800	-0.40261700
C	-3.28214200	-2.36845000	-1.27792500
C	-1.48131600	3.56254000	0.17702300
C	-0.13146600	3.70247400	-0.49396100
O	-3.27054500	-1.00955800	-0.82854600
O	-1.08432500	-2.73737000	-0.43425700
O	0.24781100	2.45314600	-1.06914700
O	-1.33611800	2.72844000	1.32852200
C	-0.13873200	-3.54250600	0.26390800
H	-0.13901400	-4.56686300	-0.13757300
H	-0.39403400	-3.59286000	1.33364900
C	1.24289600	-2.95199100	0.08436000
H	1.98515000	-3.62232300	0.53499200
H	1.47370700	-2.83583600	-0.98198700
C	1.55775100	2.48078700	-1.62859300
H	2.28932600	2.74458800	-0.85174100
H	1.62115700	3.23620300	-2.42714400
C	1.86156100	1.11517900	-2.22510100
H	2.83750600	1.12166400	-2.72220000
H	1.10557600	0.86196100	-2.97357400
C	-4.30910800	-0.66548400	0.10099200
H	-4.51689600	-1.50002200	0.78609500
H	-5.23827400	-0.43964800	-0.44070000
C	-2.55731900	2.52213300	2.04631100
H	-2.26922700	2.25960600	3.06930800
H	-3.14408800	3.44989500	2.09306300
O	1.29011300	-1.66705600	0.73525700
C	-3.83467500	0.49473700	0.85565500
C	-3.33050700	1.43200400	1.43210800
H	-1.83622800	4.55890300	0.47764300
H	-2.21270900	3.13522000	-0.52528600
H	-0.19644400	4.47419300	-1.27545400
H	0.61705400	4.02125300	0.24584800
H	-2.88201900	-2.35157900	-2.29610500
H	-4.30572000	-2.76234500	-1.31790500
H	-2.78275200	-3.28218300	0.63426400
H	-2.43264900	-4.28473100	-0.79259000
O	1.77804700	0.06009100	-1.25977800
C	2.79960300	-0.12442800	-0.34984200
C	2.53648500	-1.05026900	0.67837900
C	4.03936800	0.51842600	-0.38621700
C	3.49618000	-1.31835600	1.64870200
C	5.00011300	0.23729300	0.58990700
H	4.27346200	1.23306300	-1.16686100

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 C                  4.73461200   -0.67426400    1.60921700
 H                  3.25588300   -2.02789100    2.43520200
 H                  5.95947000    0.74372700    0.54642900
 H                  5.48026800   -0.88328300    2.36935800
 K                 -0.75309600    0.05274800   -0.03826200
Gas
HF=-1751.3861936
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 Sum of electronic and thermal Energies=            -1750.954746
 Sum of electronic and thermal Enthalpies=          -1750.953802
 Sum of electronic and thermal Free Energies=       -1751.036455
UFF
HF=-1751.4464455
Sum of electronic and zero-point Energies=          -1751.040960
 Sum of electronic and thermal Energies=            -1751.015531
 Sum of electronic and thermal Enthalpies=          -1751.014586
 Sum of electronic and thermal Free Energies=       -1751.098434
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"Misaligned"

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C                 -1.93924100    3.66047400    0.37707900
 C                 -3.10173800    2.81205600    0.85019200
 C                 -1.86682200   -3.51337300   -0.00647300
 C                 -0.48610900   -3.70304300    0.57862100
 O                 -3.09772400    1.61036800    0.08284400
 O                 -0.73040400    2.92316100    0.52392200
 O                  0.01239700   -2.45564200    1.06136000
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 C                  0.40362100    3.64949000    0.05855200
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 C                  1.64357000    2.79998600    0.21061800
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 H                 -5.13549700    1.42209000   -0.33567300
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 H                 -2.82605300   -2.28333000   -2.87889400
 H                 -3.67089400   -3.40305900   -1.79878900
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 C                 -4.05187600   -0.39002700   -0.56362900
 C                 -3.67466900   -1.36749500   -1.16901100
 H                 -2.30910000   -4.50068200   -0.20496600
 H                 -2.51145800   -2.98600500    0.71216800
 H                 -0.54613800   -4.42685200    1.40522500
 H                  0.18992200   -4.11060600   -0.18731300
 H                 -3.01037300    2.57845400    1.92154300
 H                 -4.03539700    3.37128500    0.69553200
 H                 -2.08695400    3.93179000   -0.67923900
 H                 -1.90134200    4.58811800    0.96811400
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O	1.77170400	-0.21596700	1.18920000
C	2.81744100	-0.13532900	0.29192000
C	2.68754800	0.87148000	-0.68377200
C	3.95267500	-0.94863500	0.28673000
C	3.66776400	1.04618100	-1.65385600
C	4.93702500	-0.76131100	-0.68944900
H	4.08779500	-1.72540600	1.03051300
C	4.79793700	0.22496700	-1.66301200
H	3.53063600	1.82681600	-2.39632700
H	5.81441800	-1.40074700	-0.68182400
H	5.56139900	0.36027600	-2.42218500
K	-0.72426600	0.08706300	-0.19213500

Gas
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Sum of electronic and thermal Enthalpies= -1750.954275
Sum of electronic and thermal Free Energies= -1751.037164

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Sum of electronic and thermal Enthalpies= -1751.015945
Sum of electronic and thermal Free Energies= -1751.099691

UFF
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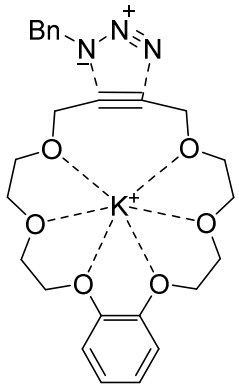

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C	-1.13451200	-3.37006300	-1.11113300
O	0.96034400	1.18124800	-0.86217900
O	-1.44273900	2.70029000	-0.68007600
O	-1.86976300	-2.19216600	-1.43854300
O	-0.08514900	-2.36450400	0.78715100
C	-2.42024400	3.49691500	-0.01761000
H	-2.55945700	4.45189100	-0.54601400
H	-2.10040600	3.71789800	1.01244500
C	-3.73582900	2.74759000	-0.01271300
H	-4.52129500	3.38601200	0.41082500

H	-4.01450200	2.46900300	-1.03550600
C	-3.19758200	-2.46251800	-1.87544600
H	-3.76290900	-2.95764500	-1.07222000
H	-3.19025800	-3.13244500	-2.74918900
C	-3.84693900	-1.14723200	-2.27747100
H	-4.85594700	-1.31766400	-2.66753500
H	-3.25386100	-0.67219500	-3.06357900
C	2.17895200	1.20431400	-0.10159800
H	2.23552400	2.12462000	0.49677700
H	3.03837500	1.19709500	-0.78738900
C	1.06021500	-2.22296200	1.63393400
H	0.67026400	-2.14830400	2.65391900
H	1.67539900	-3.13068500	1.58911300
O	-3.59017800	1.56087900	0.79230600
C	2.22103000	0.03236100	0.78422600
C	1.88814900	-1.03339100	1.33046300
H	0.78726500	-3.88650700	-0.32949400
H	0.74390800	-2.29586300	-1.12915600
H	-0.94018400	-3.95992400	-2.01941300
H	-1.70960200	-3.99157700	-0.40942600
H	0.23899400	2.07741900	-2.54149000
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H	0.24696600	3.61373400	0.11910200
H	-0.30465900	4.26774100	-1.44255900
O	-3.85816800	-0.19314500	-1.21015900
C	-4.84242600	-0.22840700	-0.24539200
C	-4.70120000	0.72320200	0.78553200
C	-5.92890000	-1.10524100	-0.22043800
C	-5.63122500	0.78907500	1.81655000
C	-6.86187700	-1.02721200	0.81901400
H	-6.06344300	-1.84926500	-0.99737800
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H	-7.70255600	-1.71426800	0.82462400
H	-7.44203100	-0.03690400	2.64460400
K	-1.35461700	0.03886000	0.12113000
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C	5.31621700	1.21504000	1.47407100
H	5.04997500	2.24838000	1.23696400
H	5.97101600	1.24693400	2.35202800
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C	6.58472000	-0.70731000	0.41240800
C	6.07950600	1.22803400	-0.93785500
C	7.21762600	-1.30199600	-0.67769500
H	6.54696900	-1.23234500	1.36408000
C	6.71621100	0.63527900	-2.03101000
H	5.65466900	2.22526200	-1.03671600
C	7.28377500	-0.63219100	-1.90273700
H	7.66814700	-2.28461300	-0.56978000
H	6.77437500	1.16663700	-2.97687100
H	7.78341900	-1.09421200	-2.74938600

Gas
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 Sum of electronic and thermal Free Energies=      -2186.101958
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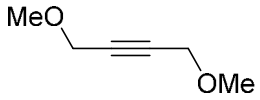


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 H                 2.12728800    0.10419300    1.53070700
 C                -2.00577200    0.44400500   -0.48678200
 H                -2.12719700    0.10397800   -1.53070900
 H                -2.39114500    1.47865800   -0.44677500
 C                 0.58929600    0.42943300    0.13276000
 C                -0.58931000    0.42951800   -0.13273900
 H                -4.29513700   -0.79442900   -0.94506200
 H                -4.56801200    0.59669200    0.14239900
 H                 4.60439300   -1.06722900   -0.79324500
 H                 4.29517000   -0.79398400    0.94522400
 H                 4.56805200    0.59666700   -0.14283800
 H                -4.60443600   -1.06692000    0.79351600
Gas
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 Sum of electronic and thermal Enthalpies=          -384.830607
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 Sum of electronic and thermal Enthalpies=          -384.840596
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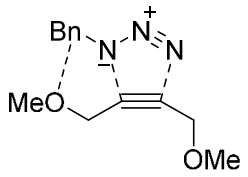

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O	4.29081200	-0.64978000	0.72826200
C	1.42628600	2.14366400	-0.27949000
H	2.25315100	2.54619500	0.33019100
H	1.50670500	2.59840400	-1.28058000
C	3.25579100	-1.33872400	0.04280100
H	3.65016700	-1.82681700	-0.86432100
H	2.83894700	-2.14214300	0.67277800
C	1.59537900	0.68874200	-0.37270300
C	2.18697900	-0.39726300	-0.31967200
H	5.81278000	-1.98935700	0.21965000
H	4.99750900	-2.31505700	1.77494400
H	-0.92356400	4.06590500	0.94827100
H	0.12556700	4.43967100	-0.44939900
N	0.88960800	-1.83098500	-1.28349200
N	-0.26363200	0.12271600	-1.49906900
N	0.00675500	-1.10554200	-1.53648000
C	-1.67466400	0.55073600	-1.47684400
H	-1.61319200	1.62975600	-1.32220600
H	-2.12129500	0.38082800	-2.46522800
H	0.83521800	4.27481300	1.18175100
H	6.08976700	-0.91004200	1.61624900
C	-2.52055800	-0.09729300	-0.39809500
C	-3.58194900	-0.94082100	-0.74137400
C	-2.24533000	0.13496900	0.95736700
C	-4.36288100	-1.54269700	0.24820200
H	-3.80017000	-1.12874100	-1.79067400
C	-3.02235100	-0.46807800	1.94514200
H	-1.41791300	0.78614000	1.22555500
C	-4.08368400	-1.30746800	1.59417900
H	-5.18504800	-2.19524200	-0.03400500
H	-2.80121700	-0.28185700	2.99310700
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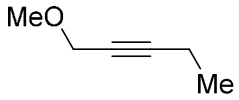


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 H                  2.78446300   -1.32106100   -0.87746900
 C                 -1.32225200    0.61570100   -0.00002300
 H                 -1.50088300    1.25293800   -0.88493700
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 C                  0.05842400    0.13753500   -0.00006300
 H                 -3.80842400    0.54423800   -0.89307900
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 C                  3.60113300    0.48739600    0.00003800
 H                  3.46465600    1.11611000   -0.88554600
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 Sum of electronic and thermal Enthalpies=           -309.643405
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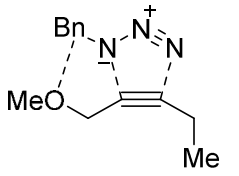


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 H                  2.22825700    2.02933300   -1.34941200
 C                  3.40361200   -1.88507600    0.57936900
 H                  3.73508800   -2.55323000   -0.22536900
 H                  2.85012700   -2.52486000    1.27826600
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C	2.03590700	0.25825300	-0.20669600
C	2.47219300	-0.88005700	0.02257000
H	-0.10588000	4.05237900	0.51161000
H	1.05060300	4.10997300	-0.84965900
N	1.04898500	-2.21468300	-0.83851100
N	0.16883100	-0.19094400	-1.38467200
N	0.27221000	-1.43977200	-1.25123400
C	-1.16610700	0.40743500	-1.55462300
H	-0.97107600	1.48202300	-1.53935300
H	-1.55673200	0.15617300	-2.54962400
C	-2.17577700	0.03459900	-0.48578800
C	-3.34068400	-0.66174700	-0.82320600
C	-1.95296500	0.37990900	0.85509700
C	-4.27419900	-1.00705400	0.15706100
H	-3.51967800	-0.93717000	-1.86055600
C	-2.88241700	0.03254900	1.83408700
H	-1.04624100	0.91707200	1.11912900
C	-4.04604400	-0.66093200	1.48853600
H	-5.17496000	-1.54830800	-0.12076000
H	-2.70042200	0.30470000	2.87077800
H	-4.76913300	-0.93000700	2.25415400
H	1.65105900	4.08820200	0.83250200
C	4.61635700	-1.25784000	1.28318400
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H	4.30049200	-0.62040000	2.11593800
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Gas
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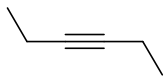

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H	2.08286200	1.43353400	0.71790000
C	-1.95432400	-0.68427000	-0.07569600
H	-2.16539900	-1.20758400	-1.01882600

H	-2.08308200	-1.43343600	0.71808300
C	2.98052700	-0.44742400	0.12020000
H	2.90022600	-1.18899300	-0.68109700
H	3.99943200	-0.04442300	0.11664000
H	2.81634200	-0.96154300	1.07265300
C	-2.98038100	0.44764000	0.12018200
H	-2.89995700	1.18908700	-0.68121500
H	-3.99938100	0.04487700	0.11674000
H	-2.81600900	0.96184100	1.07255800

Gas
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Sum of electronic and thermal Enthalpies= -234.454238
Sum of electronic and thermal Free Energies= -234.495607
UFF
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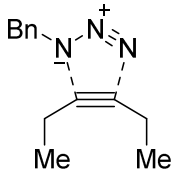
Sum of electronic and thermal Energies= -234.457895
Sum of electronic and thermal Enthalpies= -234.456951
Sum of electronic and thermal Free Energies= -234.498351



C	1.75303600	1.97868600	-0.30254200
H	1.65501200	2.28917100	-1.35051800
H	0.80909500	2.25585900	0.18462500
C	3.45958300	-1.54217400	0.48585600
H	3.80533100	-2.17315600	-0.34258500
H	2.98408700	-2.23112500	1.19543100
C	1.93654700	0.51625700	-0.24135400
C	2.43663000	-0.59936800	-0.02380700
N	1.09755100	-2.02220100	-0.82263700
N	0.04440600	-0.08621900	-1.35087400
N	0.24012500	-1.32940700	-1.22728600
C	-1.30674400	0.41282700	-1.59676800
H	-1.17368800	1.49069300	-1.75283200
H	-1.69562100	0.01473800	-2.54397600
C	-2.31387900	0.17558200	-0.48053200
C	-3.67897700	0.10947800	-0.78360800
C	-1.91100900	0.05837600	0.85469100
C	-4.62608400	-0.06098000	0.22669500
H	-4.00406100	0.18784600	-1.81932300
C	-2.85703100	-0.11585500	1.86601200
H	-0.85269400	0.09063000	1.09788800
C	-4.21699200	-0.17381700	1.55656800
H	-5.68183000	-0.11430400	-0.02635100
H	-2.52925200	-0.20983900	2.89813300
H	-4.95214500	-0.31223900	2.34483700
C	4.65477800	-0.84264800	1.14924400
H	5.16361400	-0.17902000	0.44206700
H	4.33304000	-0.24007600	2.00539600
H	5.38098000	-1.58209000	1.50610600

C	2.91432800	2.74367900	0.35633500
H	3.01146500	2.47622900	1.41362400
H	3.86424600	2.51710300	-0.13864800
H	2.74272300	3.82410200	0.29096100

Gas

Frequencies -- -362.0755

HF=-669.7184363

Sum of electronic and zero-point Energies= -669.442319

Sum of electronic and thermal Energies= -669.425494

Sum of electronic and thermal Enthalpies= -669.424550

Sum of electronic and thermal Free Energies= -669.489966

UFF

HF=-669.7243321

Sum of electronic and zero-point Energies= -669.448543

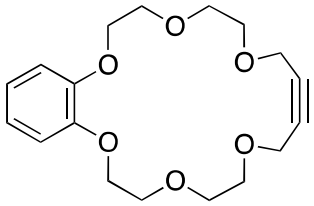
Sum of electronic and thermal Energies= -669.431654

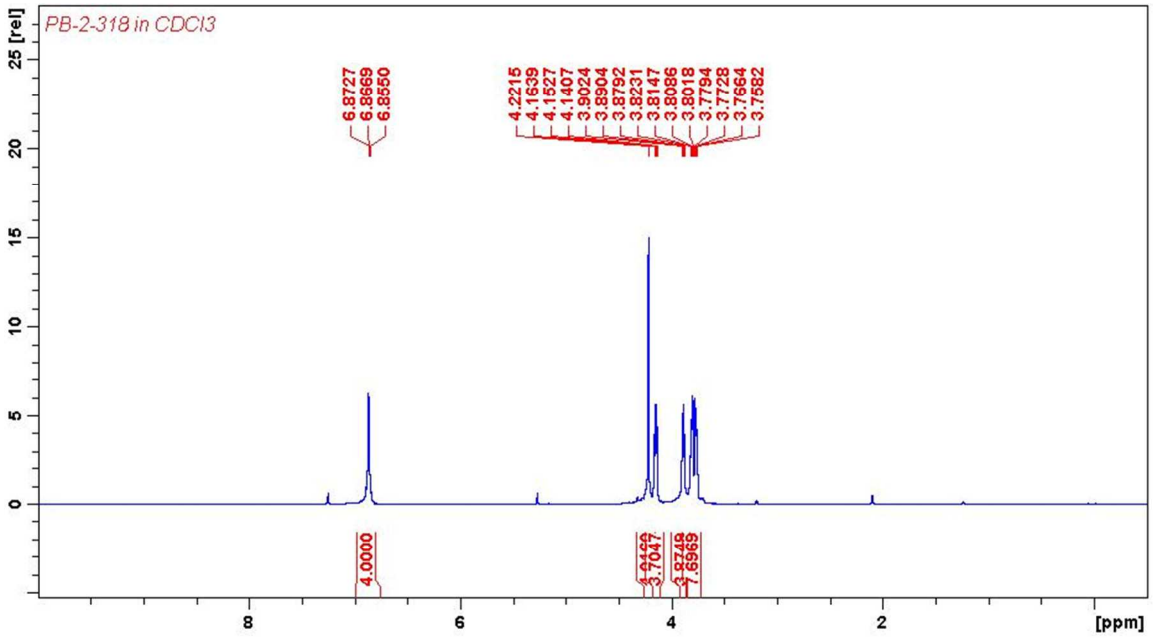
Sum of electronic and thermal Enthalpies= -669.430710

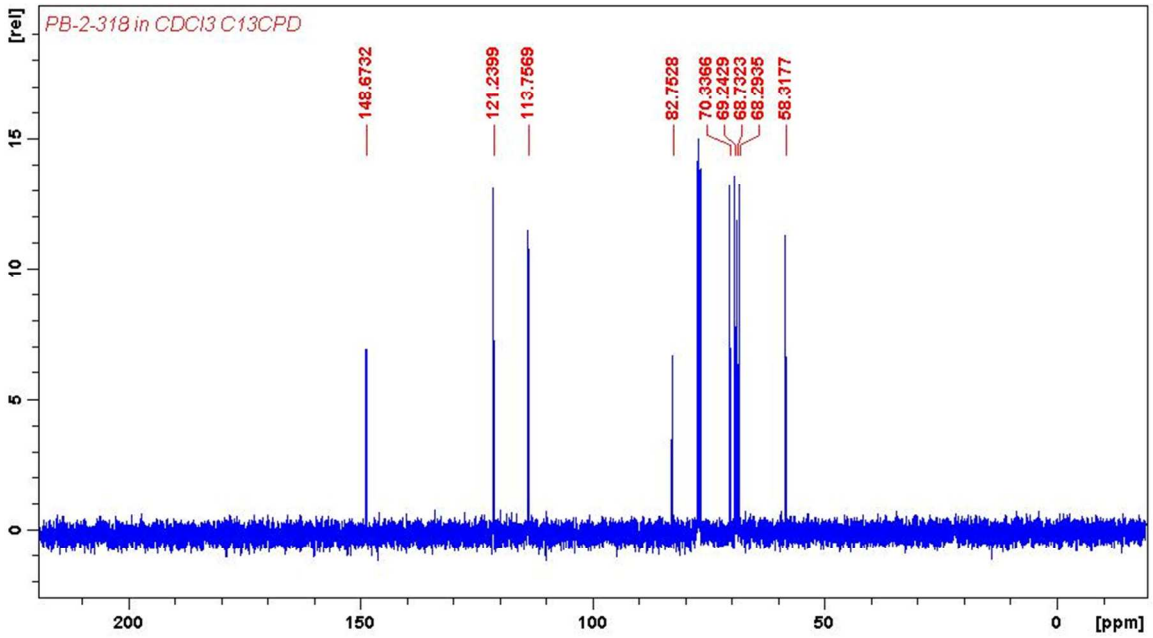
Sum of electronic and thermal Free Energies= -669.496736

NMR Spectra

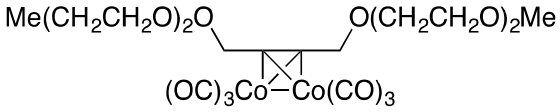
^{1}H and ^{13}C NMR Spectra of **1**

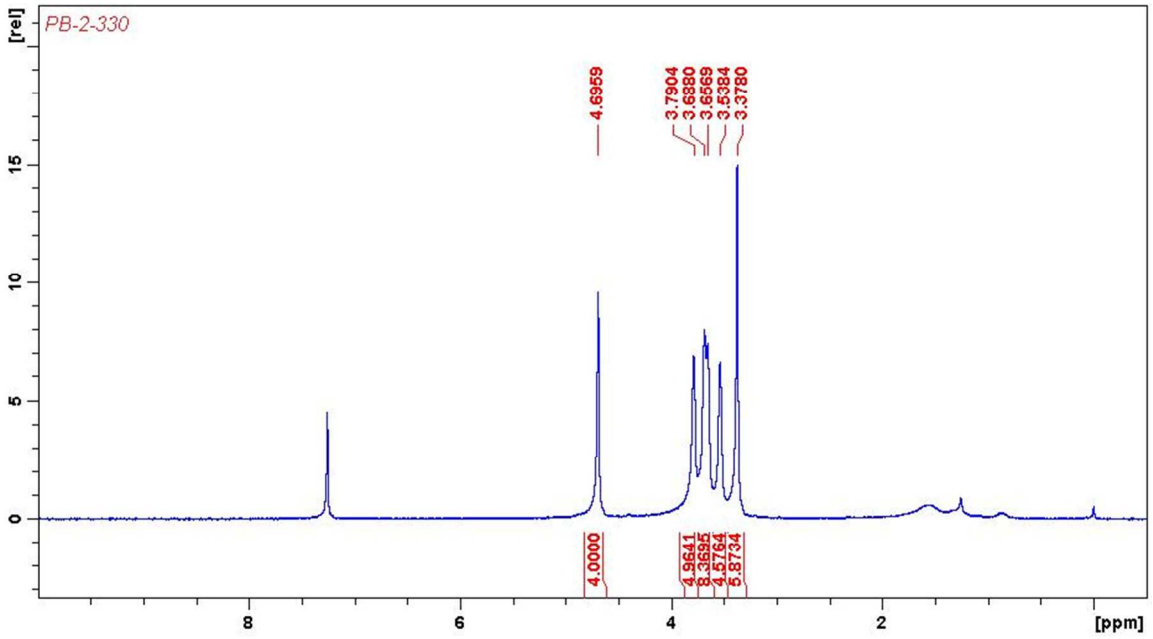


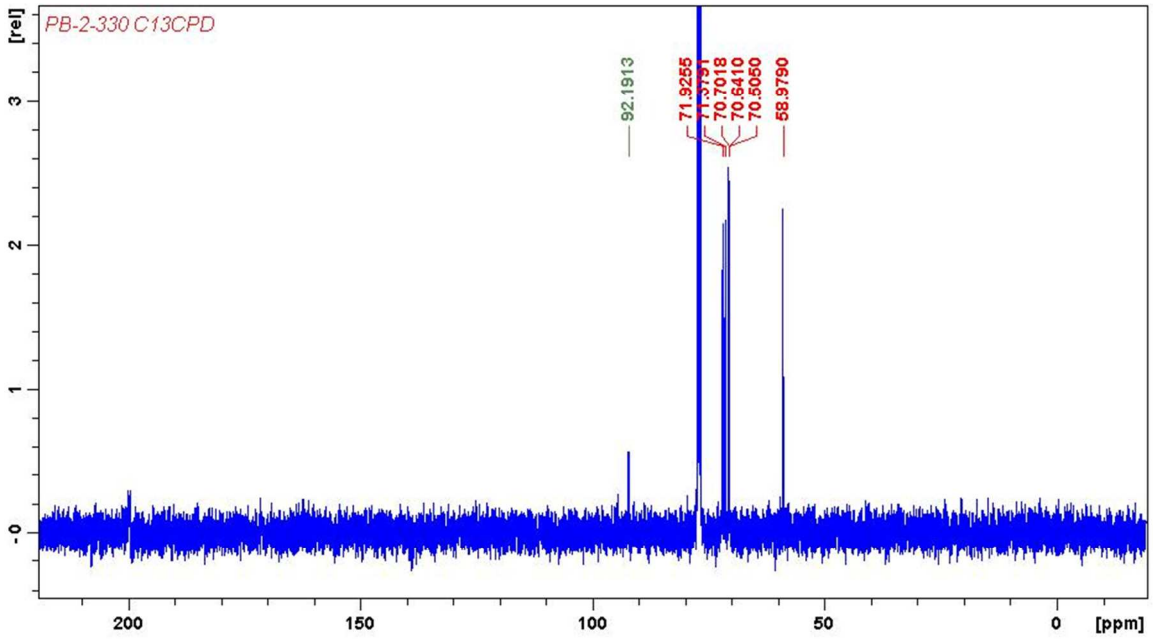




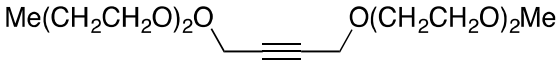
^{1}H and ^{13}C NMR Spectra of **C**

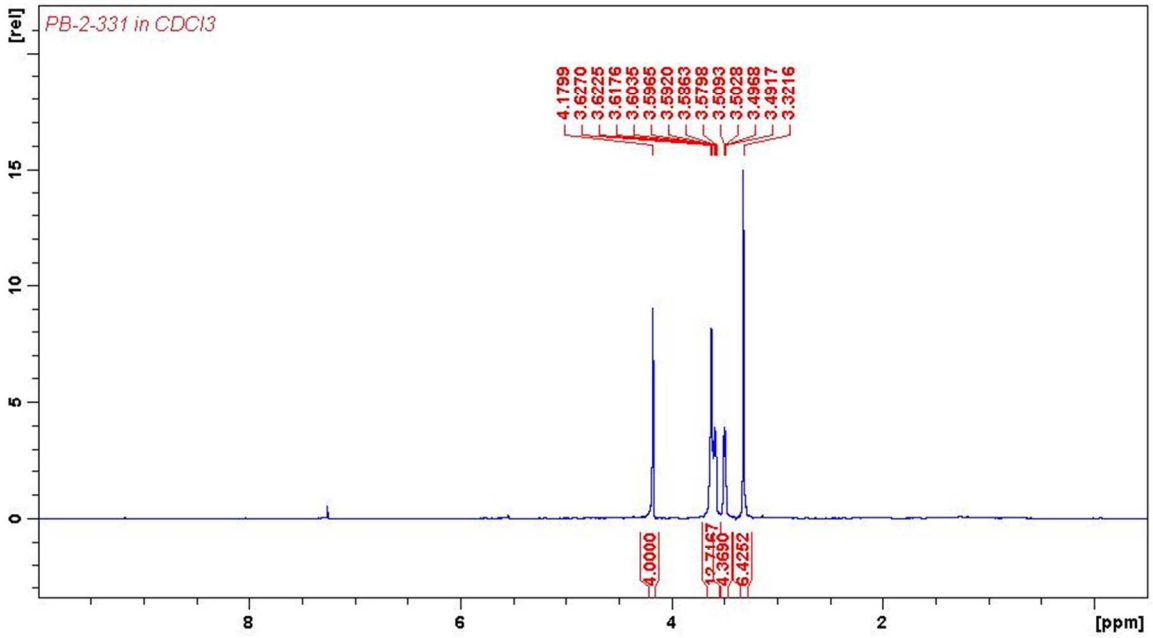


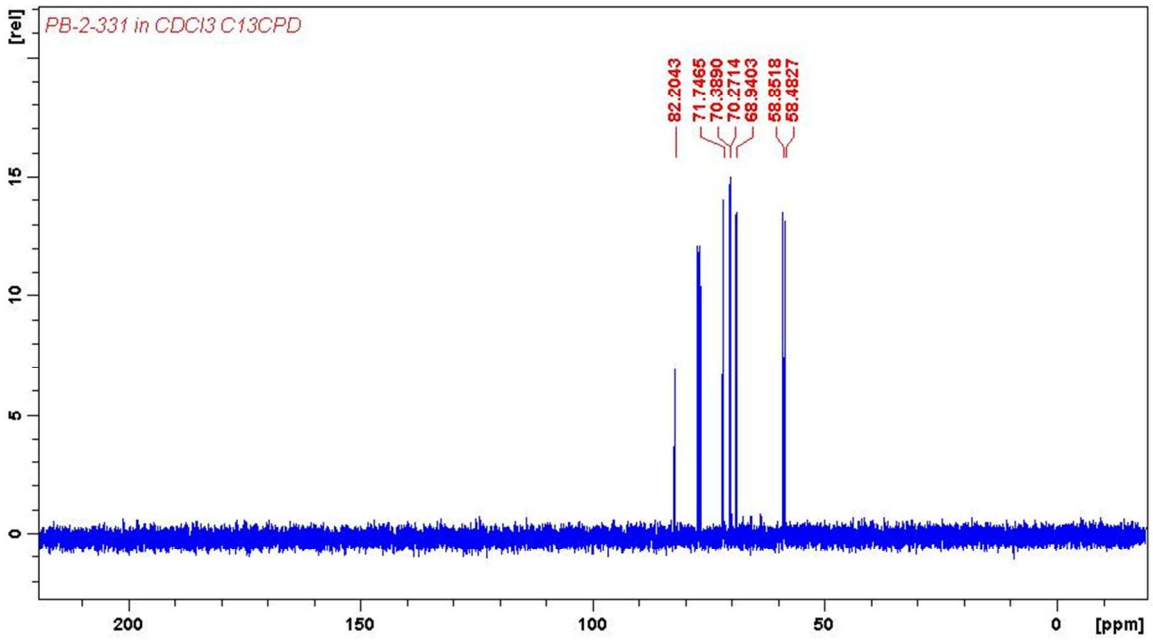




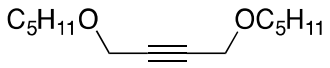
^{1}H and ^{13}C NMR Spectra of **5**

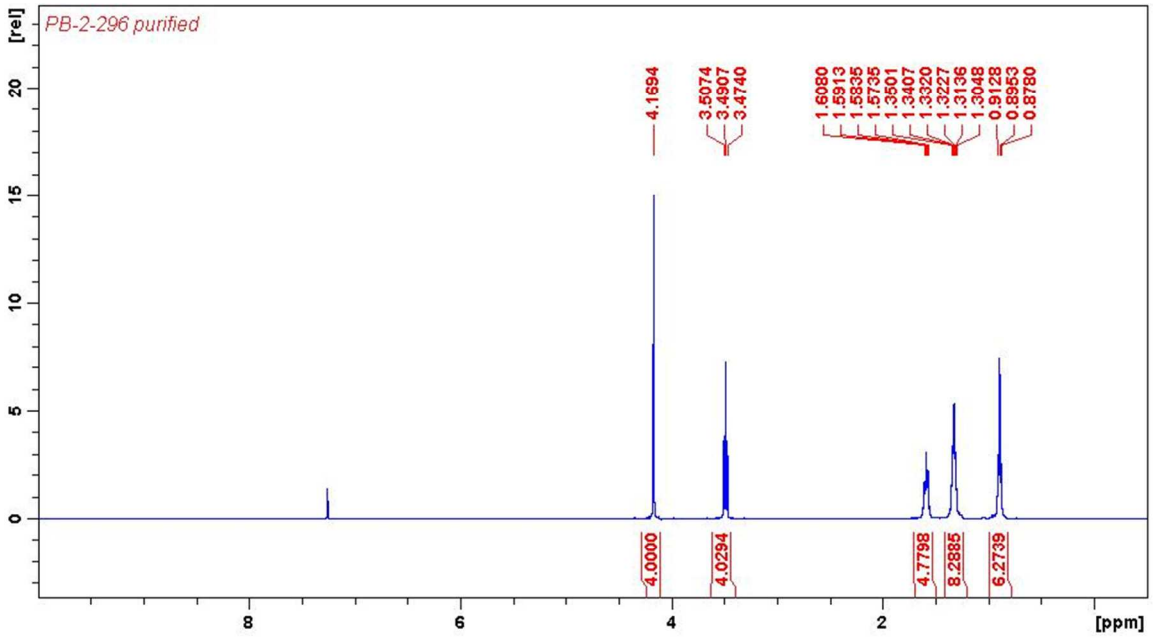


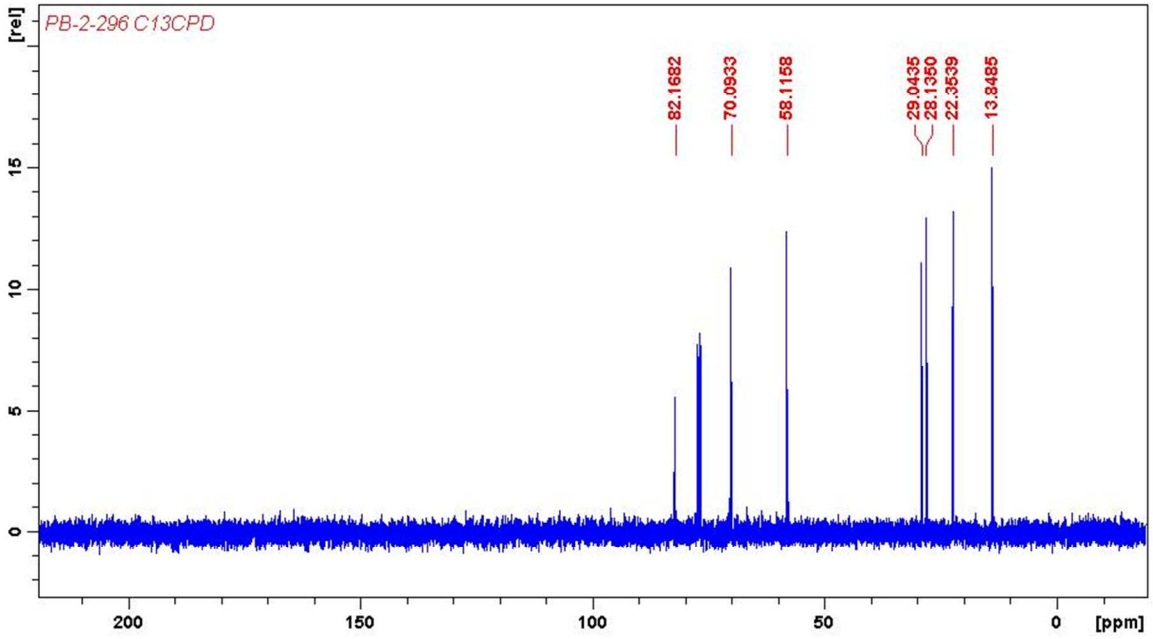




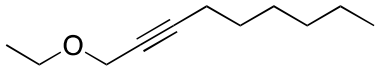
^{1}H and ^{13}C NMR Spectra of **6**

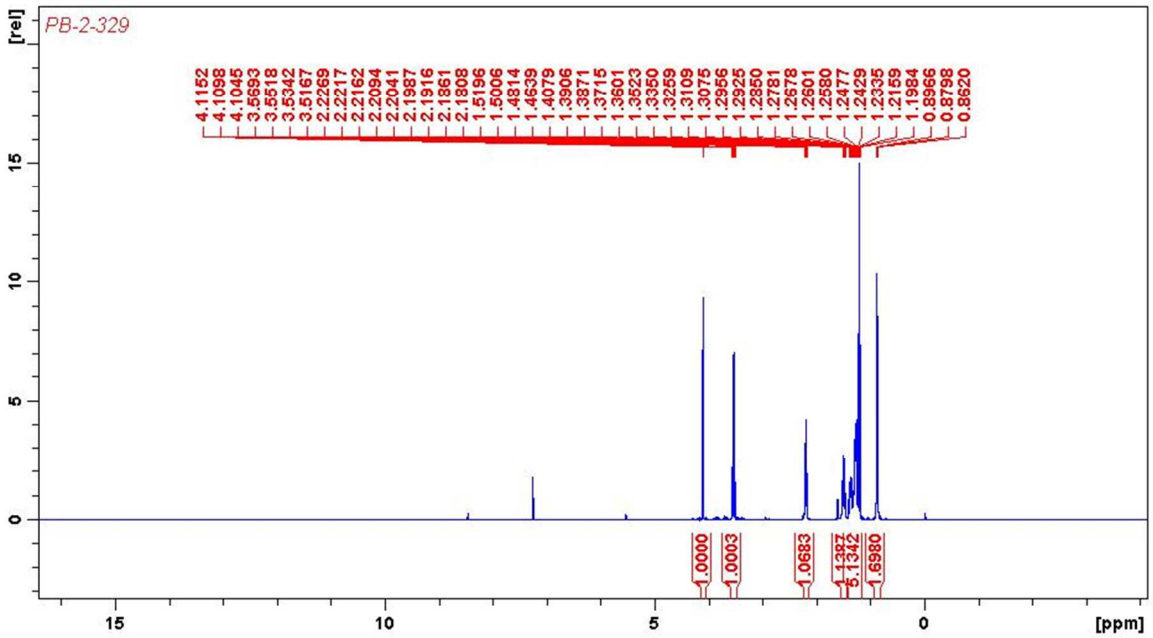


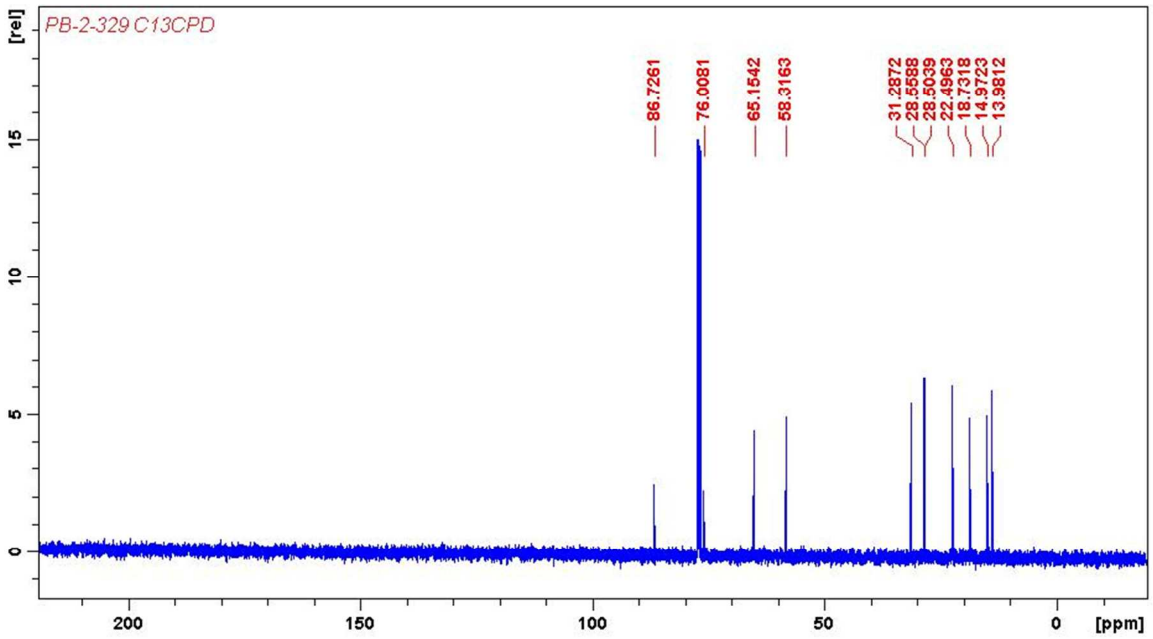




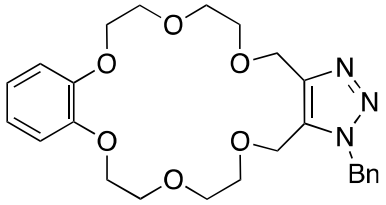
^{1}H and ^{13}C NMR Spectra of **7**

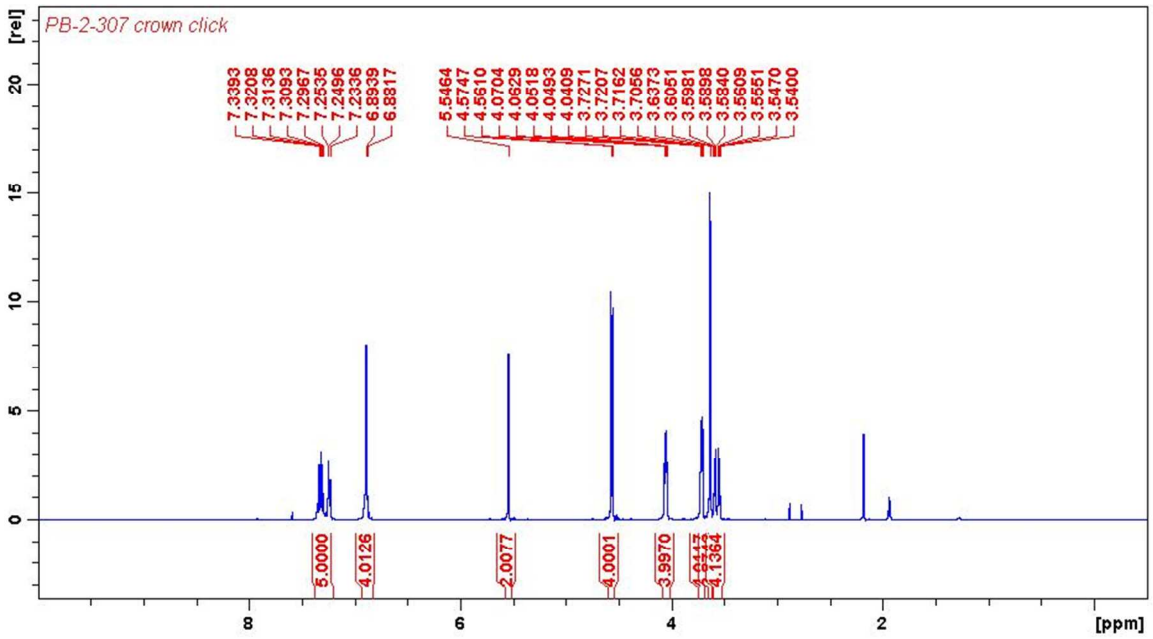


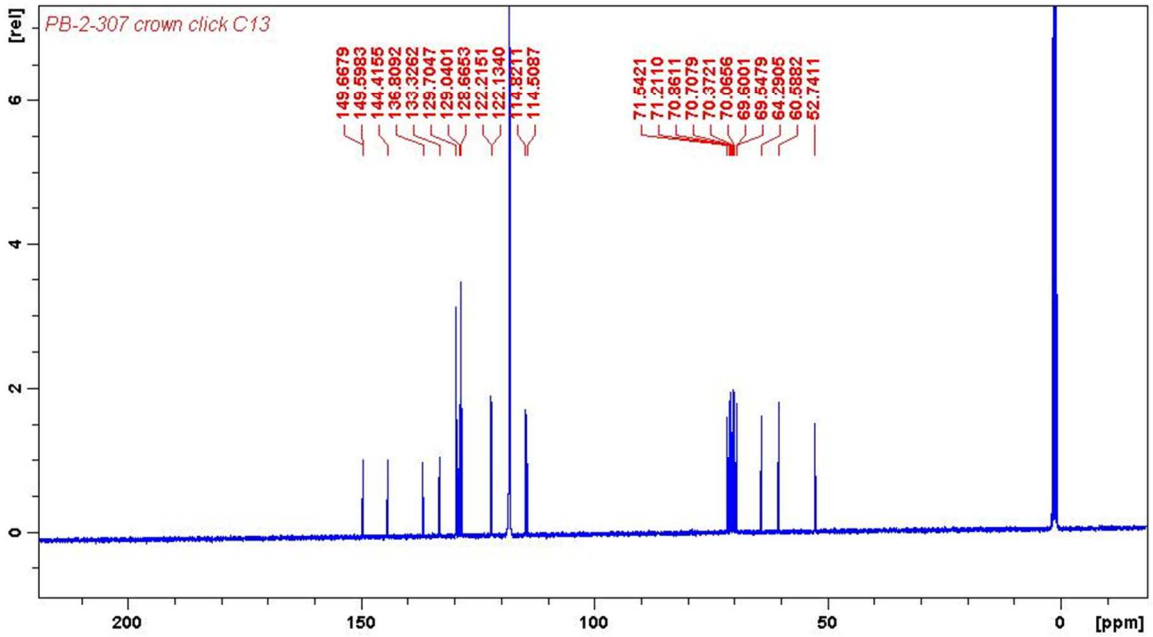




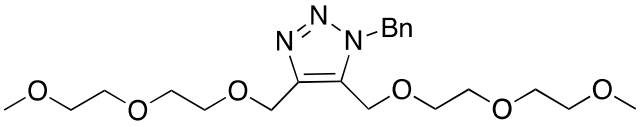
^{1}H and ^{13}C NMR Spectra of **1a**

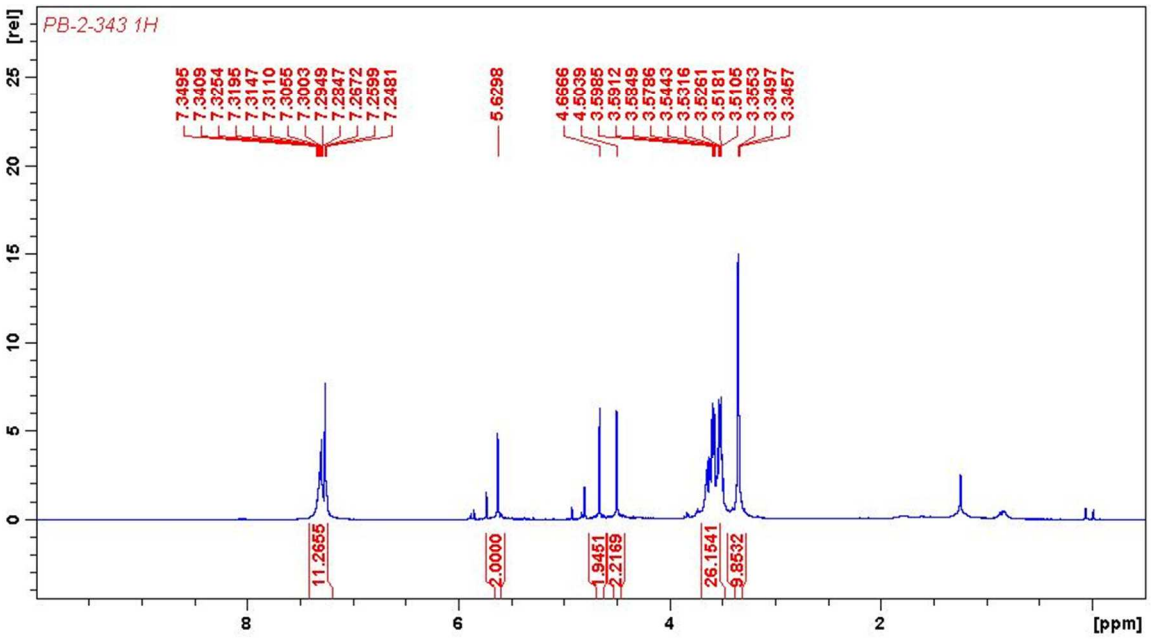


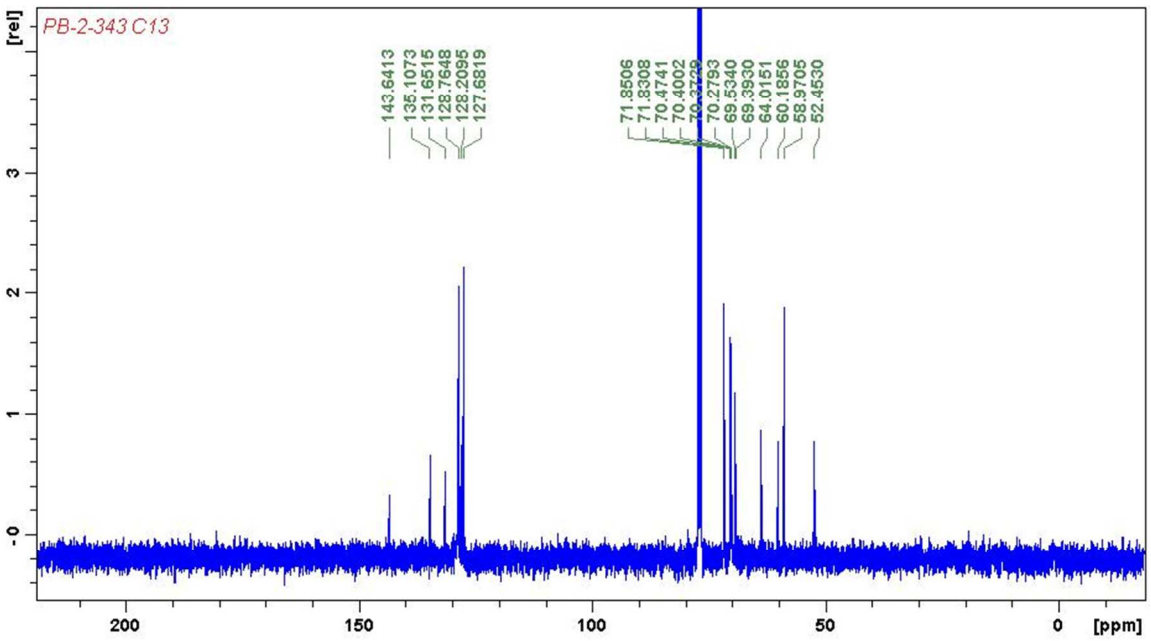




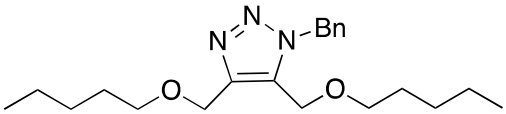
^{1}H and ^{13}C NMR Spectra of **5a**

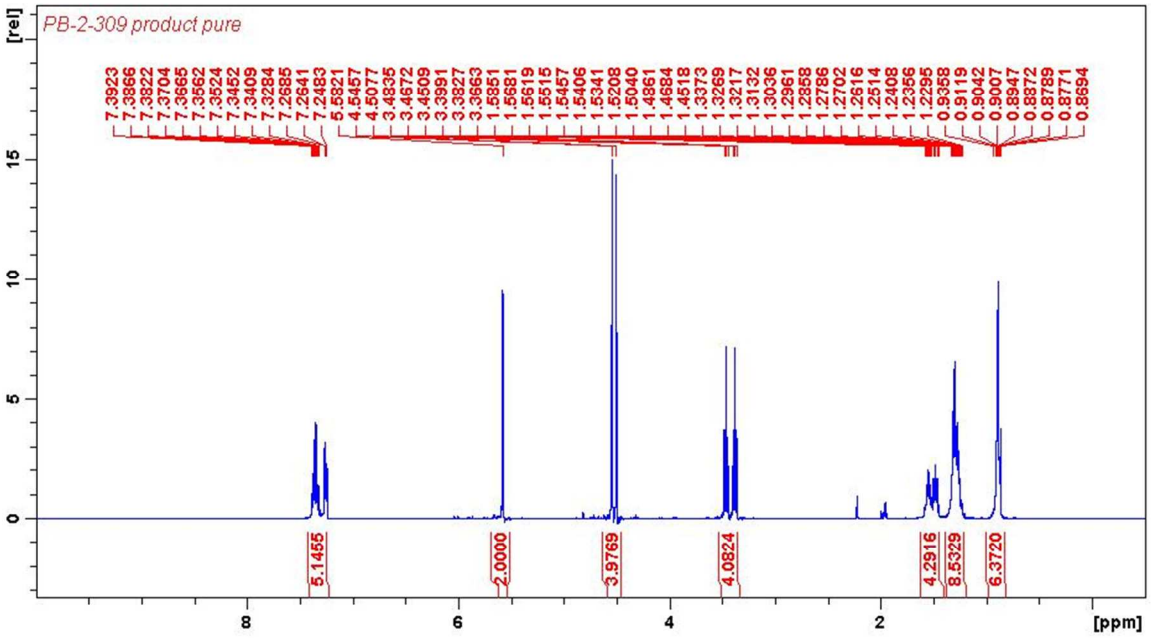


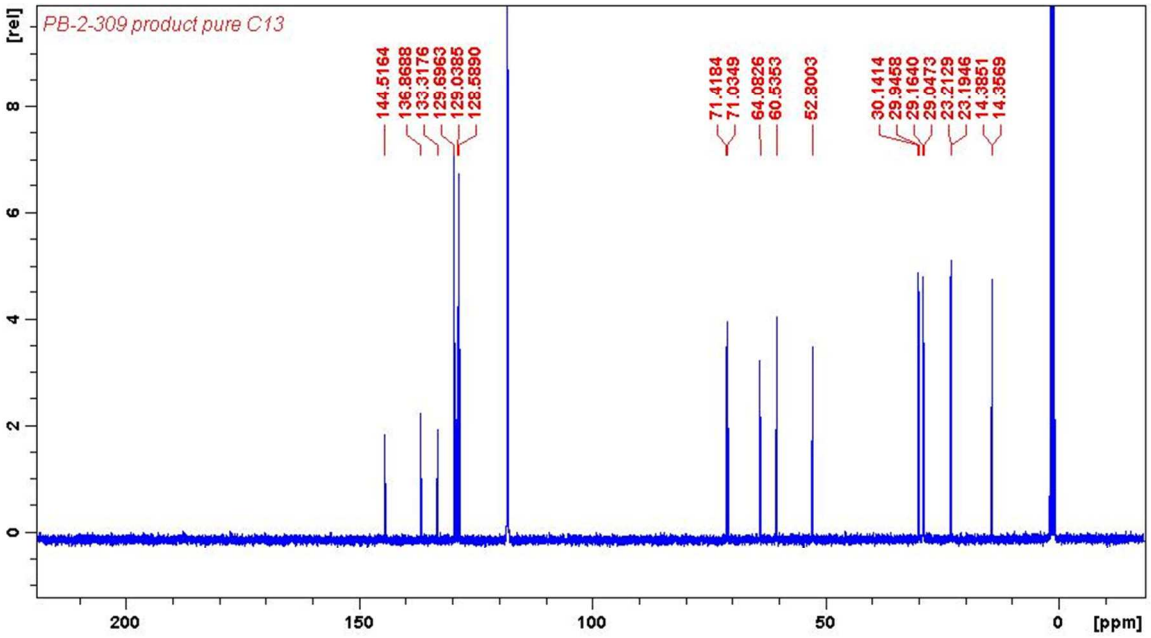




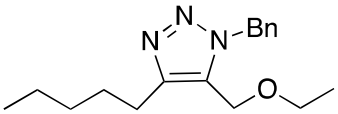
^{1}H and ^{13}C NMR Spectra of **6a**

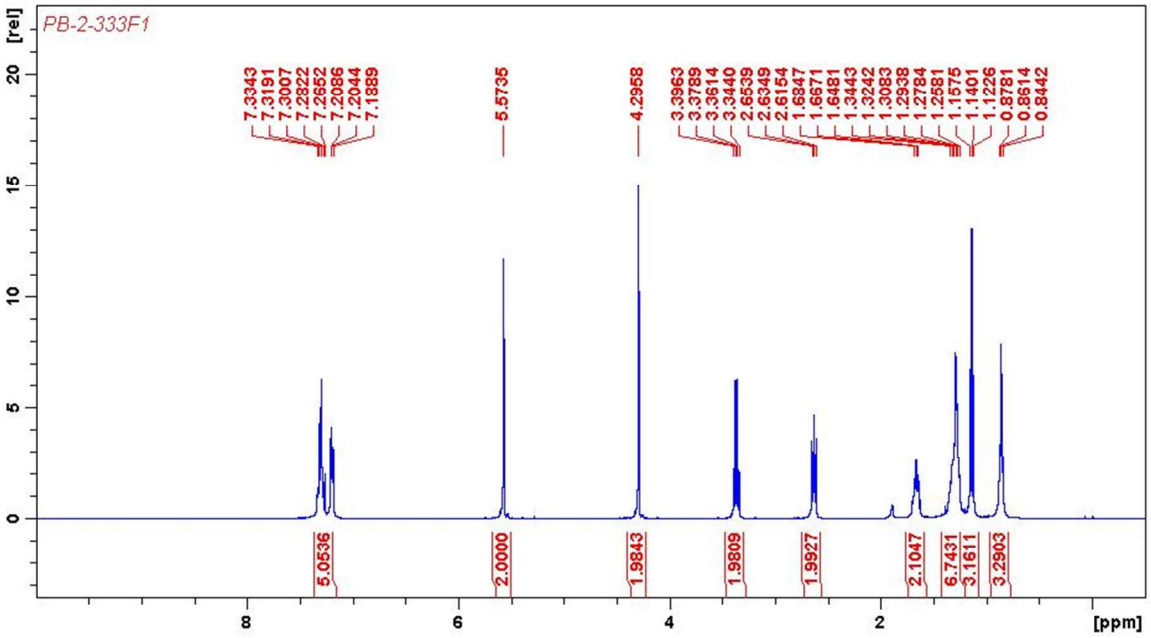


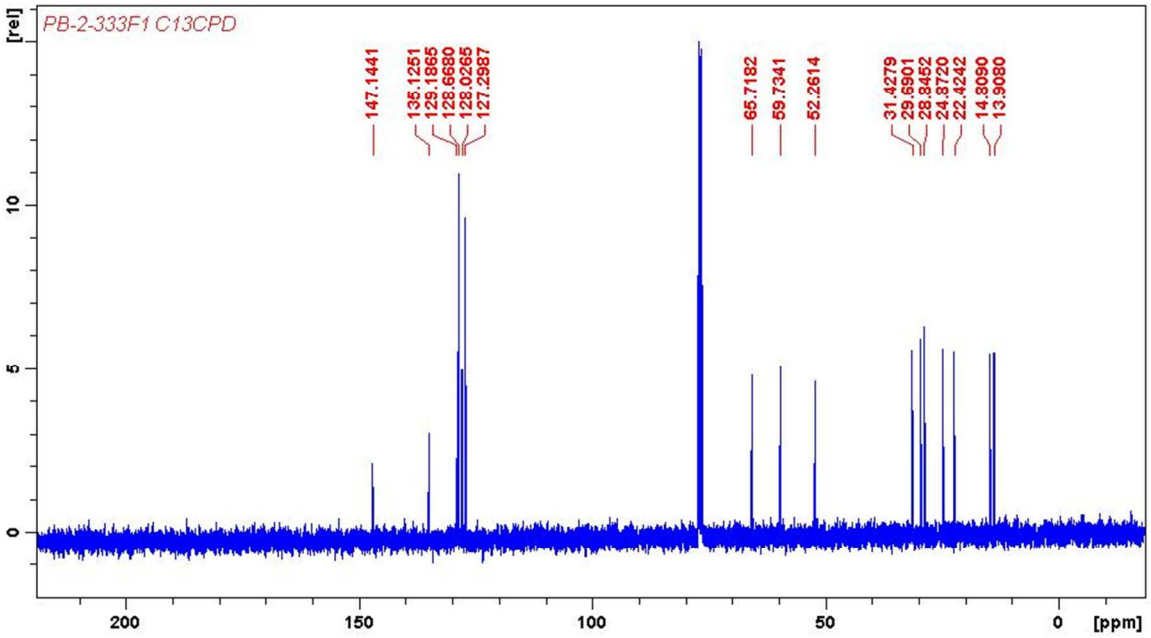


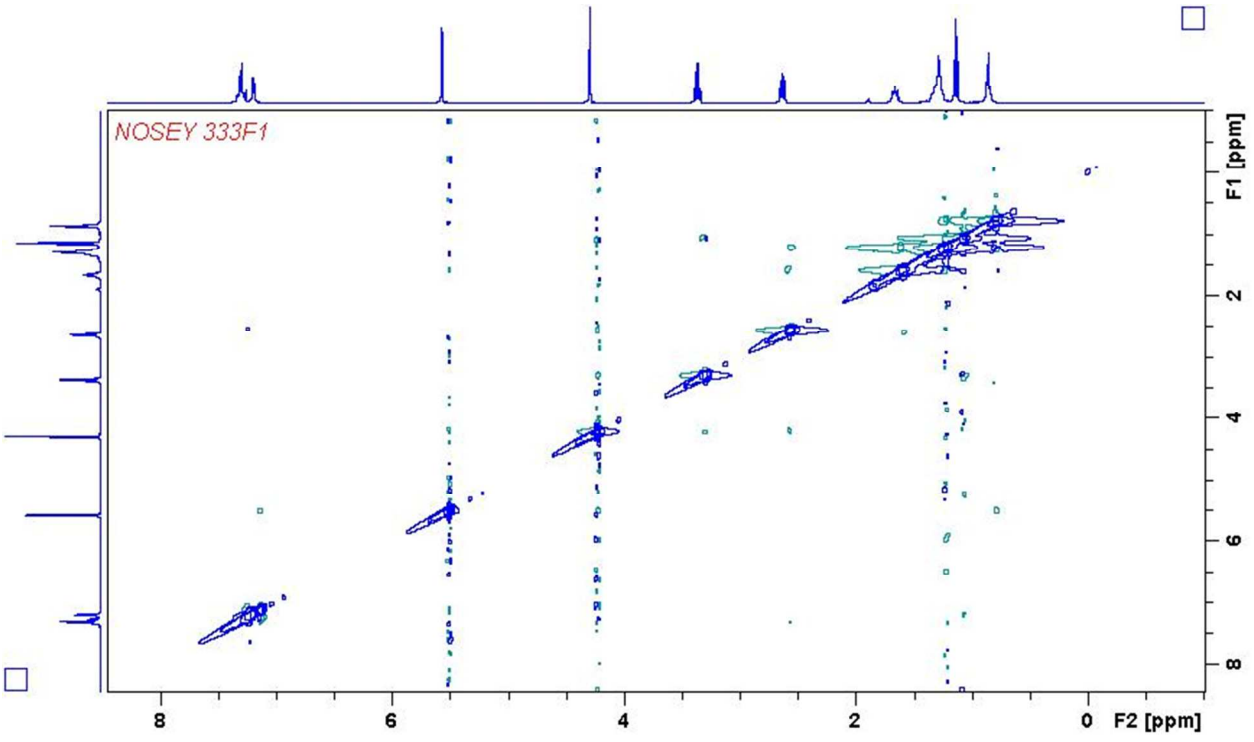


^{1}H and ^{13}C NMR Spectra of **7a1**

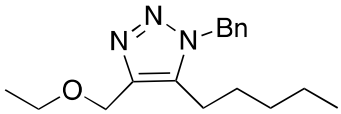


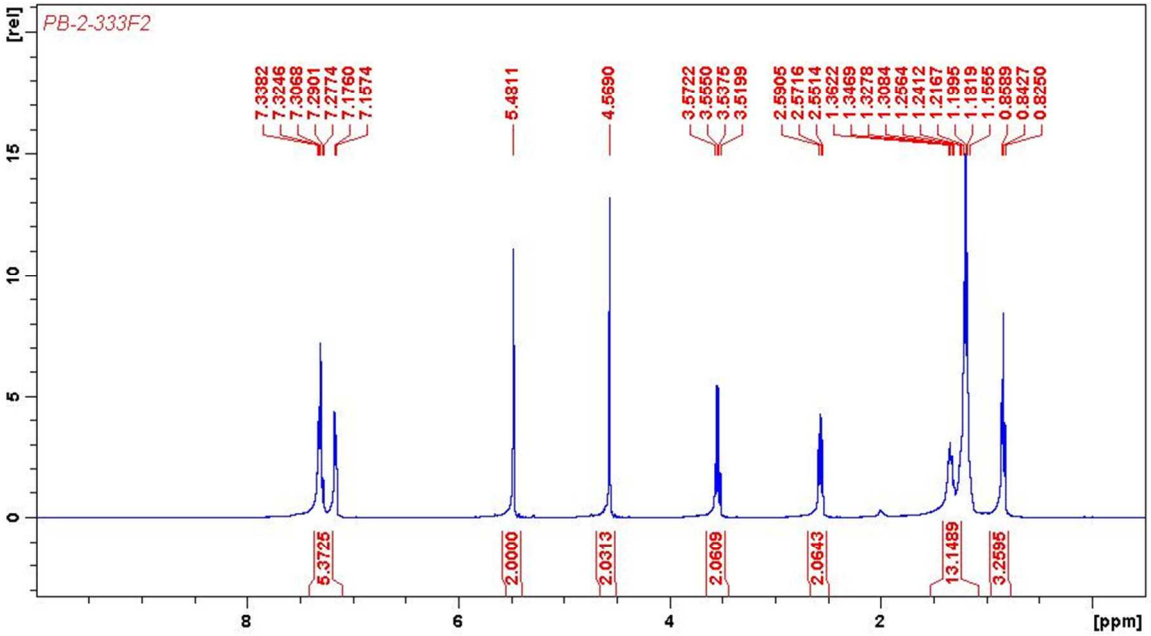


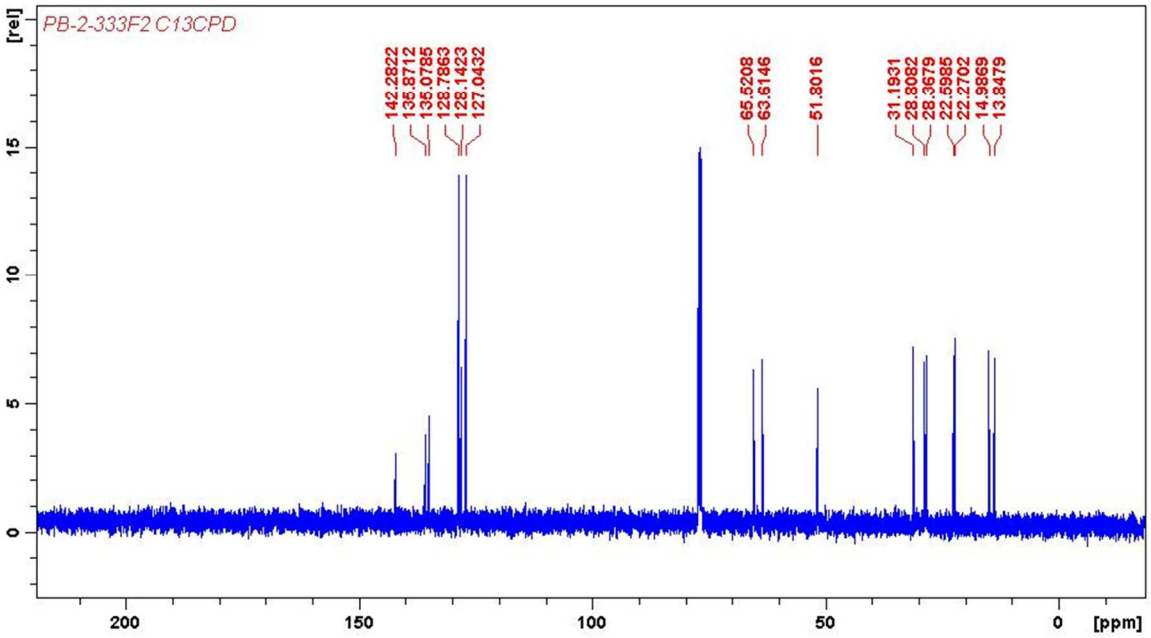


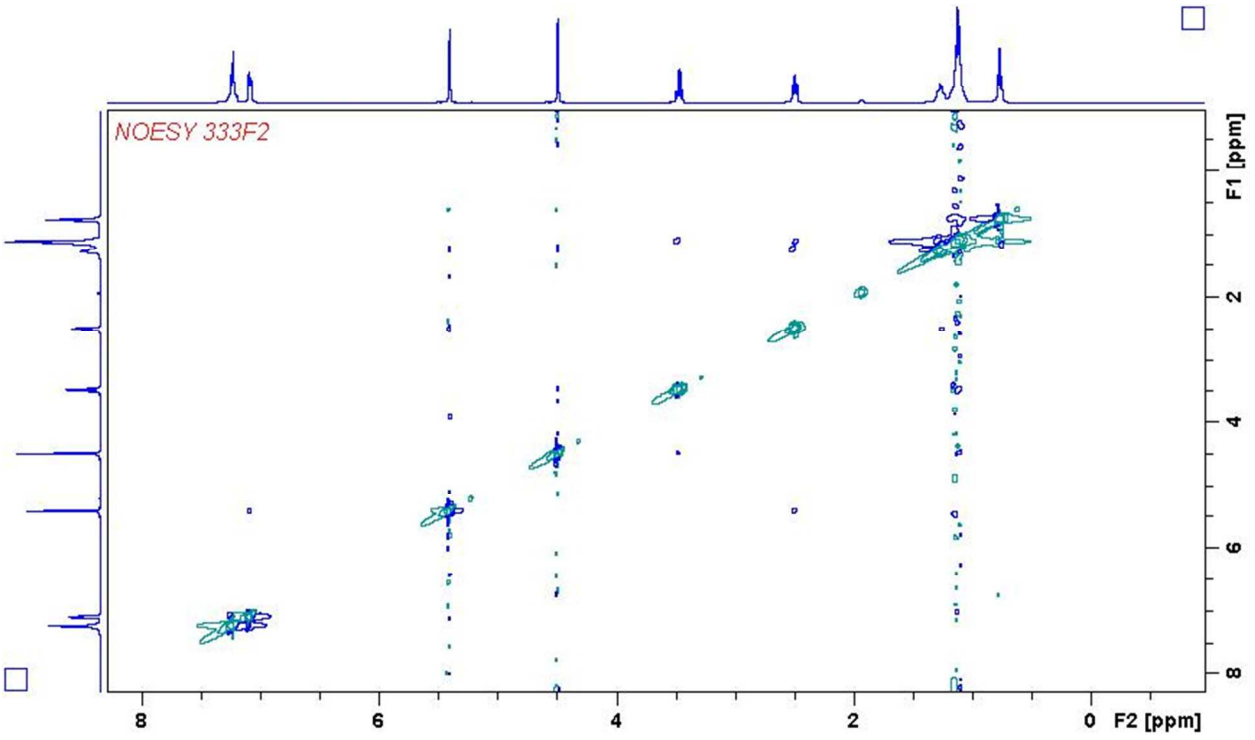

NOSEY 333F1
F1 [ppm]
F2 [ppm]
8
6
4
2
0
2
4
6
8

^{1}H and ^{13}C NMR Spectra of **7a2**








NOESY 333F2
F1 [ppm]
F2 [ppm]
8
6
4
2
0
2
4
6
8

^{1}H and ^{13}C NMR Spectra of **8a**