

Electronic Supplementary Information

Designing High Voltage Carbonyl-Containing Polycyclic Aromatic Hydrocarbon Cathode Materials Guided by Clar's Theory

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(A) Chemical structures of PYT, 9,10-anthraquinone and PTCDA

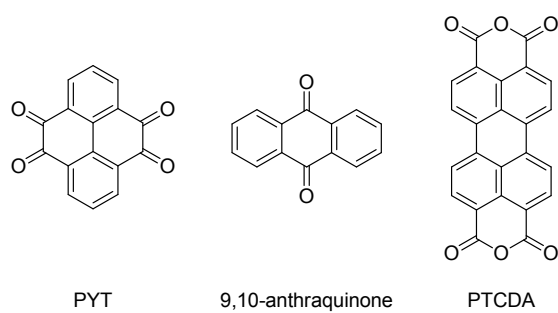
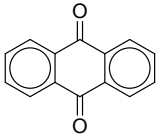
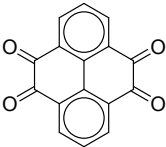
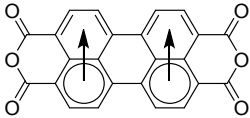
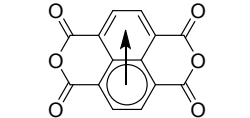
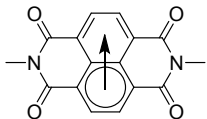
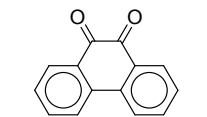
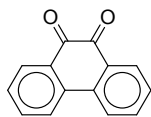


Fig. S1 Three polycyclic aromatic molecules experimentally investigated as cathode materials for Li-ion batteries.

(B) ΔC_{2Li} versus Experimental voltage

Table S1. Some C-cPAHs, their experimental voltage, and their ΔC_{2Li} value. More detail shown in Fig. S2.

Molecule	ΔC_{2Li}	Experimental Voltage (V)
	-1	2.2
	0	2.8
	0	2.3-2.4
	-2	0.9-1.3
	0	2.4
	0	2.5
	0	2.61

(C) Details about the calculations reported in Table S1

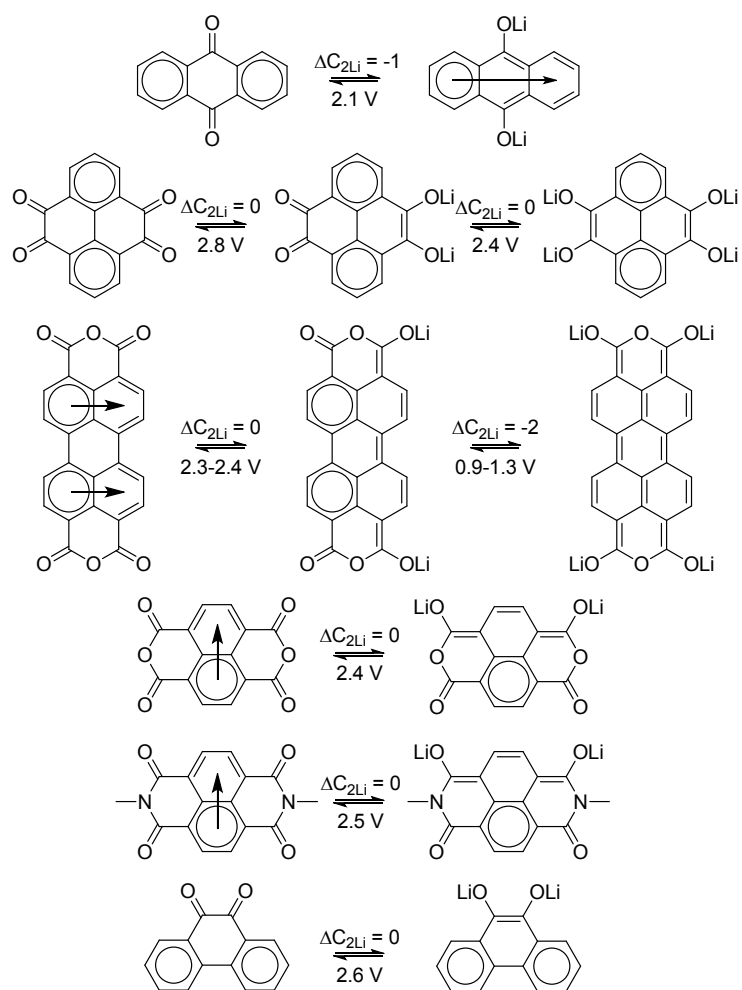
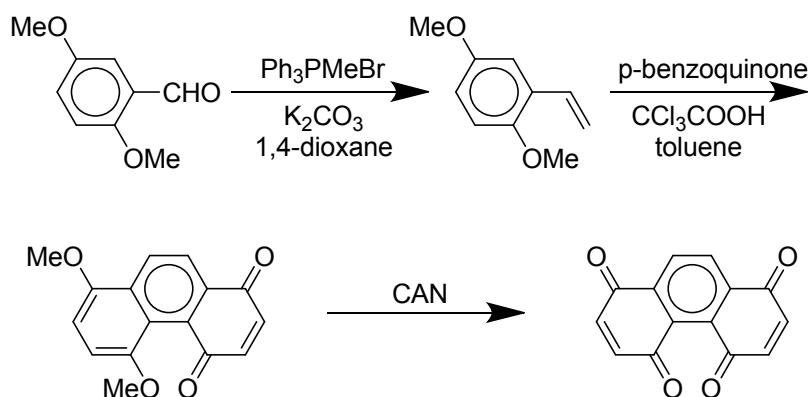


Fig. S2 Lithiation reactions of several experimentally investigated molecules.

(D) Preparation of 1,4,5,8-phenanthrenediquinone

1. Preparation of 1,4,5,8-phenanthrenediquinone: Outline.



2. Preparation of 1,4-dimethoxy-2-vinylbenzene

2,5-dimethoxybenzaldehyde (TCI, 10 mmol), K_2CO_3 (16 mmol) and methyltriphenylphosphonium bromide (12 mmol) were added to anhydrous 1,4-dioxane (10 mL), and then heated at reflux for 15 h. The mixture was purified by column chromatography (200-300 mesh silica gel, 10:1 petroleum ether/ethyl acetate) to provide 1,4-dimethoxy-2-vinylbenzene. Yield: 75%, colorless oil, ^1H NMR (400 MHz, CDCl_3) δ 7.08 – 6.98 (m, 2H), 6.85 – 6.75 (m, 2H), 5.72 (d, J = 17.7 Hz, 1H), 5.27 (d, J = 11.1 Hz, 1H), 3.81 (s, 3H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 131.5, 114.7, 113.8, 112.2, 111.9, 56.2, 55.7.

3. Preparation of 5,8-dimethoxy-1,4-phenanthrenequinone

1,4-dimethoxy-2-vinylbenzene (6 mmol) and excessive p-benzoquinone (30 mmol) were dissolved in 60 mL toluene, and 60 mg trichloroacetic acid was added as a catalyst. The solution was heated in oil bath for 20 h, and the progress was monitored with thin-layer chromatography. Solvent was then removed by rotary evaporation. The obtained solid was sublimed and then purified by column chromatography. Yield: 30%, brownish red solid, ^1H NMR (400 MHz, CDCl_3) δ 8.50 (d, J = 8.7 Hz, 1H), 8.06 (d, J = 8.7 Hz, 1H), 7.07 (d, J = 10.2 Hz, 1H), 6.95 (dd, J = 25.2, 8.5 Hz, 2H), 6.82 (d, J = 10.2 Hz, 1H), 3.98 (s, 3H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 140.7, 134.8, 127.4, 121.3, 109.3, 107.5, 56.2, 56.0.

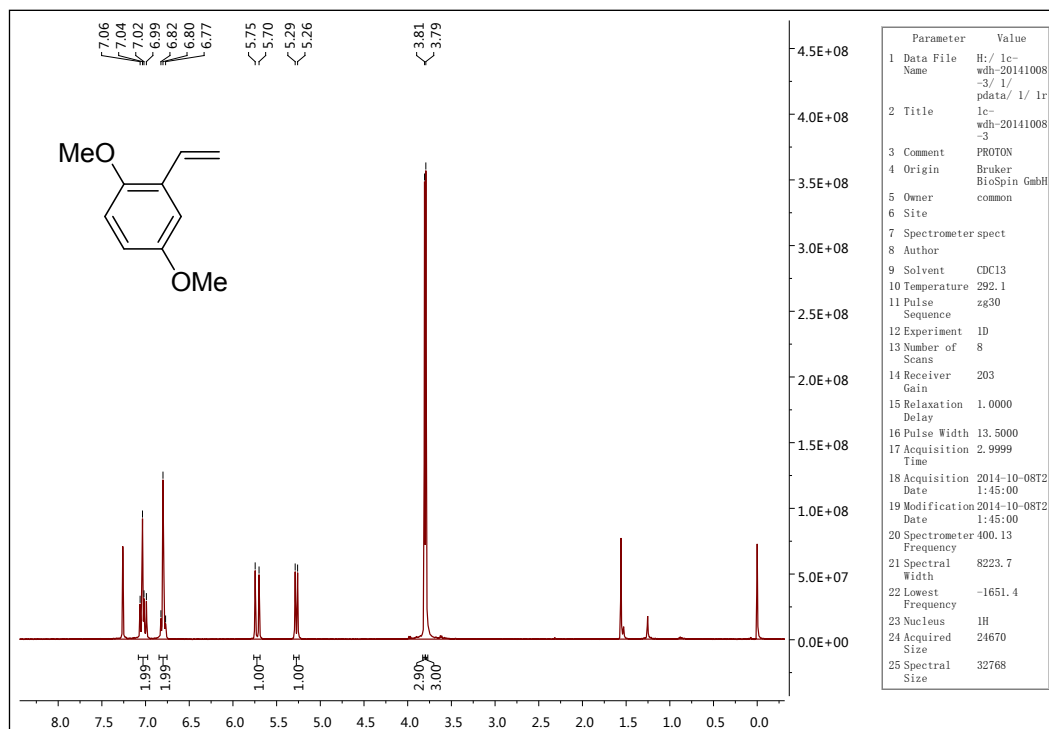
4. Preparation of 1,4,5,8-phenanthrenediquinone

5,8-dimethoxy-1,4-phenanthrenequinone (1 mmol) dissolved in acetonitrile (3 mL) was added to a solution of CAN (3 mmol) in H_2O (3 mL), after stirring for 5 min at room temperature, the reaction mixture was extracted with dichloromethane. Finally, the dichloromethane extract was concentrated under reduced pressure. Yield: 98%, yellow solid, ^1H NMR (400 MHz, CDCl_3) δ 8.41 (s, 1H), 7.18 (d, J = 10.4 Hz, 1H), 7.00 (d, J = 10.4 Hz, 1H). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ 184.0, 183.1, 140.5, 137.1, 136.3, 133.5, 129.8. The NMR spectra is in agreement with previous investigation [K. Krohn, A. Aslan, I. Ahmed, G. Pescitelli, T. Funaioli, *Eur. J. Org. Chem.*, 2009, 31, 5452].

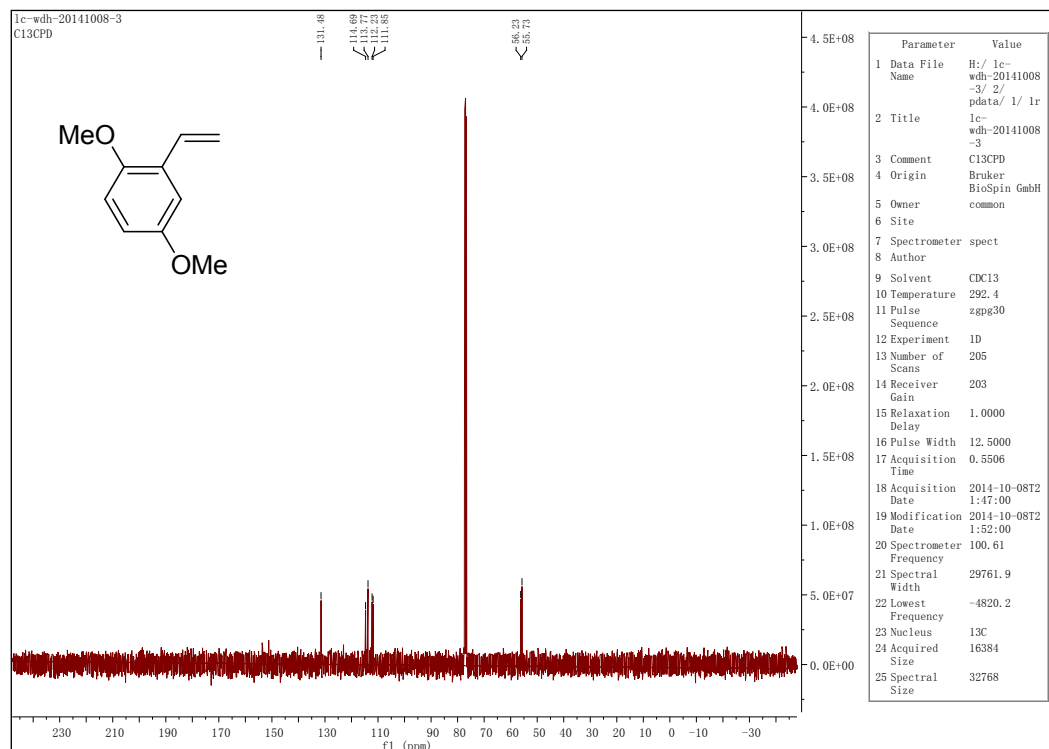
(E) NMR spectra for products of all reactions

All Nuclear Magnetic Resonance (NMR) spectra were obtained on Bruker AV 400 spectrometer at 400 MHz (^1H NMR) and 101 MHz (^{13}C NMR)

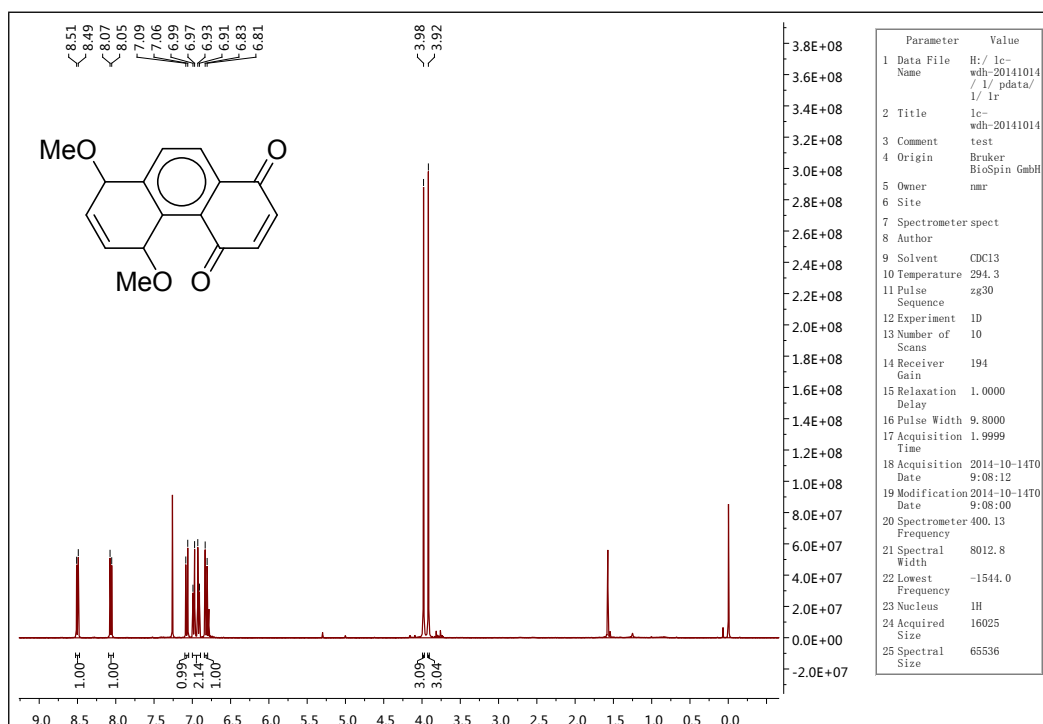
1,4-dimethoxy-2-vinylbenzene ^1H NMR (CDCl_3 , 400 M)



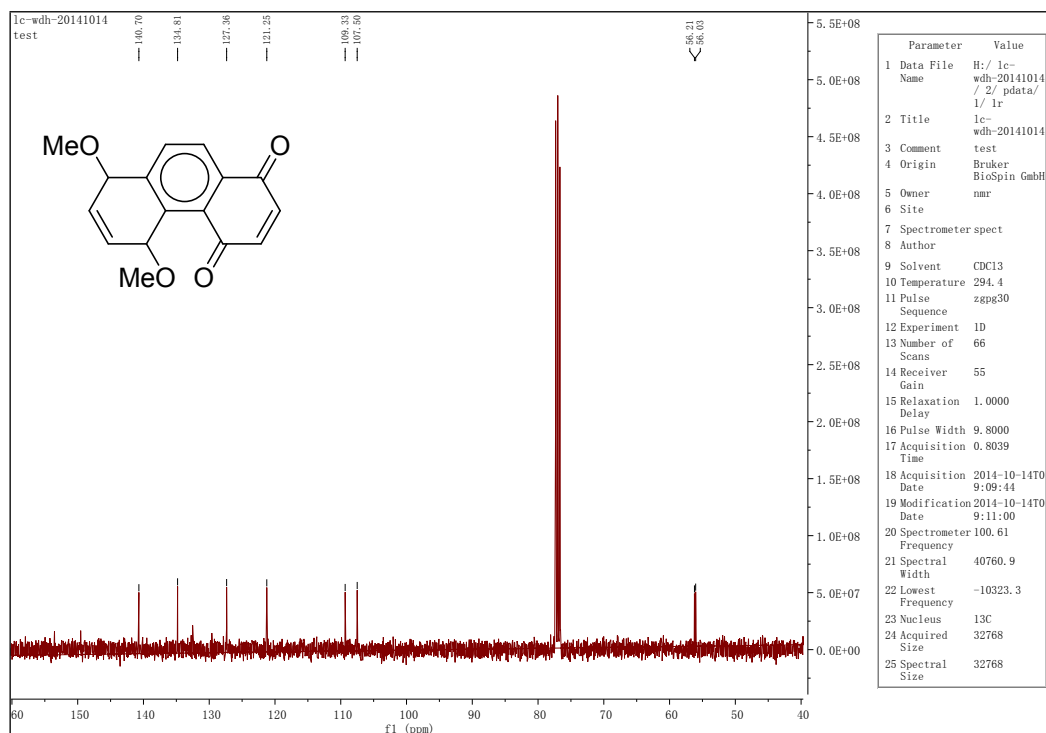
1,4-dimethoxy-2-vinylbenzene ^{13}C NMR (CDCl_3 , 400 M)



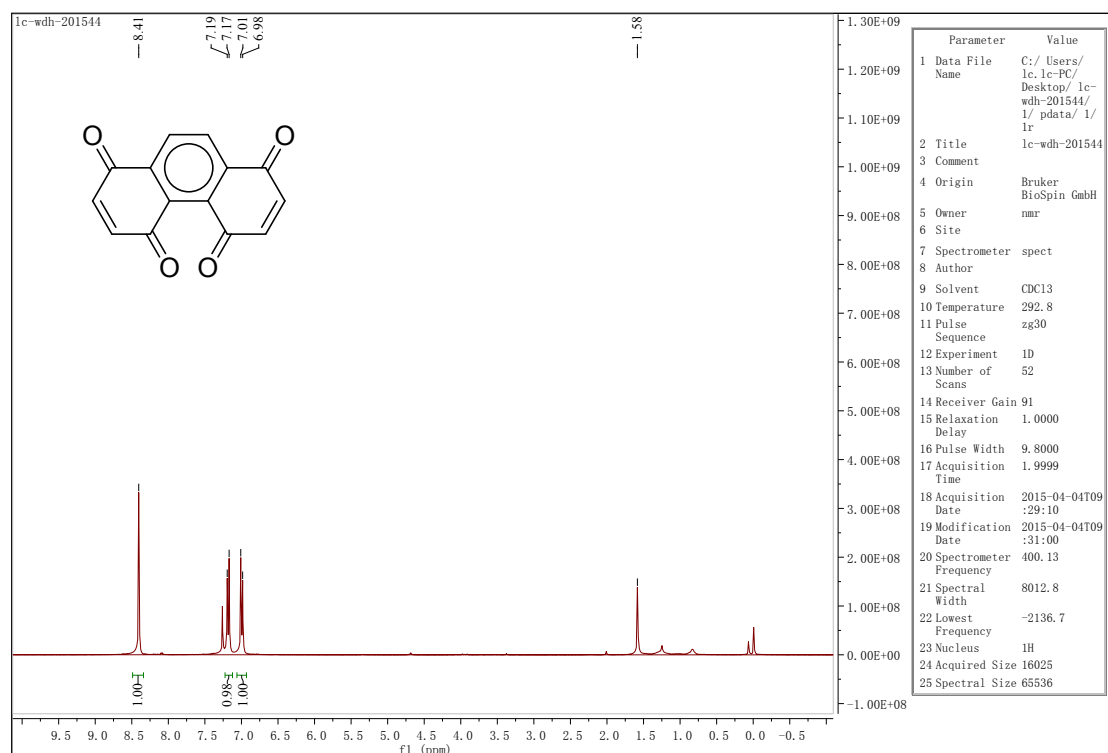
5,8-dimethoxy-1,4-phenanthrenequinone ^1H NMR (CDCl_3 , 400 M)



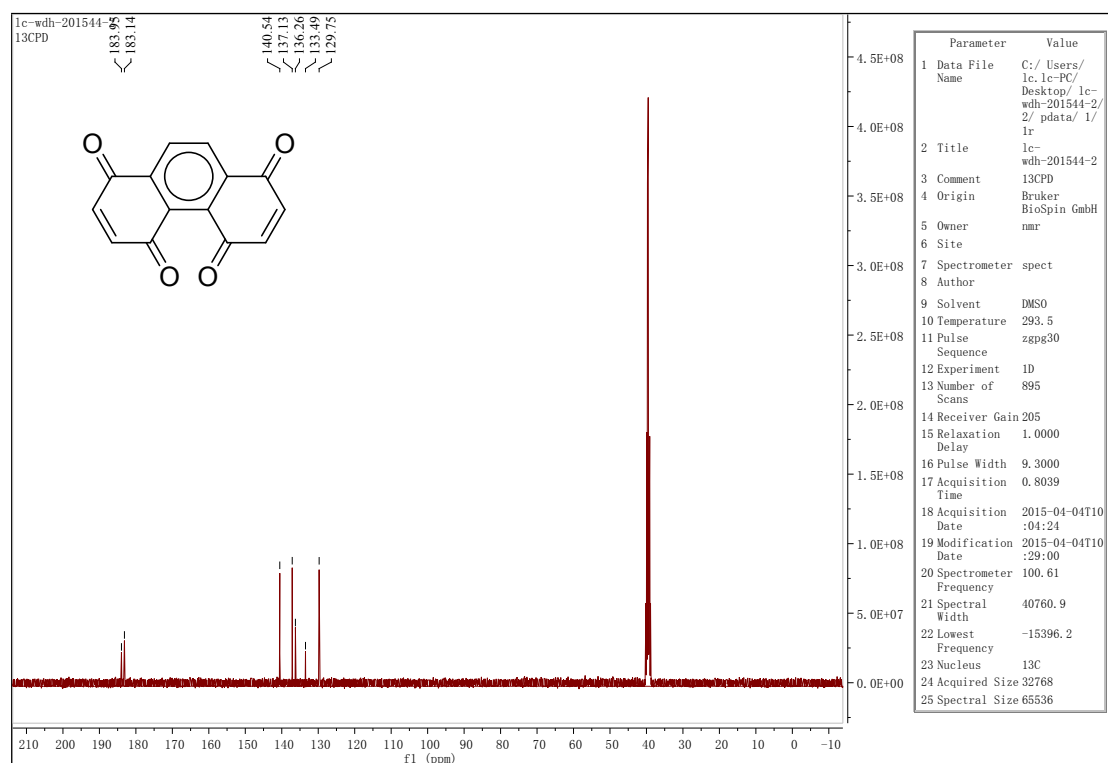
5,8-dimethoxy-1,4-phenanthrenequinone ^{13}C NMR (CDCl_3 , 400 M)



1,4,5,8-phenanthrenediquinone ¹H NMR (CDCl₃, 400 M)



1,4,5,8-phenanthrenediquinone ¹³C NMR (DMSO-d₆, 101 M)



(F) Mass Spectrometry of 1,4,5,8-phenanthrenediquinone

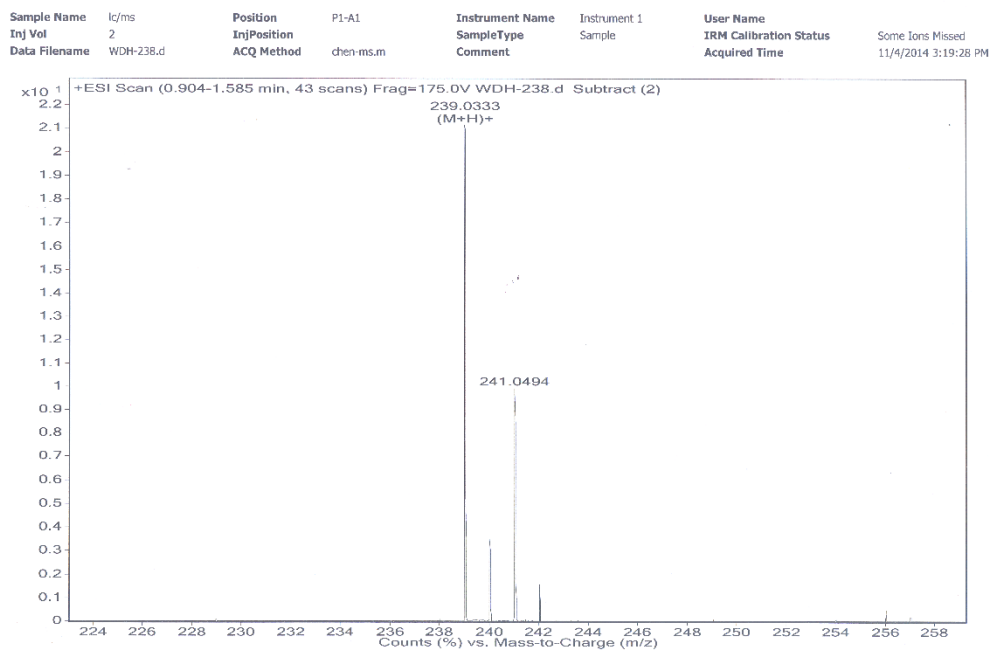


Fig. S3 ESI-MS of PADQ was recorded on Agilent 6520 Q-TQF LC/MS. The Positive-ion electrospray ionization mass spectrometry (ESI-MS) analysis clearly demonstrated the protonated molecular ion at m/z 239.

(G) The calculated voltage of molecule 3 with electron-withdrawn groups

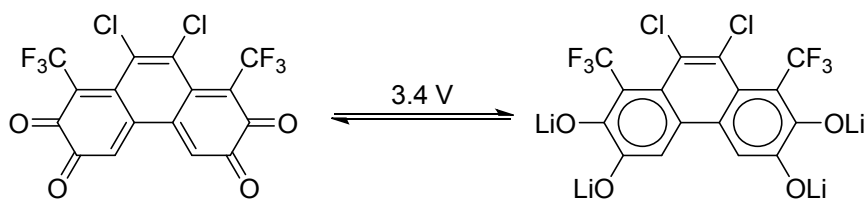


Fig. S4 Calculated voltage of molecule **3** with electron-withdrawn groups, the theoretical specific capacity is 229 mAh/g.

(H) Gaussian Archive of All Calculated Molecules

1. Previously investigated experimentally available molecules

1

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2_2Li

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3_2Li

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17172118\O,0,1.1435093677,-5.8772914412,-0.0784043044\O,0,3.3858209764
,-5.8820714131,-0.0152101436\Li,0,2.2386838139,-7.4343576952,-0.014157
0535\Li,0,4.2086989883,-4.7227174573,-1.1895972622\Li,0,-3.3203698966,
2.7625755744,1.1154022819\Version=EM64L-G09RevA.02\State=1-A\HF=-639.
9727697\RMSD=3.333e-09\Dipole=-0.38058,0.5476878,-0.4316275\Quadrupole
=3.7178681,42.9134916,-46.6313597,-59.9658525,-25.4346822,20.2079894\P
G=C01 [X(C8H6Li4O4)]\@

4

1\1\GINC-IB-COMPUTE-0-4\SP\RB3LYP\6-311+G(d)\C10H8Li2O4\ZHONGFANG\08-A
ug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=re
ad\4_1.gjf\0,1\C,0,-5.6192132298,0.0710814176,-0.0179583969\C,0,-4.2
555536156,0.6655643977,-0.0425078518\C,0,-3.1248412903,-0.0689088497,-
0.0360637715\C,0,-1.7939947087,0.4836191875,-0.0324922934\C,0,-0.66598

75703,-0.2703152973,-0.0057980548\C,0,0.665992732,0.2701131942,0.00557
35399\C,0,1.7940095201,-0.4838056137,0.0323064225\C,0,3.1248417863,0.0
687570417,0.0358593465\C,0,4.2555830398,-0.6656718929,0.0423826595\C,0
,5.6192108312,-0.0711255192,0.0177177719\O,0,-6.6119937113,0.864895147
,0.0407986519\O,0,-5.773149943,-1.1897306613,-0.0445147799\O,0,6.61203
49662,-0.8649068096,-0.0408350269\O,0,5.7730793446,1.1896976104,0.0442
045787\H,0,-4.2121279202,1.7512570158,-0.0479850769\H,0,-3.2186920351,
-1.1528043014,-0.0256605559\H,0,-1.7032881584,1.5688439178,-0.04695802
02\H,0,-0.7610464533,-1.3553490128,0.0094752298\H,0,0.7610447997,1.355
1472843,-0.0097159436\H,0,1.7033236034,-1.5690309756,0.0468519283\H,0,
3.2186599679,1.1526534888,0.0253366634\H,0,4.2122035497,-1.7513650865,
0.0479847863\Li,0,-7.7180994099,-0.7962622372,0.1259851372\Li,0,7.7181
34905,0.7962945549,-0.1253419439\\Version=EM64L-G09RevA.02\State=1-A\H
F=-702.2337768\RMSD=5.204e-09\Dipole=0.0000483,0.0000617,0.0013194\Qua
drupole=66.0844562,-32.8075715,-33.2768847,32.1283052,-5.7951898,-1.29
96867\PG=C01 [X(C10H8Li2O4)]\@

4_2Li

1\1\GINC-COMPUTE-0-38\SP\RB3LYP\6-311+G(d)\C10H8Li4O4\ZHONGFANG\08-Aug
-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
\\Title Card Required\\0,1\C,0,5.6162735883,0.1181364771,-0.086162087\
C,0,4.3771005239,-0.547824901,-0.175111481\C,0,3.114346232,0.092320937
4,0.0015857968\C,0,1.8663771642,-0.4572817558,-0.13849514\C,0,0.629940
7879,0.2420649402,0.0805255526\C,0,-0.6287096115,-0.2742054921,-0.0532
648062\C,0,-1.8632164341,0.4280446714,0.1678889535\C,0,-3.1142510984,-
0.1103400209,0.0138421309\C,0,-4.3717451472,0.5386142027,0.1981380466\
C,0,-5.6179589469,-0.1077965078,0.0773441984\O,0,6.7490616702,-0.60304
19583,-0.1598066137\O,0,5.7608354446,1.3886689115,0.0934642016\O,0,-6.
7421497181,0.6259075214,0.1678772924\O,0,-5.7788513603,-1.3688292135,-

0.151244971\H,0,4.3857518884,-1.5851660541,-0.5136342147\H,0,3.1641453
 507,1.1442379706,0.2878372519\H,0,1.7900322,-1.506884521,-0.4343013861
 \H,0,0.7175507914,1.288782088,0.3840612223\H,0,-0.7178276974,-1.320174
 4968,-0.3588205226\H,0,-1.7822627211,1.473543785,0.4768504861\H,0,-3.1
 718438016,-1.1564414193,-0.2915834986\H,0,-4.371553068,1.5655066436,0.
 5669260599\Li,0,7.642840095,1.1180763141,-0.1127422484\Li,0,-7.6610574
 782,-1.0718179475,0.0179095957\Li,0,6.2298348343,-2.0296086764,0.88395
 06976\Li,0,-6.2041274883,2.0580655013,-0.859972517\\Version=EM64L-G09R
 evA.02\State=1-A\HF=-717.4058786\RMSD=2.652e-09\Dipole=0.0513494,0.084
 2811,-0.0777405\Quadrupole=117.5760915,-47.5134503,-70.0626412,-37.498
 1468,32.8131789,-11.9536957\PG=C01 [X(C10H8Li4O4)]\\@

5

1\1\GINC-COMPUTE-0-58\SP\RB3LYP\6-311+G(d)\C8H10N2O4\ZHONGFANG\07-Aug-
 2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read\
 \Title Card Required\0,1\C,0,0.7627989571,1.2047131032,-0.1307521578\
 C,0,-0.7625293243,1.2050295388,0.1302722445\C,0,-0.7628454607,-1.23055
 94728,0.1313771537\C,0,0.7624824709,-1.2308730446,-0.1296497367\N,0,1.
 4086192784,-0.0132288609,-0.2740088343\N,0,-1.4086920808,-0.0126146555
 ,0.2745136809\O,0,-1.3393480362,-2.2878145546,0.2098810037\O,0,1.33856
 73074,-2.2883619719,-0.2080629471\O,0,1.3392309887,2.2619726647,-0.209
 7062319\O,0,-1.3386755089,2.2625115708,0.2083287465\C,0,2.8690095394,-
 0.0135418482,-0.5445966867\H,0,3.0721444828,-0.8975885419,-1.145090992
 3\H,0,3.0723591776,0.869851851,-1.1459789603\C,0,3.697297414,-0.012999
 4905,0.7366398405\H,0,3.4972161898,0.8751331817,1.3391251659\H,0,3.496
 9890948,-0.9004714637,1.3400222089\H,0,4.7590243498,-0.0132649115,0.47
 88038735\C,0,-2.8691422154,-0.0122924888,0.5447757885\H,0,-3.072631163
 4,-0.895699788,1.1460888068\H,0,-3.0724081411,0.8717409436,1.145246756
 6\C,0,-3.6971384195,-0.0128041279,-0.7366489661\H,0,-3.4967037777,0.87

46877253,-1.3399599111\H,0,-3.4969064298,-0.9009168587,-1.339114599\H,
 0,-4.7589242227,-0.0125610294,-0.4790554063\\Version=EM64L-G09RevA.02\
 State=1-A\HF=-721.5193945\RMSD=2.609e-09\Dipole=0.0000782,0.0000016,0.
 0003732\Quadrupole=13.6728379,-20.0171947,6.3443567,-0.005164,-0.77122
 82,0.0087312\PG=C01 [X(C8H10N2O4)]\\@

5_2Li

1\1\GINC-COMPUTE-0-58\SP\RB3LYP\6-311+G(d)\C8H10Li2N2O4\ZHONGFANG\07-A
 ug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=re
 ad\\Title Card Required\\0,1\C,0,-0.673437989,0.9994177744,0.137578888
 1\C,0,0.6734842755,0.999390279,-0.1376041736\C,0,0.7361121672,-1.44803
 03713,-0.1421372273\C,0,-0.736155565,-1.4480006356,0.1421610158\N,0,-1
 .3502773448,-0.2227744257,0.2748384516\N,0,1.3502785003,-0.222829713,-
 0.274840278\O,0,1.3607561521,-2.5150762665,-0.2583374154\O,0,-1.360843
 149,-2.5150219886,0.2583551936\O,0,-1.3093669357,2.1639760701,0.269873
 6729\O,0,1.309456655,2.1639222803,-0.2699186972\C,0,-2.7947250508,-0.1
 992774799,0.5618800021\H,0,-3.0070314465,-1.0540896154,1.2023900103\H,
 0,-2.992498866,0.7180926714,1.1123362515\C,0,-3.6450838097,-0.25882924
 37,-0.7063344099\H,0,-3.4486114819,0.6006304996,-1.3518964608\H,0,-3.4
 462009578,-1.1719631525,-1.2709404243\H,0,-4.7069777796,-0.2478133572,
 -0.4440427892\C,0,2.7947260727,-0.1993925857,-0.5618877236\H,0,3.00699
 80501,-1.0542257707,-1.2023811585\H,0,2.9925316491,0.7179589116,-1.112
 3635332\C,0,3.6450882023,-0.2589503216,0.7063242638\H,0,3.4486509968,0
 .6005300102,1.3518695395\H,0,3.4461730706,-1.1720652076,1.2709495985\H
 ,0,4.7069815634,-0.2479799936,0.4440281116\Li,0,0.2544704357,2.9179159
 281,1.2566406717\Li,0,-0.2543556446,2.9179024737,-1.25669422\\Version=
 EM64L-G09RevA.02\State=1-A\HF=-736.7374095\RMSD=3.412e-09\Dipole=0.000
 1381,7.5336971,0.\Quadrupole=-7.828364,0.8115965,7.0167675,0.0001583,3
 .0776013,-0.0000564\PG=C02 [X(C8H10Li2N2O4)]\\@

5_4Li

1\1\GINC-COMPUTE-0-58\SP\RB3LYP\6-311+G(d)\C8H10Li4N2O4\ZHONGFANG\07-A
ug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=re
ad\Title Card Required\0,1\C,0,0.5647800668,-1.1957422518,0.29584163
7\C,0,-0.6112460761,-1.1953768213,-0.4076487445\C,0,-0.6118455776,1.19
43090413,-0.4093466653\C,0,0.564179116,1.1962648582,0.2941435105\N,0,1
.2103841501,0.0007577501,0.7641594151\N,0,-1.3030957417,-0.0009871304,
-0.8036645715\O,0,-1.1659048555,2.3886045517,-0.7612303717\O,0,1.15901
17985,2.3874000111,0.5670458072\O,0,1.1602184114,-2.3861888288,0.57041
55349\O,0,-1.1647048462,-2.3904439369,-0.7578471253\C,0,2.6767576311,0
.0010188818,0.5923564559\H,0,3.0539964825,0.8833221354,1.1094761495\H,
0,3.0544703071,-0.8803779452,1.1106754692\C,0,3.1794231582,0.000182668
3,-0.8568546298\H,0,2.8361255802,-0.8850447561,-1.3996235061\H,0,2.835
5332599,0.8844314891,-1.4008449917\H,0,4.274440376,0.0005310265,-0.879
4885245\C,0,-2.7431955258,-0.0011211916,-0.4685116052\H,0,-3.176020779
6,0.8795340275,-0.9442389759\H,0,-3.1755729287,-0.8826296864,-0.943064
6203\C,0,-3.0914834911,-0.0002253511,1.0270428074\H,0,-2.6962270123,-0
.8830569858,1.5386913508\H,0,-2.6966482193,0.8834602836,1.5375393152\H
,0,-4.1786824484,-0.000398605,1.1597158027\Li,0,-0.6175672222,-2.99516
04419,0.9919829144\Li,0,0.6419858269,-2.8363686259,-1.2541191017\Li,0,
-0.6190956961,2.9959802355,0.9877845941\Li,0,0.6405592457,2.8347958581
, -1.2580963908\Version=EM64L-G09RevA.02\State=1-A\HF=-751.8712132\RMS
D=4.204e-09\Dipole=0.173153,-0.0000742,-0.11298\Quadrupole=-18.3139661
,21.8048063,-3.4908402,-0.023254,-18.255751,-0.0227897\PG=C01 [X(C8H10
Li4N2O4)]\@

6

I\1\GINC-IB-COMPUTE-0-11\SP\RB3LYP\6-311+G(d)\C14H8O2\ZHONGFANG\07-Aug

-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read

\Title Card Required\0,1\C,0,0.,3.6939506997,0.6986035806\C,0,0.,2.4

9033649,1.3951663839\C,0,0.,1.2746840118,0.7041015487\C,0,0.,1.2746840

118,-0.7041015487\C,0,0.,2.49033649,-1.3951663839\C,0,0.,3.6939506997,

-0.6986035806\C,0,0.,0.,1.4749906632\C,0,0.,0.,-1.4749906632\C,0,0.,-1

.2746840118,-0.7041015487\C,0,0.,-1.2746840118,0.7041015487\C,0,0.,-2.

49033649,1.3951663839\H,0,0.,-2.4761875747,2.4782706756\C,0,0.,-3.6939

506997,0.6986035806\C,0,0.,-3.6939506997,-0.6986035806\C,0,0.,-2.49033

649,-1.3951663839\H,0,0.,4.6327533142,1.2416334211\H,0,0.,2.4761875747

,2.4782706756\H,0,0.,2.4761875747,-2.4782706756\H,0,0.,4.6327533142,-1

.2416334211\H,0,0.,-4.6327533142,1.2416334211\H,0,0.,-4.6327533142,-1.

2416334211\H,0,0.,-2.4761875747,-2.4782706756\O,0,0.,0.,-2.6992497552\

O,0,0.,0.,2.6992497552\Version=EM64L-G09RevA.02\State=1-AG\HF=-688.94

77506\RMSD=5.950e-10\Dipole=0.,0.,0.\Quadrupole=-6.2023844,19.6779302,

-13.4755458,0.,0.,0.\PG=D02H [C2"(O1C1.C1O1),SG(C12H8)]\@\

6_2Li

I\1\GINC-COMPUTE-0-19\SP\RB3LYP\6-311+G(d)\C14H8Li2O2\ZHONGFANG\07-Aug

-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read

\Title Card Required\0,1\C,0,-3.6661864831,0.6931487175,-0.001655517

9\C,0,-2.4786827723,1.3821221885,-0.0033454648\C,0,-1.2161902299,0.717

9743011,-0.0021618669\C,0,-1.2089013997,-0.7301383077,0.0007754382\C,0

, -2.4646758552,-1.4069368364,0.0026665032\C,0,-3.6590394543,-0.7299285

012,0.0015517455\C,0,-0.0046702339,1.4708591399,-0.0035451195\C,0,0.01

01116199,-1.4708064859,0.001900608\C,0,1.2215413164,-0.717898543,-0.00

04941845\C,0,1.2142812011,0.7301749854,-0.0034491964\C,0,2.469960391,1

.4071746382,-0.005908774\H,0,2.456798455,2.4915652723,-0.0085913844\C,

0,3.6642285909,0.7299697376,-0.0053943972\C,0,3.6713635512,-0.69317091

99,-0.0024372502\C,0,2.4839458779,-1.3823019263,0.0000084802\H,0,-4.61
 11025026,1.2294705118,-0.0029675618\H,0,-2.476775938,2.4665763026,-0.0
 060232769\H,0,-2.4518967143,-2.4913234422,0.0048795732\H,0,-4.59851976
 16,-1.2757151538,0.0029851149\H,0,4.6037558783,1.275684089,-0.00744326
 45\H,0,4.6163135045,-1.2294433536,-0.0021790269\H,0,2.4816355508,-2.46
 67693434,0.0022578477\O,0,0.0169443795,-2.7853893398,0.0050727746\O,0,
 -0.0111831982,2.7854270957,-0.0052059887\Li,0,-0.0136772758,-4.5119895
 879,0.0157686907\Li,0,-0.0546304978,4.5117197615,0.0229694983\\Version
 =EM64L-G09RevA.02\State=1-A\HF=-704.1697238\RMSD=4.764e-09\Dipole=-0.1
 206061,-0.0000095,0.0647424\Quadrupole=-33.0695514,64.90963,-31.840078
 5,-0.4280021,-0.0045209,0.1737323\PG=C01 [X(C14H8Li2O2)]\\@

7

1\1\GINC-COMPUTE-0-36\SP\RB3LYP\6-311+G(d)\C16H10N2O4\ZHONGFANG\07-Aug
 -2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
 \\Title Card Required\0,1\C,0,-0.0097662396,2.8904815197,-1.242628638
 6\C,0,-0.003618896,1.4051724708,-1.2306734749\C,0,-0.000794156,0.70987
 46887,0.0000289916\C,0,-0.0036013894,1.4051859176,1.2307255466\C,0,-0.
 0097235234,2.8905142935,1.2427560313\C,0,-0.0034844448,0.7027660262,-2
 .4226765684\C,0,0.000794156,-0.7098746887,0.0000289916\C,0,0.003618896
 ,-1.4051724708,-1.2306734749\C,0,0.0034844448,-0.7027660262,-2.4226765
 684\C,0,0.0097662396,-2.8904815197,-1.2426286386\C,0,0.0097235234,-2.8
 905142935,1.2427560313\C,0,0.0036013894,-1.4051859176,1.2307255466\C,0
 ,0.0034754004,-0.702765783,2.4227222023\C,0,-0.0034754004,0.702765783,
 2.4227222023\H,0,-0.0069736146,1.2469710225,3.3589141038\H,0,0.0069736
 146,-1.2469710225,3.3589141038\H,0,-0.0069958307,1.2469777877,-3.35886
 55962\H,0,0.0069958307,-1.2469777877,-3.3588655962\O,0,0.0439982008,-3
 .5341438457,2.27819737\O,0,0.0441035911,-3.5342600232,-2.2779817245\O,
 0,-0.0441035911,3.5342600232,-2.2779817245\O,0,-0.0439982008,3.5341438

457,2.27819737\N,0,0.0314817124,3.5356291151,0.0000367284\N,0,-0.03148
 17124,-3.5356291151,0.0000367284\C,0,0.0498150395,5.005618808,-0.00030
 27948\H,0,0.5673362836,5.3475431272,-0.8911730089\H,0,-0.9681330781,5.
 4002822953,-0.0037870978\H,0,0.5614888454,5.3478202363,0.8937869301\C,
 0,-0.0498150395,-5.005618808,-0.0003027948\H,0,-0.5673362836,-5.347543
 1272,-0.8911730089\H,0,0.9681330781,-5.4002822953,-0.0037870978\H,0,-0
 .5614888454,-5.3478202363,0.8937869301\\Version=EM64L-G09RevA.02\State
 =1-A\HF=-1026.491205\RMSD=3.465e-09\Dipole=0.,0.,0.0001017\Quadrupole=
 7.1872827,-2.0095446,-5.1777381,1.417729,0.,0.\PG=C02 [X(C16H10N2O4)]\
 \@

7_2Li

1\1\GINC-COMPUTE-0-36\SP\RB3LYP\6-311+G(d)\C16H10Li2N2O4\ZHONGFANG\07-
 Aug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=r
 ead\\Title Card Required\\0,1\C,0,2.8525998774,-1.4194444217,-0.010993
 4136\C,0,1.4104229411,-1.3949330483,-0.0101977043\C,0,0.7209645795,-0.
 1630002831,-0.0153094618\C,0,1.4238170549,1.0780752158,-0.0164683303\C
 ,0,2.8356647394,1.0699003064,-0.0094083307\C,0,0.6827739646,-2.6241718
 466,-0.000983366\C,0,-0.7208827051,-0.1629853164,-0.015254191\C,0,-1.4
 103813474,-1.3948965071,-0.0100277825\C,0,-0.6827657451,-2.6241558134,
 -0.0008845909\C,0,-2.8525582198,-1.4193599546,-0.0106318277\C,0,-2.835
 5493088,1.0699832764,-0.0093825717\C,0,-1.4237016588,1.0781006152,-0.0
 164490127\C,0,-0.6800514777,2.3107818225,-0.0212661073\C,0,0.680183405
 6,2.3107710001,-0.0212508017\H,0,1.2261503041,3.2478386774,-0.03187120
 22\H,0,-1.2260318989,3.2478375045,-0.0319296014\H,0,1.2427253001,-3.55
 18433112,0.0063320345\H,0,-1.2427379403,-3.5518139709,0.0065159158\O,0
 ,-3.5643491647,2.1193084058,0.0025200653\O,0,-3.5346431641,-2.46344329
 86,-0.0056495102\O,0,3.5346430757,-2.4635570417,-0.0062280269\O,0,3.56
 45813907,2.1191395941,0.0027522801\Li,0,4.1789638662,3.7526645397,0.30

84219247\Li,0,-4.1801736127,3.7519460688,0.3101095092\N,0,3.4909821925
 ,-0.1626699821,-0.0167305855\N,0,-3.4909112833,-0.1625607462,-0.016473
 5249\C,0,4.9551192629,-0.1367270342,-0.0217682358\H,0,5.319713535,0.42
 06187266,-0.8851451652\H,0,5.3313144472,0.3438242133,0.8829365982\H,0,
 5.3054008876,-1.1622490901,-0.0656040374\C,0,-4.9550452069,-0.13660472
 62,-0.0214785105\H,0,-5.3312342326,0.3438605287,0.8832791415\H,0,-5.31
 96469944,0.4208080806,-0.8848049115\H,0,-5.3053331237,-1.1621226841,-0
 .0653751257\\Version=EM64L-G09RevA.02\State=1-A\HF=-1041.7233011\RMSE=
 7.953e-09\Dipole=-0.0024246,12.1172333,1.0249738\Quadrupole=17.5186768
 ,16.8478278,-34.3665046,-0.0055965,-0.0235344,7.649698\PG=C01 [X(C16H1
 0Li2N2O4)]\\@

7_4Li

1\1\GINC-COMPUTE-0-36\SP\RB3LYP\6-311+G(d)\C16H10Li4N2O4\ZHONGFANG\07-
 Aug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=r
 ead\\Title Card Required\\0,1\C,0,-2.8281936299,1.2524663636,0.0744118
 874\C,0,-1.4471232849,1.2451600421,-0.0023260941\C,0,-0.6906241327,-0.
 0060922212,0.0110631544\C,0,-1.4616855976,-1.2473492322,0.034839471\C,
 0,-2.8433671068,-1.2329170422,0.0882193714\C,0,-0.6687062004,2.4660163
 522,-0.0600546693\C,0,0.6851896826,-0.0148645343,-0.0018130134\C,0,1.4
 583289375,1.2259677999,-0.0488399861\C,0,0.6930464861,2.4574543214,-0.
 0946460752\C,0,2.8384864463,1.2118788815,-0.1032706157\C,0,2.821126225
 4,-1.2727673458,-0.0485235336\C,0,1.4410996239,-1.2664058287,0.0002725
 773\C,0,0.6610456272,-2.490191383,-0.0015965426\C,0,-0.7007477137,-2.4
 808860656,0.0216283516\H,0,-1.2449326033,-3.4217048156,0.0277568216\H,
 0,1.1927068864,-3.4379812614,-0.0127986426\H,0,-1.1954659547,3.4166515
 203,-0.0942751697\H,0,1.2309774852,3.4008530163,-0.1484937479\O,0,3.55
 46175399,-2.3534810121,-0.0880675443\O,0,3.587721002,2.2794640569,-0.1
 90649777\O,0,-3.5629962807,2.3316928116,0.1143209079\O,0,-3.5933934636

, -2.2995469844, 0.1151917269\Li, 0, -4.5592153123, -3.7250331931, -0.026504
 8953\Li, 0, 4.5255476113, -3.7709127876, -0.2429672959\Li, 0, 4.1355998675, 3
 .9003918862, -0.4533895181\Li, 0, -3.8221435336, 3.9838436438, 0.6244059766
 \N, 0, 3.552235301, -0.0358570589, -0.1265726341\N, 0, -3.5439939555, 0.01456
 00574, 0.1747968828\C, 0, -4.9150449992, 0.0183267485, -0.3200709873\H, 0, -5
 .3857161721, 0.9579935349, -0.0473510207\H, 0, -4.9613579192, -0.0831583466
 , -1.4207868698\H, 0, -5.4691125531, -0.808051741, 0.1176648456\C, 0, 4.83442
 68144, -0.0267778335, 0.5746813825\H, 0, 5.3825647517, 0.8718004312, 0.30581
 49299\H, 0, 4.7060525055, -0.0383761993, 1.6749536015\H, 0, 5.4124026197, -0.
 9026805815, 0.2921267441\\Version=EM64L-G09RevA.02\State=1-A\HF=-1056.8
 105596\RMSD=9.412e-09\Dipole=-0.0544344, 0.7720165, -0.0082959\Quadrupol
 e=28.5872698, 50.2123547, -78.7996245, 3.0388134, -9.8402817, 6.4290086\PG=
 C01 [X(C16H10Li4N2O4)]\@

8

1\1\GINC-IB-COMPUTE-0-0\SP\RB3LYP\6-311+G(d)\C16H6O4\ZHONGFANG\07-Aug-
 2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read\
 \Title Card Required\0, 1\C, 0, 0.0000044676, 3.5699013611, 0.0003458803\C
 , 0, 1.1975376813, 2.8661509465, -0.0194730518\C, 0, 1.2083707784, 1.46544642
 33, -0.0170471204\C, 0, 0.0000009284, 0.738238768, 0.0001617839\C, 0, -1.2083
 677048, 1.4654465363, 0.0174359447\C, 0, -1.1975306744, 2.8661508749, 0.0200
 4839\C, 0, 2.5160449458, 0.774241745, -0.033696486\C, 0, -0.0000003862, -0.73
 82388586, 0.0000049424\C, 0, 1.2083689224, -1.4654480184, 0.0171783001\C, 0,
 2.5160420906, -0.7742438816, 0.0339199538\C, 0, 1.1975360826, -2.8661527493
 , 0.0194700319\H, 0, 2.1468961156, -3.3880602132, 0.0350157508\C, 0, 0.000003
 2721, -3.5699013959, -0.0004405494\C, 0, -1.1975315307, -2.8661491967, -0.02
 00972306\C, 0, -1.2083690268, -1.4654451152, -0.0173462073\C, 0, -2.51604876
 74, -0.7742434704, -0.0337338841\C, 0, -2.5160466941, 0.7742452455, 0.033883
 3474\H, 0, 0.0000057333, 4.653443937, 0.0004201759\H, 0, 2.1468980037, 3.3880

569352,-0.0350491571\H,0,-2.1468904178,3.3880567191,0.035669904\H,0,0.
 0000045314,-4.6534439613,-0.0006179901\H,0,-2.1468909909,-3.3880536041
 ,-0.0357821388\O,0,3.5778508115,-1.3581681516,0.0942373936\O,0,3.57784
 4517,1.3581493216,-0.0943377698\O,0,-3.5778412064,-1.3581389606,-0.094
 620037\O,0,-3.5778525227,1.3581607635,0.0943398237\\Version=EM64L-G09R
 evA.02\State=1-A\HF=-914.4520231\RMSD=3.503e-09\Dipole=-0.0000027,-0.0
 00002,0.0004001\Quadrupole=-33.6889671,26.7275369,6.9614302,0.0000263,
 -0.0006901,0.0023941\PG=C01 [X(C16H6O4)]\\@

8_2Li

1\1\GINC-C02\SP\RB3LYP\6-311+G(d)\C16H6Li2O4\ZHOU\22-Apr-2015\0\\#p b3
 lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1
 \C,0,-0.0164146,3.54423548,0.17094678\C,0,-0.01760668,2.83522049,-1.01
 563793\C,0,-0.00823971,1.41888789,-1.03225\C,0,-0.00191023,0.71690687,
 0.21284254\C,0,0.00484387,1.46884949,1.42172596\C,0,-0.0020271,2.86032
 45,1.3947498\C,0,-0.00441841,0.70362791,-2.27711693\C,0,0.00191023,-0.
 71690687,0.21284254\C,0,0.00823971,-1.41888789,-1.03225\C,0,0.00441841
 ,-0.70362791,-2.27711693\C,0,0.01760668,-2.83522049,-1.01563793\H,0,0.
 02550004,-3.35240279,-1.96830202\C,0,0.0164146,-3.54423548,0.17094678\
 C,0,0.0020271,-2.8603245,1.3947498\C,0,-0.00484387,-1.46884949,1.42172
 596\C,0,-0.0251583,-0.77854644,2.72322461\C,0,0.0251583,0.77854644,2.7
 2322461\H,0,-0.02535863,4.62921475,0.15802615\H,0,-0.02550004,3.352402
 79,-1.96830202\H,0,0.00262283,3.4032622,2.33263829\H,0,0.02535863,-4.6
 2921475,0.15802615\H,0,-0.00262283,-3.4032622,2.33263829\O,0,0.0080084
 6,-1.31151563,-3.46857417\O,0,-0.00800846,1.31151563,-3.46857417\O,0,-
 0.08060521,-1.35423951,3.79697731\O,0,0.08060521,1.35423951,3.79697731
 \Li,0,-1.26743793,-0.00739899,-4.24602176\Li,0,1.26743793,0.00739899,-
 4.24602176\\Version=EM64L-G09RevB.01\State=1-A\HF=-929.7191461\RMSD=4.
 254e-09\Dipole=0.,0.,-7.880079\Quadrupole=-0.0843057,-10.4294738,10.51

37795,-0.3082553,0.,0.\PG=C02 [X(C16H6Li2O4)]\@

8_4Li

1\1\GINC-C02\SP\RB3LYP\6-311+G(d)\C16H6Li4O4\ZHOU\22-Apr-2015\0\#p b3
lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\Title Card Required\0,1
\C,0,0,3.52444044,0.\C,0,-1.213659,2.83779356,0.\C,0,-1.23960129,1.43
096107,0.\C,0,0,0.71002227,0.\C,0,1.23960129,1.43096107,0.\C,0,1.2136
59,2.83779356,0.\C,0,-2.48245676,0.70138928,0.\C,0,0,-0.71002227,0.\C
,0,-1.23960129,-1.43096107,0.\C,0,-2.48245676,-0.70138928,0.\C,0,-1.21
3659,-2.83779356,0.\H,0,-2.15519274,-3.37516929,0.\C,0,0,-3.52444044,
0.\C,0,1.213659,-2.83779356,0.\C,0,1.23960129,-1.43096107,0.\C,0,2.482
45676,-0.70138928,0.\C,0,2.48245676,0.70138928,0.\H,0,0,4.61174549,0.
\H,0,-2.15519274,3.37516929,0.\H,0,2.15519274,3.37516929,0.\H,0,0,-4.
61174549,0.\H,0,2.15519274,-3.37516929,0.\O,0,-3.68450595,-1.31494712,
0.\O,0,-3.68450595,1.31494712,0.\O,0,3.68450595,-1.31494712,0.\O,0,3.6
8450595,1.31494712,0.\Li,0,-4.40765255,0.,1.25680589\Li,0,-4.40765255,
0.,-1.25680589\Li,0,4.40765255,0.,1.25680589\Li,0,4.40765255,0.,-1.256
80589\Version=EM64L-G09RevB.01\State=1-AG\HF=-944.9628839\RMSE=5.209e
-09\Dipole=0.,0.,0.\Quadrupole=58.8610521,-49.7986681,-9.0623841,0.,0.
,0.\PG=D02H [C2'(H1C1C1.C1C1H1),SG'(Li4),SG"(C12H4O4)]\@

9

1\1\GINC-COMPUTE-0-41\SP\RB3LYP\6-311+G(d)\C14H4O6\ZHONGFANG\07-Aug-20
14\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read\T
itle Card Required\0,1\C,0,-0.0000444509,2.8775108002,1.2364575319\C,
0,-0.0000211275,1.3999828472,1.2345097713\C,0,-0.0000117318,0.70942479
4,-0.0000000042\C,0,-0.0000211275,1.3999828326,-1.2345097878\C,0,-0.00
00444509,2.8775107856,-1.2364575658\C,0,-0.0000064846,0.7024962329,2.4

294743972\C,0,0.0000117318,-0.709424794,0.0000000042\C,0,0.0000211275,
-1.3999828326,1.2345097878\C,0,0.0000064846,-0.7024962042,2.4294744055
\C,0,0.0000444509,-2.8775107856,1.2364575658\C,0,0.0000444509,-2.87751
08002,-1.2364575319\C,0,0.0000211275,-1.3999828472,-1.2345097713\C,0,0
.0000064846,-0.7024962329,-2.4294743972\C,0,-0.0000064846,0.7024962042
,-2.4294744055\H,0,-0.0000131799,1.2463915444,-3.3656358294\H,0,0.0000
131799,-1.2463915841,-3.3656358147\H,0,-0.0000131799,1.2463915841,3.36
56358147\H,0,0.0000131799,-1.2463915444,3.3656358294\O,0,0.0000112204,
-3.506755203,0.0000000207\O,0,-0.000055565,-3.5730650663,-2.2133343667
\O,0,-0.000055565,-3.5730650402,2.2133344088\O,0,0.000055565,3.5730650
663,2.2133343667\O,0,-0.0000112204,3.506755203,-0.0000000207\O,0,0.000
055565,3.5730650402,-2.2133344088\\Version=EM64L-G09RevA.02\State=1-AG
\HF=-987.5729732\RMSD=6.568e-10\Dipole=0.,0.,0.\Quadrupole=16.6697099,
-30.8364316,14.1667217,-0.0000906,0.,0.0000003\PG=D02H [C2"(O1C1.C1O1)
,SG(C12H4O4)]\@

9_2Li

1\1\GINC-COMPUTE-0-41\SP\RB3LYP\6-311+G(d)\C14H4Li2O6\ZHONGFANG\07-Aug
-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
\\Title Card Required\\0,1\C,0,2.8394091207,1.3939783811,0.0196325198\
C,0,1.4032602734,1.3859961672,0.010952544\C,0,0.7202056596,0.149876060
4,0.0053588039\C,0,1.4164178017,-1.0961287236,0.0090575619\C,0,2.81852
80131,-1.0843052669,0.0155870866\C,0,0.6823908503,2.6196158434,0.00751
44146\C,0,-0.7201888923,0.1499575654,-0.0048881396\C,0,-1.4031353314,1
.3861249858,-0.0078626653\C,0,-0.6821765749,2.6196802411,-0.001784139\
C,0,-2.8393112174,1.3942187394,-0.016470752\C,0,-2.818614185,-1.084052
3123,-0.0176043438\C,0,-1.4165257451,-1.0959962115,-0.0112567903\C,0,-
0.6783475332,-2.3355658429,-0.0072999185\C,0,0.6781494719,-2.335628173
5,0.0024970971\H,0,1.2345922894,-3.2657198041,0.0055717908\H,0,-1.2348
S27

61368,-3.2656058214,-0.0124003913\H,0,1.2421738474,3.5473119949,0.0122
 968064\H,0,-1.2418926944,3.5474238899,-0.004656512\O,0,-3.4589959674,0
 .143955015,-0.0198977559\O,0,-3.593314652,-2.0734979293,-0.020257498\O
 ,0,-3.585026758,2.3647056271,-0.0205359069\O,0,3.5852606347,2.36434140
 46,0.0258113307\O,0,3.4590094309,0.1435822356,0.0204681672\O,0,3.59308
 78052,-2.0738666414,0.0162905684\Li,0,5.4257784111,-2.1890926703,-0.06
 77190214\Li,0,-5.4257668307,-2.1894935136,0.0621727025\\Version=EM64L-
 G09RevA.02\State=1-A\HF=-1002.8301533\RMSD=8.600e-09\Dipole=0.0003239,
 -6.8344922,-0.0094524\Quadrupole=66.3125788,-32.3744305,-33.9381483,0.
 0102439,-2.9237564,0.01048\PG=C01 [X(C14H4Li2O6)]\\@

9_2Li_2

1\1\GINC-COMPUTE-0-41\SP\RB3LYP\6-311+G(d)\C14H4Li2O6\ZHONGFANG\07-Aug
 -2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
 \\Title Card Required\0,1\C,0,2.8380811623,1.4030435133,-0.0022436114
 \C,0,1.4031934134,1.3861971145,-0.0008757255\C,0,0.7206184364,0.147793
 9835,-0.000580553\C,0,1.4133617827,-1.1012580906,-0.0013688642\C,0,2.8
 135524282,-1.0921553469,-0.0025268745\C,0,0.6817278412,2.6199452333,0.
 0000412577\C,0,-0.7206325419,0.1477508528,0.0005905686\C,0,-1.40329601
 89,1.3861041904,0.0014845762\C,0,-0.6819157881,2.619902499,0.001241996
 9\C,0,-2.8381873167,1.4028966191,0.0026433892\C,0,-2.8134761456,-1.092
 3436446,0.0018500823\C,0,-1.4132983513,-1.1013378787,0.0008518417\C,0,
 -0.677815085,-2.3421782143,0.000208991\C,0,0.6779470279,-2.3421356431,
 -0.0008487624\H,0,1.2360502436,-3.2712138535,-0.001371496\H,0,-1.23586
 33159,-3.2712892716,0.0005949422\H,0,1.2414317581,3.547634276,-0.00025
 66922\H,0,-1.2416759465,3.5475560233,0.0019626212\O,0,-3.4555229632,0.
 1461034197,0.0022046013\O,0,-3.619009902,-2.0536988266,0.0024295889\O,
 0,-3.5864911724,2.3694038113,0.0038075486\O,0,3.586362837,2.3695739876
 ,-0.0030141945\O,0,3.4554251365,0.1462833641,-0.0031085267\O,0,3.61914

39485,-2.053509029,-0.0029809334\Li,0,5.3582662976,-1.2311576187,-0.00
 44239047\Li,0,-5.3578808158,-1.2303487002,0.0044305128\\Version=EM64L-
 G09RevA.02\State=1-A\HF=-1002.8283046\RMSD=3.112e-09\Dipole=0.0008874,
 -3.6015067,0.0003475\Quadrupole=67.8933913,-43.1083892,-24.7850021,-0.
 0169086,-0.0766977,-0.0042641\PG=C01 [X(C14H4Li2O6)]\\@

10TCNQ

1\1\GINC-COMPUTE-0-58\SP\RB3LYP\6-311+G(d)\C12H4N4\ZHONGFANG\07-Aug-20
 14\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read\\N
 3.gjf\\0,1\C,0,-1.4223935664,-0.0000000605,-0.0002972579\C,0,-0.676041
 2826,-1.2386564028,-0.000218667\C,0,0.6760412576,-1.2386563877,-0.0000
 646279\C,0,1.4223935176,-0.0000000008,0.0000371218\C,0,0.676041223,1.2
 386562907,-0.0001470535\C,0,-0.6760413108,1.2386562676,-0.0002984133\C
 ,0,2.8078457681,0.0000000282,0.0003434578\C,0,3.5672629114,1.204615075
 6,0.000477614\C,0,3.5672629485,-1.2046150033,0.0005769\C,0,-2.80784586
 46,-0.0000000896,-0.0003483434\C,0,-3.5672630668,1.2046149163,-0.00040
 27336\C,0,-3.5672630176,-1.2046151646,-0.0003293477\N,0,-4.1935274497,
 2.1765366944,-0.0004385112\N,0,-4.1935273039,-2.1765370051,-0.00031005
 86\N,0,4.1935269235,2.1765370901,0.0005832182\N,0,4.193527482,-2.17653
 66695,0.0007676287\H,0,-1.2143740606,-2.1787333179,-0.0002699332\H,0,1
 .2143740249,-2.1787333014,0.0000107497\H,0,1.2143739913,2.1787332149,-
 0.0001331376\H,0,-1.2143741252,2.1787331599,-0.0004076054\\Version=EM6
 4L-G09RevA.02\State=1-A\HF=-678.7615107\RMSD=7.383e-09\Dipole=0.000000
 3,-0.0000002,-0.0004752\Quadrupole=-24.8273308,5.2875087,19.5398221,-0
 .0000008,-0.0056736,0.0006233\PG=C01 [X(C12H4N4)]\\@

10TCNQ_Li

1\1\GINC-IB-COMPUTE-0-0\SP\UB3LYP\6-311+G(d)\C12H4LiN4(2)\ZHONGFANG\0

```

7-Aug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess
=read\N3_Li.gjf\0,2\C,0,-1.4069600474,0.1870347311,0.0103279959\C,0,
-0.8376759459,-1.1163182027,0.01615613\C,0,0.5217834422,-1.3040144552,
0.0117533132\C,0,1.4228247924,-0.2017079605,0.0005613629\C,0,0.8522017
682,1.102489955,-0.0046887096\C,0,-0.5075829527,1.2885246501,0.0004449
837\C,0,2.8367477133,-0.3963512827,-0.0053326796\C,0,3.7388152262,0.68
96704443,-0.0178246376\C,0,3.4100302741,-1.6864682766,0.0004980681\C,0
,-2.8273950719,0.3877037337,0.0134346387\C,0,-3.4035194289,1.676463404
9,0.0122169095\C,0,-3.7292592326,-0.6821948934,0.0134200863\N,0,-3.877
7497938,2.7370324402,0.011011616\N,0,-4.4877085896,-1.5639319596,0.011
3511558\N,0,4.478408855,1.5850906392,-0.028319521\N,0,3.8762412518,-2.
7502918142,0.0053672571\H,0,-1.4877203266,-1.984773168,0.0248870051\H,
0,0.9160402725,-2.3142638745,0.016911023\H,0,1.5036502134,1.9694428855
,-0.0131695001\H,0,-0.9021650465,2.2986158388,-0.0041540643\Li,0,-5.96
46333731,-2.9116828355,-0.0750724333\\Version=EM64L-G09RevA.02\State=2
-A\HF=-686.4162065\S2=0.760407\S2-1=0.\S2A=0.750082\RMSD=9.714e-09\Dip
ole=-9.7191575,-5.0610267,-0.1284813\Quadrupole=22.6343704,-9.5783541,
-13.0560163,61.7500354,1.6961367,0.7761959\PG=C01 [X(C12H4Li1N4)]\ \@

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10TCNQ_2Li

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1\1\GINC-COMPUTE-0-58\SP\RB3LYP\6-311+G(d)\C12H4Li2N4\ZHONGFANG\07-Aug
-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
\N3_Li.gjf\0,1\C,0,-1.4212368151,0.1982190046,-0.0000497524\C,0,-0.8
533172159,-1.0888432653,0.0001442528\C,0,0.5236808063,-1.2814386855,0.
0002239818\C,0,1.4212533076,-0.1981912359,0.0001145137\C,0,0.853333470
1,1.088875944,-0.0000830016\C,0,-0.5236641935,1.2814720121,-0.00016135
96\C,0,2.8804253523,-0.4061612207,0.0002050372\C,0,3.7673805791,0.6553
804457,0.0001799995\C,0,3.4398815227,-1.6918604535,0.0003492805\C,0,-2
.8804024591,0.4061609446,-0.0001357924\C,0,-3.4398992725,1.6918496024,

```

-0.0003453396\C,0,-3.76735629,-0.6553872911,-0.0000745078\N,0,-3.89049
 74265,2.768590589,-0.0005185966\N,0,-4.5091736252,-1.5623060981,-0.000
 0308662\N,0,4.5091713109,1.5623221623,0.0001646398\N,0,3.8904390188,-2
 .7686176299,0.0004701172\H,0,-1.4986835562,-1.9625935232,0.0002365205\
 H,0,0.9082040358,-2.2969366172,0.0003775053\H,0,1.4986965032,1.9626276
 436,-0.0001802786\H,0,-0.90818728,2.2969693141,-0.0003163637\Li,0,5.85
 72858654,2.9764039838,0.0006417775\Li,0,-5.8573266384,-2.9765286257,-0
 .0008357672\\Version=EM64L-G09RevA.02\State=1-A\HF=-694.0479847\RMSD=1
 .319e-09\Dipole=-0.0001302,-0.0002947,-0.0004431\Quadrupole=66.8388262
 ,-19.9001225,-46.9387036,124.600291,0.0218893,0.0186147\PG=C01 [X(C12H
 4Li2N4)]\@

2. Reactants and products of four reactions

Reactant and product of Reaction 1 is the same with **6** above.

Reaction 2 Reactant

1\1\GINC-IB-COMPUTE-0-14\SP\RB3LYP\6-311+G(d)\C14H8O2\ZHONGFANG\14-Aug
 -2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
 \\Title Card Required\\0,1\C,0,2.6806010861,2.189794798,0.\C,0,2.49755
 41849,0.7198932,0.\C,0,1.101898197,0.209534658,0.\C,0,-0.000462164,1.1
 212792412,0.\C,0,0.2379932157,2.5882144058,0.\C,0,1.6470254141,3.04451
 39914,0.\C,0,0.8680888185,-1.1483071618,0.\C,0,-1.290193812,0.63697324
 32,0.\C,0,-1.5536786885,-0.7546919486,0.\C,0,-0.4494518968,-1.66811017
 53,0.\C,0,-0.7091737872,-3.0626199268,0.\H,0,0.1271255984,-3.754227194
 4,0.\C,0,-2.0029904865,-3.5318630162,0.\C,0,-3.09318454,-2.6299900445,
 0.\C,0,-2.8747003067,-1.271144808,0.\H,0,1.7128305945,-1.828617167,0\
 H,0,3.7083207285,2.5382863454,0.\H,0,1.7960290443,4.1194163206,0.\H,0,
 -2.1163369825,1.3396991505,0.\H,0,-2.1925197026,-4.599840144,0.\H,0,-4

.1066424571,-3.0164464985,0.\H,0,-3.7106192311,-0.5791648262,0.\O,0,-0
.6741171189,3.4072380014,0.\O,0,3.4738922919,-0.0213844442,0.\Version
=EM64L-G09RevA.02\State=1-A\HF=-688.9329338\RMSD=4.581e-09\Dipole=-0.
915812,-1.1053356,0.\Quadrupole=-0.7520291,4.0708912,-3.3188621,12.572
511,0,0.\PG=CS [SG(C14H8O2)]\@

Reaction 2 Product

1\1\GINC-COMPUTE-0-39\SP\RB3LYP\6-311+G(d)\C14H8Li2O2\ZHONGFANG\14-Aug
-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
\\Title Card Required\0,1\C,0,-3.2011891384,-0.7258807123,0.004503002
\C,0,-2.0359653269,-1.4811082175,0.0039466517\C,0,-0.7885702397,-0.731
0959683,0.0030515072\C,0,-0.794803875,0.7218326622,0.0011785631\C,0,-2
.0486156968,1.4610788719,0.0009590752\C,0,-3.2072869355,0.6958240221,0
.0031048545\C,0,0.4417870506,-1.3948356747,0.0036662852\C,0,0.42982092
08,1.3960946033,-0.0005580288\C,0,1.6614165032,0.7271777719,-0.0001707
596\C,0,1.6675959701,-0.7153790822,0.0022876161\C,0,2.9263099108,-1.39
30367128,0.0031287475\H,0,2.9316345598,-2.4800095489,0.0051760222\C,0,
4.1067291091,-0.6968065148,0.0014055883\C,0,4.1006203548,0.7294599789,
-0.0013009011\C,0,2.9142896011,1.4155712613,-0.0020277\H,0,0.436417275
8,-2.4801071427,0.0054123459\H,0,-4.1528068744,-1.2542732492,0.0054590
256\H,0,-4.163398771,1.2160454645,0.0032123262\H,0,0.4151938889,2.4812
836065,-0.002210413\H,0,5.0540773714,-1.2272129663,0.0020848103\H,0,5.
0433947299,1.2679535422,-0.0027393082\H,0,2.9103332773,2.5025510729,-0
.0040233304\O,0,-2.048815462,2.7796795825,-0.0012431164\O,0,-2.0246584
014,-2.7997030076,0.0035233241\Li,0,-2.1317839657,4.5036319645,-0.0041
902826\Li,0,-2.0964788369,-4.5243686072,-0.0148959051\\Version=EM64L-G
09RevA.02\State=1-A\HF=-704.168768\RMSD=4.152e-09\Dipole=-1.2341402,-0
.0061243,-0.0365122\Quadrupole=-26.7519142,61.1719466,-34.4200325,-0.3
225431,0.147239,0.1881006\PG=C01 [X(C14H8Li2O2)]\@

Reaction 3 Reactant

1\1\GINC-COMPUTE-0-39\SP\RB3LYP\6-311+G(d)\C14H8O2\ZHONGFANG\14-Aug-20
14\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read\T
itle Card Required\0,1\C,0,4.2339574696,0.457321896,0.0000510875\C,0,
3.1352909798,1.2898188814,-0.0000048229\C,0,1.8257610829,0.7511661196,
-0.0000074916\C,0,1.6611523778,-0.6711914407,0.0000488567\C,0,2.810076
0951,-1.5003161557,0.0001046488\C,0,4.0715689846,-0.9463033033,0.00010
60165\C,0,0.6692992505,1.5757913865,-0.0000611442\C,0,0.3477638776,-1.
2057902201,0.0000452856\C,0,-0.7603705411,-0.38784967,-0.0000097307\C,
0,-0.6009378226,1.0379402272,-0.0000608857\C,0,-1.7726128607,1.8969648
544,-0.0001057625\H,0,-1.5981989906,2.9691635063,-0.0001460363\C,0,-3.
0416620097,1.4318952323,-0.0000869975\C,0,-3.3310177698,0.0039918603,-
0.0000253747\C,0,-2.1186006117,-0.9781113126,-0.0000194758\H,0,0.79643
41943,2.6541490017,-0.0001014788\H,0,5.2328854571,0.8800888087,0.00005
3082\H,0,3.263692569,2.367455892,-0.000046735\H,0,2.682523576,-2.57799
08862,0.0001457842\H,0,4.9465402621,-1.587142457,0.000149478\H,0,0.208
6960671,-2.2817098671,0.0000832459\H,0,-3.8912830511,2.1062937408,-0.0
001108055\O,0,-2.332227533,-2.1749585082,0.0000505591\O,0,-4.461701053
3,-0.4538915864,0.0000256969\\Version=EM64L-G09RevA.02\State=1-A\HF=-6
88.9258379\RMSD=3.697e-09\Dipole=3.501066,2.0775675,-0.0000627\Quadrup
ole=-7.4233131,7.6940515,-0.2707385,-11.8483173,0.0005478,-0.000767\PG
=C01 [X(C14H8O2)]\ \@

Reaction 3 Product

1\1\GINC-COMPUTE-0-33\SP\RB3LYP\6-311+G(d)\C14H8Li2O2\ZHONGFANG\14-Aug
-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
\Title Card Required\0,1\C,0,4.4740422374,0.2339756346,0.0001082779\

C,0,3.4530983219,1.1463257815,0.0000390447\C,0,2.0856454391,0.72698315
 67,0.0000190846\C,0,1.7946169614,-0.6899256022,0.0000670373\C,0,2.8932
 826915,-1.6079036042,0.0001388488\C,0,4.188546347,-1.1646895815,0.0001
 598905\C,0,1.0212157572,1.6350004194,-0.0000375077\C,0,0.4615632662,-1
 .1127813923,0.0000477815\C,0,-0.6077293336,-0.2032911901,-0.000002262\
 C,0,-0.3170788003,1.2197566031,-0.0000421585\C,0,-1.4003783741,2.14544
 17044,-0.0000725646\H,0,-1.1845349817,3.2100962998,-0.0001122543\C,0,-
 2.7018865095,1.6979588469,-0.0000444635\C,0,-3.0160079678,0.309611877,
 0.000006222\C,0,-1.971449091,-0.6435438342,-0.0000044869\H,0,1.2387262
 298,2.700870212,-0.0000718154\H,0,5.5065697396,0.5690197819,0.00012510
 5\H,0,3.6693187469,2.2114327056,0.000000189\H,0,2.6786677137,-2.673201
 5012,0.0001781507\H,0,5.0084920368,-1.876260499,0.000216973\H,0,0.2360
 227635,-2.1742482131,0.0000796653\H,0,-3.5281610915,2.4047849899,-0.00
 00548429\O,0,-2.3321237156,-1.9369233283,0.0000215706\O,0,-4.273192188
 6,-0.1664665841,0.0000772915\Li,0,-3.8107698154,-1.6109721878,-1.26442
 78883\Li,0,-3.8106703829,-1.6109824947,1.2646271117\\Version=EM64L-G09
 RevA.02\State=1-A\HF=-704.1798173\RMSD=5.088e-09\Dipole=-3.2671452,-2.
 2813403,0.0002017\Quadrupole=10.826535,-3.3711533,-7.4553817,23.143805
 4,-0.0010379,-0.0010534\PG=C01 [X(C14H8Li2O2)]\@

Reaction 4 Reactant

1\1\GINC-COMPUTE-0-33\SP\UB3LYP\6-311+G(d)\C14H8O2(3)\ZHONGFANG\09-Aug
 -2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=read
 \\Title Card Required\0,3\C,0,4.2916227508,-0.7067413926,0.011028488\
 C,0,3.103473858,-1.4060587557,0.0215889973\C,0,1.8626521587,-0.7206197
 753,0.0105928344\C,0,1.8625087574,0.7209317123,-0.0091784412\C,0,3.103
 1688796,1.4066647853,-0.020377588\C,0,4.2914757785,0.7076057306,-0.011
 1170958\C,0,0.6307799262,-1.4066088922,0.0172825213\C,0,0.6304979398,1
 .4066531421,-0.0149835195\C,0,-0.5986451561,0.732151952,-0.0051014916\
 S34

C,0,-0.5985171484,-0.7323912401,0.0071514129\C,0,-1.8155397056,-1.4310
062859,0.0053819183\H,0,-1.820054071,-2.5164466217,0.0082483207\C,0,-3
.0930160151,-0.7704831268,-0.0046741894\C,0,-3.0931135631,0.7699260795
,0.0100687529\C,0,-1.815762588,1.43061037,-0.003492825\H,0,0.633156687
5,-2.4920242732,0.0303437948\H,0,5.2348202579,-1.241814699,0.019729013
3\H,0,3.1061706135,-2.4910090884,0.0388894487\H,0,3.1056004148,2.49164
70718,-0.0358764258\H,0,5.2345547522,1.2428840744,-0.0201234619\H,0,0.
6326379107,2.4920901241,-0.0263852887\H,0,-1.8204071096,2.5160521057,-
0.0066852939\O,0,-4.1624471795,1.3850513152,0.032559034\O,0,-4.1623134
436,-1.3857608353,-0.0245048977\\Version=EM64L-G09RevA.02\State=3-A\HF
=-688.8829231\S2=2.025949\S2-1=0.\S2A=2.000403\RMSD=7.804e-09\Dipole=5
.7820887,0.0004719,-0.0028423\Quadrupole=-18.6236658,14.3925462,4.2311
196,-0.0025021,0.0300172,-0.3128906\PG=C01 [X(C14H8O2)]\\@

Reaction 4 Product

1\1\GINC-IB-COMPUTE-0-10\SP\RB3LYP\6-311+G(d)\C14H8Li2O2\ZHONGFANG\14-
Aug-2014\0\#p sp b3lyp/6-311+g* scrf=(solvent=thf) geom=check guess=r
ead\\Title Card Required\\0,1\C,0,-4.5740503065,-0.711494441,-0.000069
702\C,0,-3.3883300533,-1.4028263676,-0.0000439627\C,0,-2.1344975576,-0
.720913914,0.0000047888\C,0,-2.1344982121,0.7208680344,0.0000181079\C,
0,-3.3883313302,1.4027793593,-0.0000045832\C,0,-4.5740509552,0.7114463
514,-0.0000457077\C,0,-0.903817729,-1.3986203693,0.0000474489\C,0,-0.9
03819002,1.3985756161,0.0000309347\C,0,0.3214550507,0.7256952831,0.000
0523645\C,0,0.3214557065,-0.7257389347,0.0000672997\C,0,1.573468653,-1
.41860902,0.0000975944\H,0,1.5782149092,-2.506280328,0.0001928928\C,0,
2.7728659633,-0.7422312049,0.0000418278\C,0,2.7728653066,0.7421897893,
0.0000706322\C,0,1.573467361,1.4185665126,0.0000329988\H,0,-0.90568377
95,-2.4865449559,0.000048427\H,0,-5.5181576451,-1.2475944457,-0.000107
3999\H,0,-3.3890370148,-2.4897938146,-0.0000615099\H,0,-3.3890392579,2

.4897468042,0.0000083663\H,0,-5.5181587727,1.2475455103,-0.0000657259\
H,0,-0.9056860191,2.4865001943,0.0000184872\H,0,1.57821265,2.506237823
1,-0.0000631372\O,0,3.9819428561,1.2926863067,-0.0001051287\O,0,3.9819
440237,-1.2927266451,0.0002211397\Li,0,4.774835443,-0.0001642617,-1.26
26888229\Li,0,4.7748197117,0.0001241177,1.2628551765\\Version=EM64L-G0
9RevA.02\State=1-A\HF=-704.1881806\RMSD=6.552e-09\Dipole=5.4002171,0.0
000017,0.0001248\Quadrupole=36.4515752,-23.3805646,-13.0710106,0.00002
02,0.0016662,0.002107\PG=C01 [X(C14H8Li2O2)]\\@

3. All designed molecules and PADQ (9)

1

1\1\GINC-C03\FOpt\RB3LYP/6-311+G(d)\C14H8O2\ZHOU\15-Apr-2015\0\#p opt
freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Requi
red\\0,1\C,0,-3.58175411,-0.28207227\C,0,-2.78672921,0.94483555\C,0.
,-1.42234201,0.93570834\C,0,-0.69348728,-0.33561874\C,0,-1.4824638,-
1.55703544\C,0,-2.83090249,-1.54313622\C,0,-0.67273255,2.17681619\C,
0.,0.69348728,-0.33561874\C,0.,1.42234201,0.93570834\C,0.,0.67273255,2
.17681619\C,0.,2.78672921,0.94483555\H,0.,3.33480526,1.88142559\C,0.,3
.58175411,-0.28207227\C,0.,2.83090249,-1.54313622\C,0.,1.4824638,-1.55
703544\H,0.,-1.22973321,3.10749528\H,0.,-3.33480526,1.88142559\H,0.,-0
.97558522,-2.51265333\H,0.,-3.40600762,-2.46238698\H,0.,1.22973321,3.1
0749528\H,0.,3.40600762,-2.46238698\H,0.,0.97558522,-2.51265333\O,0.,-
4.81709302,-0.25635813\O,0.,4.81709302,-0.25635813\\Version=EM64L-G09R
evB.01\State=1-A1\HF=-688.8935201\RMSD=6.384e-09\RMSF=6.466e-06\Dipole
=0.,0.,0.1383525\Quadrupole=8.5422727,-33.9816572,25.4393845,0.,0.,0.\
PG=C02V [SGV(C14H8O2)]\\@

1_2Li

1\1\GINC-C02\SP\RB3LYP\6-311+G(d)\C14H8Li2O2\ZHOU\22-Apr-2015\0\#p b3

lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1
\\C,0,-3.61628885,-0.3088594,-0.0041952\\C,0,-2.85436002,0.87006243,-0.0
0272559\\C,0,-1.44317042,0.86578792,0.00069559\\C,0,-0.72013496,-0.36402
872,0.00293967\\C,0,-1.49255421,-1.55102509,0.00170725\\C,0,-2.87228293,
-1.53077131,-0.00171421\\C,0,-0.70280588,2.09861438,0.00163057\\C,0,0.73
346848,-0.34645016,0.00554996\\C,0,1.42730718,0.90039314,0.00535299\\C,0
,0.65745518,2.11505161,0.00382001\\C,0,2.83815533,0.93884444,0.0060521\\
H,0,3.33883479,1.9049142,0.00547507\\C,0,3.62695874,-0.2218511,0.006390
67\\C,0,2.91216832,-1.46127041,0.00828278\\C,0,1.53343164,-1.51478447,0.
00766279\\H,0,-1.25824947,3.03339314,0.00030095\\H,0,-3.37671502,1.82478
275,-0.00447353\\H,0,-0.99711704,-2.51670288,0.0032421\\H,0,-3.42871349,
-2.46481593,-0.00270777\\H,0,1.19016879,3.06290813,0.00422922\\H,0,3.490
46128,-2.38209973,0.00973952\\H,0,1.06100609,-2.49189924,0.00863898\\O,0
, -4.92560888,-0.31414807,-0.00752732\\O,0,4.93552297,-0.1944843,0.00492
458\\Li,0,-6.60705995,0.14659477,-0.01132984\\Li,0,6.67059439,-0.2440335
, -0.05193627\\Version=EM64L-G09RevB.01\\State=1-A\\HF=-704.1858998\\RMSD=
3.265e-09\\Dipole=0.0779015,0.344539,-0.1062384\\Quadrupole=101.9143493,
-46.5111745,-55.4031748,-10.2527423,-1.0636082,0.0211501\\PG=C01 [X(C14
H8Li2O2)]\\@

2

1\1\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C24H8O6\ZHOU\20-Apr-2015\0\#p opt

freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Requi
red\\0,1\\C,0.3663259839,-3.5233515188,0.\\C,0.2126992902,-2.7803705149,
-1.2460847429\\C,0.0168837658,-1.431375328,-1.2626653289\\C,0.0011477382
, -0.6879702274,0.\\C,0.0168837658,-1.431375328,1.2626653289\\C,0.2126992
902,-2.7803705149,1.2460847429\\C,-0.0581700647,-0.6812093031,-2.520375

862\C,-0.0011477382,0.6879702274,0.\C,-0.0168837658,1.431375328,-1.262
6653289\C,0.0581700647,0.6812093031,-2.520375862\C,-0.2126992902,2.780
3705149,-1.2460847429\H,-0.2735315851,3.3596161442,-2.1534230946\C,-0.
3663259839,3.5233515188,0.\C,-0.2126992902,2.7803705149,1.2460847429\C
,-0.0168837658,1.431375328,1.2626653289\C,0.0581700647,0.6812093031,2.
520375862\C,-0.0581700647,-0.6812093031,2.520375862\H,0.2735315851,-3.
3596161442,-2.1534230946\H,0.2735315851,-3.3596161442,2.1534230946\H,-
0.2735315851,3.3596161442,2.1534230946\C,0.3376863873,1.3920543267,-3.
8203927737\C,-0.3376863873,-1.3920543267,-3.8203927737\C,0.3376863873,
1.3920543267,3.8203927737\C,-0.3376863873,-1.3920543267,3.8203927737\C
,0.1452118001,0.6511640494,5.0822694859\C,-0.1452118001,-0.6511640494,
5.0822694859\C,0.1452118001,0.6511640494,-5.0822694859\C,-0.1452118001
,-0.6511640494,-5.0822694859\H,0.2880391747,1.222630994,-5.9925951616\
H,-0.2880391747,-1.222630994,-5.9925951616\H,-0.2880391747,-1.22263099
4,5.9925951616\H,0.2880391747,1.222630994,5.9925951616\O,0.7893752798,
2.525434129,3.857613573\O,-0.7893752798,-2.525434129,3.857613573\O,0.6
053356934,-4.7349817603,0.\O,-0.6053356934,4.7349817603,0.\O,0.7893752
798,2.525434129,-3.857613573\O,-0.7893752798,-2.525434129,-3.857613573
\\Version=EM64L-G09RevB.01\State=1-AG\HF=-1370.9878912\RMSD=6.137e-09\
RMSF=4.332e-05\Dipole=0.,0.,0.\Quadrupole=7.2466819,-48.4340084,41.187
3265,-3.8515866,0.,0.\PG=C02H [SGH(C4O2),X(C20H8O4)]\\@

2_2Li

1\1\GINC-C04\FOpt\RB3LYP\6-311+G(d)\C24H8Li2O6\ZHOU\23-Apr-2015\0\#p
opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Re
quired\\0,1\C,0.0113489704,0.7033845063,0.013705966\C,-0.0113489704,-0
.7033845063,-0.013705966\C,0.2487183635,3.5575722153,0.0706614639\C,-0
.2487183635,-3.5575722153,-0.0706614639\C,-0.1437159919,-2.8050060287,
-1.2626137877\C,0.1437159919,2.8050060287,1.2626137877\C,-0.1441455074

, -2.853060832, 1.1504547136\C, 0.1441455074, 2.853060832, -1.1504547136\C,
 -0.0126079906, -1.414483237, -1.2711308926\C, 0.0126079906, 1.414483237, 1.
 2711308926\C, -0.0147366891, -1.4638056251, 1.2146225401\C, 0.0147366891, 1.
 4638056251, -1.2146225401\C, 0.0447816997, -0.7459803022, 2.4736766819\C,
 0.0512510466, -0.6477172419, -2.5004771743\C, -0.0447816997, 0.7459803022,
 -2.4736766819\C, -0.0512510466, 0.6477172419, 2.5004771743\C, 0.2929340597
 , -1.476142501, 3.7534998409\C, 0.305430327, -1.3280177594, -3.8062280353\C
 , -0.2929340597, 1.476142501, -3.7534998409\C, -0.305430327, 1.3280177594, 3.
 8062280353\C, 0.1251045067, -0.7506176535, 5.0287603668\C, 0.1319880451, -
 0.5570994718, -5.0535791974\C, -0.1319880451, 0.5570994718, 5.0535791974\C
 , -0.1251045067, 0.7506176535, -5.0287603668\H, 0.1779655914, 3.3517858878,
 2.1908321901\H, -0.1779655914, -3.3517858878, -2.1908321901\H, -0.17826813
 3, -3.4362732552, 2.0561222655\H, 0.178268133, 3.4362732552, -2.0561222655\
 H, 0.252850905, -1.3429161224, 5.9286912078\H, 0.2583645212, -1.1152106346,
 -5.9753105849\H, -0.2583645212, 1.1152106346, 5.9753105849\H, -0.252850905
 , 1.3429161224, -5.9286912078\O, 0.4230123432, 4.8426201657, 0.0959029712\O
 , -0.4230123432, -4.8426201657, -0.0959029712\O, 0.6923617233, -2.638496854
 7, 3.8126172186\O, 0.7146628772, -2.4840415495, -3.9072445039\O, -0.6923617
 233, 2.6384968547, -3.8126172186\O, -0.7146628772, 2.4840415495, 3.90724450
 39\Li, 0.5044352335, 6.5926643275, 0.1752769157\Li, -0.5044352335, -6.59266
 43275, -0.1752769157\\Version=EM64L-G09RevB.01\State=1-AG\HF=-1386.3130
 117\RMSD=9.061e-09\RMSF=9.537e-06\Dipole=0., 0., 0.\Quadrupole=-47.77269
 89, 98.139856, -50.3671571, 22.0875067, 0.7442096, 4.9853997\PG=CI [X(C24H8
 Li2O6)]\@

2_4Li

1\1\GINC-C04\FOpt\RB3LYP\6-311+G(d)\C24H8Li4O6\ZHOU\17-Apr-2015\0\#p
 opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Re
 quired\0, 1\C, 0., 0.7020021991, -0.0956927771\C, 0., -0.7020021991, -0.0956

927771\C,0.,3.5602693243,-0.1054946193\C,0.,-3.5602693243,-0.105494619
 3\C,0.,-2.8227659281,1.1047268686\C,0.,2.8428241277,-1.3091520115\C,0.
 , -2.8428241277,-1.3091520115\C,0.,2.8227659281,1.1047268686\C,0.,-1.43
 41973371,1.1643426968\C,0.,1.4402323702,-1.3529214996\C,0.,-1.44023237
 02,-1.3529214996\C,0.,1.4341973371,1.1643426968\C,0.,-0.7119619152,-2.
 608808683\C,0.,-0.7224070081,2.4524094872\C,0.,0.7224070081,2.45240948
 72\C,0.,0.7119619152,-2.608808683\C,0.,-1.4438624081,-3.8983569022\C,0
 .,-1.4446585122,3.7067891285\C,0.,1.4446585122,3.7067891285\C,0.,1.443
 8624081,-3.8983569022\C,0.,-0.6688110326,-5.1388721951\C,0.,-0.6856991
 845,4.8996428462\C,0.,0.6688110326,-5.1388721951\C,0.,0.6856991845,4.8
 996428462\H,0.,3.397960811,-2.229113246\H,0.,-3.3771350197,2.024035189
 8\H,0.,-3.397960811,-2.229113246\H,0.,3.3771350197,2.0240351898\H,0.,-
 1.2507897176,-6.0553852829\H,0.,-1.2390869341,5.835706294\H,0.,1.25078
 97176,-6.0553852829\H,0.,1.2390869341,5.835706294\Li,0.,6.2209716589,-
 1.2577461017\Li,0.,-6.2209716589,-1.2577461017\O,0.,4.8686389108,-0.07
 95128132\O,0.,-4.8686389108,-0.0795128132\O,0.,-2.6869288698,-4.036081
 5606\O,0.,-2.7511711729,3.8389118247\O,0.,2.7511711729,3.8389118247\O,
 0.,2.6869288698,-4.0360815606\Li,0.,4.380257792,4.4861763565\Li,0.,-4.
 380257792,4.4861763565\\Version=EM64L-G09RevB.01\State=1-A1\HF=-1401.5
 513944\RMSD=6.375e-09\RMSF=1.976e-06\Dipole=0.,0.,5.4543785\Quadrupole
 =-78.5542418,118.3007175,-39.7464757,0.,0.,0.\PG=C02V [SGV(C24H8Li4O6)
]\@

2_6Li

1\I\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C24H8Li6O6\ZHOU\17-Apr-2015\0\#p
 opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Re
 quired\\0,1\C,0.,0.,0.717683073\C,0.,0.,-0.717683073\C,0.,0.,3.5690441
 611\C,0.,0.,-3.5690441611\C,0.,1.1965950545,-2.8434824447\C,0.,-1.1965
 950545,2.8434824447\C,0.,-1.1965950545,-2.8434824447\C,0.,1.1965950545

.2.8434824447\C,0.,1.2440670456,-1.4374028989\C,0.,-1.2440670456,1.437
4028989\C,0.,-1.2440670456,-1.4374028989\C,0.,1.2440670456,1.437402898
9\C,0.,-2.5422287099,-0.7243846535\C,0.,2.5422287099,-0.7243846535\C,0
.,2.5422287099,0.7243846535\C,0.,-2.5422287099,0.7243846535\C,0.,-3.80
22293276,-1.4454152401\C,0.,3.8022293276,-1.4454152401\C,0.,3.80222932
76,1.4454152401\C,0.,-3.8022293276,1.4454152401\C,0.,-4.9842880957,-0.
6906281835\C,0.,4.9842880957,-0.6906281835\C,0.,-4.9842880957,0.690628
1835\C,0.,4.9842880957,0.6906281835\H,0.,-2.1241504371,3.3850194685\H,
0.,2.1241504371,-3.3850194685\H,0.,-2.1241504371,-3.3850194685\H,0.,2.
1241504371,3.3850194685\H,0.,-5.9241947695,-1.2396664144\H,0.,5.924194
7695,-1.2396664144\H,0.,-5.9241947695,1.2396664144\H,0.,5.9241947695,1
.2396664144\Li,0.,0.,6.6139324595\Li,0.,0.,-6.6139324595\O,0.,0.,4.900
5254387\O,0.,0.,-4.9005254387\O,0.,-3.9446342499,-2.7660920032\O,0.,3.
9446342499,-2.7660920032\O,0.,3.9446342499,2.7660920032\O,0.,-3.944634
2499,2.7660920032\Li,0.,4.5942852686,4.3655745846\Li,0.,4.5942852686,-
4.3655745846\Li,0.,-4.5942852686,4.3655745846\Li,0.,-4.5942852686,-4.3
655745846\\Version=EM64L-G09RevB.01\State=1-AG\HF=-1416.7596557\RMSD=6
.279e-09\RMSF=1.118e-05\Dipole=0.,0.,0.\Quadrupole=-126.9434483,-43.25
37272,170.1971755,0.,0.,0.\PG=D02H [C2"(Li1O1C1C1.C1C1O1Li1),SG(C20H8L
i4O4)]\\@

3

1\1\GINC-C04\FOpt\RB3LYP\6-311+G(d)\C14H6O4\ZHOU\15-Apr-2015\0\#p opt
freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Requi
red\\0,1\C,0.0272864676,3.6576430858,0.090436243\C,0.0533276104,2.8145
185104,1.2734980863\C,0.0301013461,1.4548018643,1.2017649153\C,-0.0076
702982,0.7410340153,-0.1044886097\C,-0.0642154142,1.4605363008,-1.2529
558793\C,-0.0497215005,2.9249092699,-1.2723062621\C,0.0210115863,0.676
0958084,2.4136098404\C,0.0076702982,-0.7410340153,-0.1044886097\C,-0.0

301013461,-1.4548018643,1.2017649153\C,-0.0210115863,-0.6760958084,2.4
 136098404\C,-0.0533276104,-2.8145185104,1.2734980863\H,-0.0833490897,-
 3.3159717481,2.2351047702\C,-0.0272864676,-3.6576430858,0.090436243\C,
 0.0497215005,-2.9249092699,-1.2723062621\C,0.0642154142,-1.4605363008,
 -1.2529558793\H,0.0381279644,1.2147182693,3.3544776707\H,0.0833490897,
 3.3159717481,2.2351047702\H,-0.1216250502,0.9960215374,-2.2292380064\H
 ,-0.0381279644,-1.2147182693,3.3544776707\H,0.1216250502,-0.9960215374
 ,-2.2292380064\O,0.0551869214,4.8756999205,0.1275249535\O,-0.055186921
 4,-4.8756999205,0.1275249535\O,-0.0921027705,3.559771658,-2.309313502\
 O,0.0921027705,-3.559771658,-2.309313502\\Version=EM64L-G09RevB.01\Sta
 te=1-A\HF=-838.1466706\RMSD=7.738e-09\RMSF=1.573e-05\Dipole=0.,0.,3.05
 49421\Quadrupole=17.8081566,-38.094329,20.2861724,0.1387653,0.,0.\PG=C
 02 [X(C14H6O4)]\ \@

3_2Li

1\1\GINC-C04\SP\RB3LYP\6-311+G(d)\C14H6Li2O4\ZHOU\22-Apr-2015\0\#p b3
 lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1
 \C,0,-3.62116966,0.04676321,-0.01638811\C,0,-2.85160693,1.22059277,-0.
 02830701\C,0,-1.45044167,1.179295,-0.01144149\C,0,-0.76871393,-0.06715
 175,0.01037323\C,0,-1.54521294,-1.25533545,0.03740603\C,0,-2.93399614,
 -1.234377,0.03226704\C,0,-0.69770738,2.41721722,-0.00783284\C,0,0.6830
 1124,-0.0928647,-0.00275811\C,0,1.41477959,1.21333478,0.01490158\C,0,0
 .6526305,2.44028197,0.01254344\C,0,2.77868736,1.25720004,0.02809801\H,
 0,3.29944158,2.20978873,0.04720525\C,0,3.59701052,0.06111084,0.0145543
 3\C,0,2.84886721,-1.298314,-0.04430941\C,0,1.41412754,-1.25970904,-0.0
 3883824\H,0,-1.25580207,3.34911491,-0.01595097\H,0,-3.36323337,2.17918
 954,-0.04986485\H,0,-1.06876356,-2.22854969,0.07030253\H,0,1.19644189,
 3.37884886,0.02304071\H,0,0.92684411,-2.22626652,-0.07283976\O,0,-4.93
 45082,-0.00430128,-0.03563028\O,0,4.82114937,0.08781787,0.04441406\O,0

, -3.72481636, -2.30233293, 0.06480348 \O, 0, 3.50611333, -2.33922734, -0.0928
 5158 \Li, 0, -5.07036944, -1.53975491, 1.28648243 \Li, 0, -5.01667295, -1.62038
 294, -1.26904746 \\\Version=EM64L-G09RevB.01\State=1-A\HF=-853.446495\RMS
 D=6.519e-09\Dipole=-9.6932763, -0.0739428, 0.0226927\Quadrupole=8.163384
 3, -8.4558144, 0.2924301, 36.2885901, -0.1035912, 0.3038946\PG=C01 [X(C14H6
 Li2O4)]\@

3_4Li

1\1\GINC-C04\FOpt\RB3LYP\6-311+G(d)\C14H6Li4O4\ZHOU\17-Apr-2015\0\#p
 opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\Title Card Re
 quired\0, 1\C, 0, 3.5934293, 0.20337573\C, 0, 2.85056617, 1.36977359\C, 0, .
 1.42709763, 1.35795468\C, 0, 0.72677862, 0.11432232\C, 0, 1.4979979, -1.081
 80774\C, 0, 2.88466691, -1.07245149\C, 0, 0.68356622, 2.57898719\C, 0, -0.7
 2677862, 0.11432232\C, 0, -1.42709763, 1.35795468\C, 0, -0.68356622, 2.5789
 8719\C, 0, -2.85056617, 1.36977359\H, 0, -3.37131306, 2.32574352\C, 0, -3.5
 934293, 0.20337573\C, 0, -2.88466691, -1.07245149\C, 0, -1.4979979, -1.0818
 0774\H, 0, 1.22991971, 3.51953317\H, 0, 3.37131306, 2.32574352\H, 0, 1.0103
 997, -2.05121869\H, 0, -1.22991971, 3.51953317\H, 0, -1.0103997, -2.0512186
 9\O, 0, 4.9329428, 0.12042074\O, 0, -4.9329428, 0.12042074\O, 0, 3.66661696
 , -2.16150694\O, 0, -3.66661696, -2.16150694\Li, -1.26162248, 4.95661032, -1
 .38179431\Li, 1.26162248, 4.95661032, -1.38179431\Li, -1.26162248, -4.95661
 032, -1.38179431\Li, 1.26162248, -4.95661032, -1.38179431\Version=EM64L-G
 09RevB.01\State=1-A1\HF=-868.7223114\RMSD=2.730e-09\RMSF=4.829e-05\Dip
 ole=0, 0, -3.7779694\Quadrupole=-17.5116659, 55.792471, -38.2808051, 0, 0
 , 0.\PG=C02V [SGV(C14H6O4), X(Li4)]\@

4

1\1\GINC-C04\SP\RB3LYP\6-311+G(d)\C18H6O6\ZHOU\16-Apr-2015\0\#p b3lyp

/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1\C,
0,-0.74767451,-3.74780099,-0.19932638\C,0,-1.40578416,-2.44430224,-0.2
5781314\C,0,-0.74107986,-1.27820363,-0.05001732\C,0,0.74107986,-1.2782
0363,0.05001732\C,0,1.40578416,-2.44430224,0.25781314\C,0,0.74767451,-
3.74780099,0.19932638\C,0,1.47749674,-0.00269217,-0.05001732\C,0,0.736
41689,1.2808958,0.05001732\C,0,1.41393575,2.43959592,0.25781314\H,0,0.
90609398,3.37924471,0.43805627\C,0,2.87185361,2.52140561,0.19932638\C,
0,3.61952812,1.22639538,-0.19932638\C,0,2.81971992,0.00470632,-0.25781
314\H,0,-2.47346478,-2.47432276,-0.43805627\H,0,2.47346478,-2.47432276
,0.43805627\H,0,3.37955875,-0.90492195,-0.43805627\C,0,-2.81971992,0.0
0470632,0.25781314\C,0,-3.61952812,1.22639538,0.19932638\C,0,-2.871853
61,2.52140561,-0.19932638\C,0,-1.41393575,2.43959592,-0.25781314\C,0,-
0.73641689,1.2808958,-0.05001732\C,0,-1.47749674,-0.00269217,0.0500173
2\H,0,-3.37955875,-0.90492195,0.43805627\H,0,-0.90609398,3.37924471,-0
.43805627\O,0,-4.81536618,1.2439128,0.41712763\O,0,-3.48494318,3.54827
304,-0.41712763\O,0,1.33042301,-4.79218584,0.41712763\O,0,-1.33042301,
-4.79218584,-0.41712763\O,0,3.48494318,3.54827304,0.41712763\O,0,4.815
36618,1.2439128,-0.41712763\\Version=EM64L-G09RevB.01\State=1-A1\HF=-1
141.0548286\RMSD=8.895e-09\Dipole=-0.0021535,-0.0012433,0.\Quadrupole=
-15.5017187,-15.4942288,30.9959475,-0.0064864,0.0041424,-0.0071749\PG=
D03 [X(C18H6O6)]\\@

4_2Li

1\1\GINC-C02\SP\RB3LYP\6-311+G(d)\C18H6Li2O6\ZHOU\22-Apr-2015\0\\#p b3
lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1
\C,0,-3.70188338,0.96461407,0.11165336\C,0,-2.8448402,-0.18677803,0.00
426274\C,0,-1.47290692,-0.12413818,-0.02310321\C,0,-0.81306326,1.20158
462,0.01060388\C,0,-1.55426103,2.33092849,0.1876496\C,0,-3.00737328,2.
32839091,0.24605686\C,0,0.64587131,1.28309713,-0.11307944\C,0,1.455776

35,0.06759053,0.13314771\C,0,2.80967443,0.19898621,0.32490203\H,0,3.42
802461,-0.6515134,0.57980157\C,0,3.52313571,1.43736213,0.15280702\C,0,
2.70367204,2.63441658,-0.35808174\C,0,1.26113696,2.45743278,-0.4242016
8\H,0,-3.36596613,-1.13418175,-0.02236718\H,0,-1.08891281,3.30253636,0
.29728082\H,0,0.69688538,3.33555641,-0.71314536\C,0,-1.23225339,-2.587
52763,-0.16620901\C,0,-0.48567705,-3.76423412,-0.13156657\C,0,0.972580
32,-3.66935588,0.02864092\C,0,1.55249838,-2.40604718,0.12372937\C,0,0.
79182747,-1.22315893,0.08876925\C,0,-0.64205889,-1.31691578,-0.0509295
4\H,0,-2.30118832,-2.69627425,-0.2916676\H,0,2.63080722,-2.37080927,0.
20356095\O,0,-0.95877619,-4.97097192,-0.23438454\O,0,1.60660132,-4.805
70202,0.05011489\O,0,-3.65958894,3.3542584,0.38884975\O,0,-4.93030654,
0.89831833,0.12458258\O,0,4.73077292,1.56259797,0.35065026\O,0,3.25177
063,3.68639478,-0.65902299\Li,0,0.27470056,-5.86242663,1.15092207\Li,0
,0.50998859,-5.75437071,-1.37586188\\Version=EM64L-G09RevB.01\State=1-
A\HF=-1156.3850706\RMSD=6.772e-09\Dipole=0.821044,-12.6217929,-0.31364
23\Quadrupole=-82.1964024,73.2595058,8.9368965,-10.5322069,0.7217494,1
.7758525\PG=C01 [X(C18H6Li2O6)]\@

4_4Li

1\1\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C18H6Li4O6\ZHOU\17-Apr-2015\0\#p
opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Re
quired\\0,1\C,-0.0476871038,2.8624170188,-2.2704553542\C,-0.0557196043
,1.4618143789,-2.2310840295\C,-0.0033329259,0.7401169102,-1.0287112768
\C,0.0434919381,1.4585071839,0.1953003898\C,0.0583910043,2.88284735,0.
1576679394\C,0.0222379985,3.599325952,-1.0243859852\C,0.0496815779,0.7
476047662,1.4600554625\C,-0.0496815779,-0.7476047662,1.4600554625\C,-0
.1271307595,-1.4094286861,2.6663486832\H,-0.2176410503,-2.4870747465,2
.7064230607\C,-0.0758594176,-0.7660550947,3.9462263489\C,0.0758594176,
0.7660550947,3.9462263489\C,0.1271307595,1.4094286861,2.6663486832\H,-

0.1137469561,0.9544434348,-3.1862151027\H,0.0880075618,3.4581478912,1.0749505948\H,0.2176410503,2.4870747465,2.7064230607\C,0.0557196043,-1.4618143789,-2.2310840295\C,0.0476871038,-2.8624170188,-2.2704553542\C,-0.0222379985,-3.599325952,-1.0243859852\C,-0.0583910043,-2.88284735,0.1576679394\C,-0.0434919381,-1.4585071839,0.1953003898\C,0.0033329259,-0.7401169102,-1.0287112768\H,0.1137469561,-0.9544434348,-3.1862151027\H,-0.0880075618,-3.4581478912,1.0749505948\O,0.1051901188,-3.5883874653,-3.3696178559\O,-0.024164717,-4.929567388,-1.1431999513\O,0.024164717,4.929567388,-1.1431999513\O,-0.1051901188,3.5883874653,-3.3696178559\O,-0.1389751702,-1.3778980244,5.0175628284\O,0.1389751702,1.3778980244,5.0175628284\Li,-1.1781830351,-4.9827092176,-2.7354834172\Li,1.3384789689,-4.9792896442,-2.5502520949\Li,-1.3384789689,4.9792896442,-2.5502520949\Li,1.1781830351,4.9827092176,-2.7354834172\\Version=EM64L-G09 RevB.01\State=1-A\HF=-1171.6647859\RMSD=9.748e-09\RMSF=1.618e-05\Dipole=0.,0.,-11.7981514\Quadrupole=-10.7253201,80.6133899,-69.8880698,-4.2334871,0.,0.\PG=C02 [X(C18H6Li4O6)]\\@

4_6Li

1\1\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C18H6Li6O6\ZHOU\18-Apr-2015\0\#p
 opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1\C,0.0746427574,1.237270686,-3.5814088788\C,0.0875963145,0.0536167624,-2.8604752232\C,0.0064421529,0.0141533444,-1.4404261264\C,-0.071851747,1.2426199624,-0.7310913303\C,-0.113575778,2.4539117054,-1.4766936401\C,-0.0526060308,2.4872439875,-2.8610654542\C,-0.071851747,1.2426199624,0.7310913303\C,0.0064421529,0.0141533444,1.4404261264\C,0.0875963145,0.0536167624,2.8604752232\H,0.1798718956,-0.8645539854,3.430398302\C,0.0746427574,1.237270686,3.5814088788\C,-0.0526060308,2.4872439875,2.8610654541\C,-0.113575778,2.4539117054,1.4766936401\H,0.1798718956,-0.8645539854,-3.430398302\H,-0.1847052319,3.409815585,-0.9693

124449\H,-0.1847052319,3.409815585,0.9693124449\C,-0.0136230999,-2.502
8855505,-1.3891918897\C,-0.0299029919,-3.7186137477,-0.7242568022\C,-0
.0299029919,-3.7186137477,0.7242568022\C,-0.0136230999,-2.5028855505,1
.3891918897\C,0.0027730461,-1.2523722472,0.7102091445\C,0.0027730461,-
1.2523722472,-0.7102091445\H,-0.02873638,-2.539391067,-2.4731677616\H,
-0.02873638,-2.539391067,2.4731677616\O,-0.0559563495,-4.9313251103,-1
.3085022716\O,-0.0559563495,-4.9313251103,1.3085022716\O,-0.0791186947
,3.5990891451,-3.6197664941\O,0.1766209983,1.3413812111,-4.920447219\O
,0.1766209983,1.3413812111,4.920447219\O,-0.0791186947,3.5990891451,3.
6197664941\Li,-1.3145004023,-5.6674346581,0.\Li,1.1898053488,-5.681890
695,0.\Li,-1.1687435919,2.7424424774,-4.9972406884\Li,1.3285246423,2.9
226089584,-4.8040259794\Li,-1.1687435919,2.7424424774,4.9972406884\Li,
1.3285246423,2.9226089584,4.8040259794\\Version=EM64L-G09RevB.01\State
=1-A\HF=-1186.9229298\RMSD=3.701e-09\RMSF=2.540e-05\Dipole=0.222241,-
0.0773902,0.\Quadrupole=-30.1336679,15.7203015,14.4133664,5.2057275,0.
,0.\PG=CS [SG(Li2),X(C18H6Li4O6)]\@

5

1\1\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C24H10O4\ZHOU\15-Apr-2015\0\#p op
t freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Requ
ired\0,1\C,0.,3.546157,0.\C,1.197057,2.849998,-0.039205\C,1.221791,1.
447184,-0.061343\C,0.,0.733298,0.\C,-1.221791,1.447184,0.061343\C,-1.1
97057,2.849998,0.039205\C,2.509463,0.735142,-0.111042\C,0.,-0.733298,0
.\C,1.221791,-1.447184,0.061343\C,2.509463,-0.735142,0.111042\C,1.1970
57,-2.849998,0.039205\H,2.119245,-3.414139,0.041762\C,0.,-3.546157,0.\
C,-1.197057,-2.849998,-0.039205\C,-1.221791,-1.447184,-0.061343\C,-2.5
09463,-0.735142,-0.111042\C,-2.509463,0.735142,0.111042\H,0.,4.629815,
0.\H,2.119245,3.414139,-0.041762\H,-2.119245,3.414139,0.041762\H,0.,-4
.629815,0.\H,-2.119245,-3.414139,-0.041762\C,3.682946,-1.389915,0.3281

59\H,3.72021,-2.445097,0.563437\C,3.682946,1.389915,-0.328159\H,3.72021,2.445097,-0.563437\C,-3.682946,-1.389915,-0.328159\H,-3.72021,-2.445097,-0.563437\C,-3.682946,1.389915,0.328159\H,-3.72021,2.445097,0.563437\C,-4.978909,-0.740951,-0.22315\C,-4.978909,0.740951,0.22315\C,4.978909,-0.740951,0.22315\C,4.978909,0.740951,-0.22315\O,6.032625,-1.316802,0.439428\O,6.032625,1.316802,-0.439428\O,-6.032625,-1.316802,-0.439428\O,-6.032625,1.316802,0.439428\\Version=EM64L-G09RevB.01\State=1-A\HF=-1221.7403251\RMSD=6.837e-09\RMSF=9.139e-06\Dipole=0.,0.,0.\Quadrupole=-76.1842952,50.266339,25.9179562,0.,0.,0.\PG=D02 [C2(H1C1C1.C1C1H1).X(C20H8O4)]\\@

5_2Li

1\1\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C24H10Li2O4\ZHOU\17-Apr-2015\0\#p

opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,1\C,0.015602,3.535315,-0.224115\C,0.039757,2.845439,-1.432248\C,0.058202,1.447565,-1.458827\C,0.015602,0.723011,-0.231563\C,0.007016,1.427285,1.007102\C,0.009217,2.838982,0.969157\C,0.100339,0.73782,-2.743726\C,-0.015602,-0.723011,-0.231563\C,-0.058202,-1.447565,-1.458827\C,-0.100339,-0.73782,-2.743726\C,-0.039757,-2.845439,-1.432248\H,-0.024376,-3.415012,-2.35144\C,-0.015602,-3.535315,-0.224115\C,-0.009217,-2.838982,0.969157\C,-0.007016,-1.427285,1.007102\C,0.000968,-0.709759,2.275709\C,-0.000968,0.709759,2.275709\H,-0.002026,4.619818,-0.22087\H,0.024376,3.415012,-2.35144\H,-0.003517,3.404378,1.890744\H,0.002026,-4.619818,-0.22087\H,0.003517,-3.404378,1.890744\C,-0.304521,-1.39095,-3.925213\H,-0.527884,-2.449072,-3.961634\C,0.304521,1.39095,-3.925213\H,0.527884,2.449072,-3.961634\C,0.002958,-1.395148,3.51769\H,0.003907,-2.477611,3.559655\C,-0.002958,1.395148,3.51769\H,-0.003907,2.477611,3.559655\C,0.001627,-0.727733,4.733329\C,-0.001627,0.727733,4.733329\C,-0.20662,-0.743988,-5.215875\C,0.20662,0.743988,-5.215875\O,-0.4090

59,-1.32577,-6.274876\O,0.409059,1.32577,-6.274876\O,0.002412,-1.30073
 3,5.932609\O,-0.002412,1.300733,5.932609\Li,-1.265643,-0.001463,6.7310
 54\Li,1.265643,0.001463,6.731054\\Version=EM64L-G09RevB.01\State=1-A\H
 F=-1237.0394286\RMSD=4.921e-09\RMSF=5.038e-06\Dipole=0.,0.,10.5514513\
 Quadrupole=-7.0505369,-9.0205587,16.0710957,-1.1186349,0.,0.\PG=C02 [X
 (C24H10Li2O4)]\\@

5_4Li

1\1\GINC-C03\FOpt\RB3LYP\6-311+G(d)\C24H10Li4O4\ZHOU\17-Apr-2015\0\#p
 opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card R
 equired\\0,1\C,0.,-3.528034111,0.\C,1.2050345164,-2.839572144,0.\C,1.2
 398918252,-1.4350066807,0.\C,0.,-0.7211351393,0.\C,-1.2398918252,-1.43
 50066807,0.\C,-1.2050345164,-2.839572144,0.\C,2.5086696207,-0.70770019
 81,0.\C,0.,0.7211351393,0.\C,1.2398918252,1.4350066807,0.\C,2.50866962
 07,0.7077001981,0.\C,1.2050345164,2.839572144,0.\H,2.123933087,3.41051
 36982,0.\C,0.,3.528034111,0.\C,-1.2050345164,2.839572144,0.\C,-1.23989
 18252,1.4350066807,0.\C,-2.5086696207,0.7077001981,0.\C,-2.5086696207,
 -0.7077001981,0.\H,0.,-4.6142440836,0.\H,2.123933087,-3.4105136982,0.\
 H,-2.123933087,-3.4105136982,0.\H,0.,4.6142440836,0.\H,-2.123933087,3.
 4105136982,0.\C,3.7534923926,1.3917904756,0.\H,3.7930091702,2.47478101
 33,0.\C,3.7534923926,-1.3917904756,0.\H,3.7930091702,-2.4747810133,0.\
 C,-3.7534923926,1.3917904756,0.\H,-3.7930091702,2.4747810133,0.\C,-3.7
 534923926,-1.3917904756,0.\H,-3.7930091702,-2.4747810133,0.\C,-4.96928
 21156,0.7260544515,0.\C,-4.9692821156,-0.7260544515,0.\C,4.9692821156,
 0.7260544515,0.\C,4.9692821156,-0.7260544515,0.\O,6.1740716509,1.30354
 73869,0.\O,6.1740716509,-1.3035473869,0.\O,-6.1740716509,1.3035473869,
 0.\O,-6.1740716509,-1.3035473869,0.\Li,-6.9511591976,0.,1.2590452404\L
 i,-6.9511591976,0.,-1.2590452404\Li,6.9511591976,0.,1.2590452404\Li,6.
 9511591976,0.,-1.2590452404\\Version=EM64L-G09RevB.01\State=1-AG\HF=-1

252.3246078\RMSD=2.607e-09\RMSF=3.376e-05\Dipole=0.,0.,0.\Quadrupole=1
22.3657999,-76.1811079,-46.184692,0.,0.,0.\PG=D02H [C2'(H1C1C1.C1C1H1)
,SG'(Li4),SG''(C20H8O4)]\@

6

1\1\GINC-C04\FOpt\RB3LYP\6-311+G(d)\C30H10O8\ZHOU\21-Apr-2015\0\#p op
t freq b3lyp/6-311+g(d) scf=xqc scrf=(solvent=thf) symm=loose\Title C
ard Required\0,1\C,3.5428394985,3.6881029746,-0.856830378\C,2.7828121
083,2.4709983694,-0.6012200261\C,1.4645520372,2.4755268801,-0.27139351
62\C,0.731651466,3.7630442042,-0.1523577328\C,1.3456739721,4.936500266
9,-0.4514205742\C,2.7635158044,5.0208296321,-0.7949512349\C,-0.6913616
592,3.7503806318,0.2309315826\C,-1.4663019306,2.4900369337,0.075304405
2\C,-2.8239671086,2.5267175157,0.1130919049\H,-3.4353835339,1.64925384
48,-0.0507268903\C,-3.5711515424,3.733862348,0.4450703887\C,-2.7411686
767,4.960841765,0.8892807253\C,-1.2944089934,4.8709489741,0.7029246363
\H,3.3455635944,1.5555254102,-0.7266597304\H,0.8095377605,5.8769575911
, -0.4591977111\H,-0.7352117666,5.7683583334,0.9359928004\C,1.368630058
,0.0000001733,-0.0000000443\C,0.7083617175,-1.2267488975,0.0850615337\
C,-0.7107218302,-1.2304417892,0.024799472\C,-1.3701700743,-0.000000402
7,-0.0000000443\C,-0.7107223477,1.2304412612,-0.0247995607\C,0.7083612
016,1.2267489663,-0.0850616224\H,2.4462278557,0.0000003999,-0.00000004
43\H,-2.4475150263,-0.0000006292,-0.0000000443\O,3.3231303909,6.076402
8133,-1.0217543721\O,4.7301072184,3.6835323613,-1.1263147243\O,-4.7871
564129,3.7894027546,0.4270217241\O,-3.2895107002,5.9512596417,1.333290
9209\C,1.4645530784,-2.4755264932,0.2713934275\C,-1.4663008833,-2.4900
377795,-0.0753044938\C,-0.6913600818,-3.7503811517,-0.2309316713\C,0.7
316530488,-3.7630441255,0.1523576441\C,2.7828131476,-2.470997428,0.601
2199375\H,3.3455642486,-1.5555242321,0.7266596417\C,3.5428410497,-3.68
81017135,0.8568302894\C,2.7635179161,-5.0208286989,0.7949511463\C,1.34

56760484,-4.93649993,0.4514204856\H,0.8095402323,-5.8769574797,0.45919
 76224\C,-1.2944069447,-4.8709497476,-0.702924725\H,-0.7352093404,-5.76
 83588717,-0.9359928891\C,-2.7411665902,-4.960843147,-0.8892808139\C,-2
 .8239660459,-2.5267189325,-0.1130919936\H,-3.4353828402,-1.6492555188,
 0.0507268016\C,-3.5711499719,-3.7338640791,-0.4450704774\O,4.730108767
 7,-3.6835306008,1.1263146356\O,3.3231329467,-6.0764016446,1.0217542834
 \O,-3.2895081971,-5.9512612544,-1.3332910095\O,-4.7871548191,-3.789404
 9971,-0.4270218128\\Version=EM64L-G09RevB.01\State=1-A\HF=-1751.330024
 2\RMSD=8.663e-09\RMSF=3.921e-06\Dipole=0.1052388,0.,0.\Quadrupole=-34.
 6495133,-18.7545928,53.4041061,-0.0000033,-0.0000002,0.8652849\PG=C02
 [C2(H1C1C1H1),X(C28H8O8)]\@

6_2Li

1\1\GINC-C04\SP\RB3LYP\6-311+G(d)\C30H10Li2O8\ZHOU\22-Apr-2015\0\#p b
 3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,
 1\C,0,-3.29771218,4.00811506,-0.05184391\C,0,-2.1491198,3.12721102,0.1
 3627475\C,0,-2.2245986,1.77638403,0.0119507\C,0,-3.54535938,1.12610757
 ,-0.20029975\C,0,-4.64094093,1.91303564,-0.4835118\C,0,-4.62082135,3.3
 4607262,-0.47776972\C,0,-3.6420444,-0.3124241,-0.0524586\C,0,-2.466907
 01,-1.11114205,0.1264886\C,0,-2.60042096,-2.49702314,0.2867702\H,0,-1.
 73952799,-3.1340222,0.44406279\C,0,-3.84806714,-3.13484369,0.26738462\
 C,0,-5.05009997,-2.32268262,0.09249379\C,0,-4.90636358,-0.95001497,-0.
 05708341\H,0,-1.22197282,3.63642049,0.36660633\H,0,-5.60303363,1.47093
 528,-0.70574388\H,0,-5.81591431,-0.37216753,-0.15750505\C,0,0.25445651
 ,1.49100085,0.03164722\C,0,1.43684191,0.73572578,0.08379436\C,0,1.3125
 905,-0.67736365,0.1437004\C,0,0.03169942,-1.2378312,0.14700991\C,0,-1.
 1445375,-0.48372798,0.12726162\C,0,-1.01737407,0.93183478,0.07343687\H
 ,0,0.33905726,2.56040549,-0.07843326\H,0,-0.04989015,-2.31221479,0.125
 76148\O,0,-5.59012607,4.05263469,-0.75973435\O,0,-3.21820165,5.2181479

9,0.09722548\O,0,-4.04202503,-4.41376588,0.40873759\O,0,-6.18214463,-2
.98720338,0.10545268\C,0,2.74544291,1.38630295,0.08838619\C,0,2.496986
63,-1.54190087,0.11945\C,0,3.80323991,-0.91970879,-0.21571977\C,0,3.95
409279,0.53526893,-0.05185089\C,0,2.88438266,2.73634908,0.24600777\H,0
,2.02976727,3.38622731,0.37927531\C,0,4.16424709,3.41148408,0.28570119
\C,0,5.4165657,2.5225543,0.17928449\C,0,5.19376057,1.0887918,0.0330029
8\H,0,6.09142758,0.48417122,0.01026786\C,0,4.83811288,-1.69839097,-0.6
3082106\H,0,5.76770475,-1.27412767,-0.98895271\C,0,4.79134887,-3.15422
007,-0.57714322\C,0,2.42619286,-2.88457433,0.33433185\H,0,1.51575721,-
3.36547715,0.66779707\C,0,3.54145917,-3.78040352,0.08084796\O,0,4.2811
4422,4.62329835,0.41409676\O,0,6.53490626,3.00896919,0.22082989\O,0,5.
69558273,-3.86299352,-0.98573319\O,0,3.50888281,-4.97725603,0.3202864\
Li,0,-5.7411245,-4.30713079,1.56456851\Li,0,-5.59119337,-4.57495718,-0
.9453827\\Version=EM64L-G09RevB.01\State=1-A\HF=-1766.6456938\RMSE=8.8
55e-09\Dipole=-8.0793688,-10.0776873,0.8017518\Quadrupole=0.3852644,-2
4.1125099,23.7272455,111.8236623,-10.8975377,-4.1975098\PG=C01 [X(C30H
10Li2O8)]\\@

6_4Li

1\1\GINC-C02\SP\RB3LYP\6-311+G(d)\C30H10Li4O8\ZHOU\22-Apr-2015\0\#p b
3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,
1\C,0,3.07267055,-4.17782012,0.1611451\C,0,2.01399878,-3.18609456,0.28
923397\C,0,2.21248936,-1.85349072,0.10200025\C,0,3.59123004,-1.3399885
6,-0.13711567\C,0,4.61778816,-2.24808151,-0.32858705\C,0,4.47003584,-3
.66359891,-0.22672902\C,0,3.81513696,0.08680704,-0.10700713\C,0,2.7265
3305,0.99182767,0.07337914\C,0,2.99144632,2.36114389,0.18526162\H,0,2.
19688409,3.07719622,0.355297\C,0,4.29158198,2.88345539,0.09583679\C,0,
5.4042536,1.96908639,-0.12630809\C,0,5.13434311,0.61680163,-0.20892036
\H,0,1.03979125,-3.59327856,0.52845267\H,0,5.62350432,-1.91085214,-0.5

4083665\H,0,5.98256347,-0.04256131,-0.34095357\C,0,-0.23915724,-1.3468
 4303,0.10420157\C,0,-1.34167514,-0.48777204,0.11485429\C,0,-1.08686512
 ,0.90095672,0.12400757\C,0,0.23915724,1.34684303,0.10420157\C,0,1.3416
 7514,0.48777204,0.11485429\C,0,1.08686512,-0.90095672,0.12400757\H,0,-
 0.41918765,-2.40856076,0.04413257\H,0,0.41918765,2.40856076,0.04413257
 \O,0,5.38620418,-4.4756218,-0.40433314\O,0,2.86611834,-5.37256781,0.33
 44514\O,0,4.59933452,4.1492377,0.19949684\O,0,6.59876295,2.53974632,-0
 .20725338\C,0,-2.72653305,-0.99182767,0.07337914\C,0,-2.21248936,1.853
 49072,0.10200025\C,0,-3.59123004,1.33998856,-0.13711567\C,0,-3.8151369
 6,-0.08680704,-0.10700713\C,0,-2.99144632,-2.36114389,0.18526162\H,0,-
 2.19688409,-3.07719622,0.355297\C,0,-4.29158198,-2.88345539,0.09583679
 \C,0,-5.4042536,-1.96908639,-0.12630809\C,0,-5.13434311,-0.61680163,-0
 .20892036\H,0,-5.98256347,0.04256131,-0.34095357\C,0,-4.61778816,2.248
 08151,-0.32858705\H,0,-5.62350432,1.91085214,-0.54083665\C,0,-4.470035
 84,3.66359891,-0.22672902\C,0,-2.01399878,3.18609456,0.28923397\H,0,-1
 .03979125,3.59327856,0.52845267\C,0,-3.07267055,4.17782012,0.1611451\O
 ,0,-4.59933452,-4.1492377,0.19949684\O,0,-6.59876295,-2.53974632,-0.20
 725338\O,0,-5.38620418,4.4756218,-0.40433314\O,0,-2.86611834,5.3725678
 1,0.3344514\Li,0,6.33349533,3.88160159,1.22467761\Li,0,6.03042337,4.11
 017633,-1.26356551\Li,0,-6.33349533,-3.88160159,1.22467761\Li,0,-6.030
 42337,-4.11017633,-1.26356551\\Version=EM64L-G09RevB.01\State=1-A\HF=-
 1781.9462925\RMSE=4.188e-09\Dipole=0.,0.,0.2412439\Quadrupole=55.86107
 18,-44.347375,-11.5136968,224.6429732,0.,0.\PG=C02 [X(C30H10Li4O8)]\@

6_6Li

1\1\GINC-C02\SP\RB3LYP\6-311+G(d)\C30H10Li6O8\ZHOU\22-Apr-2015\0\#p b
 3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,
 1\C,0,-3.48740773,-4.03607688,-0.45770657\C,0,-2.35391456,-3.14901635,
 -0.38263898\C,0,-2.44861003,-1.79709222,-0.17546371\C,0,-3.7979564,-1.

17095865,-0.07319907\C,0,-4.91467089,-1.9875626,-0.11745467\C,0,-4.875
 41314,-3.40468379,-0.28840012\C,0,-3.9021956,0.26689399,0.05635699\C,0
 ,-2.73234539,1.08249492,0.08708021\C,0,-2.88028648,2.47214743,0.217340
 51\H,0,-2.01828636,3.12664703,0.25687671\C,0,-4.13099538,3.08954905,0.
 31421771\C,0,-5.33012283,2.26422624,0.27368625\C,0,-5.17916626,0.89733
 273,0.15068271\H,0,-1.39426859,-3.63544985,-0.50465554\H,0,-5.91008435
 ,-1.57164272,-0.0342256\H,0,-6.08681371,0.3075292,0.12739486\C,0,0.025
 61425,-1.49090373,-0.04042285\C,0,1.20333573,-0.73138059,0.00486704\C,
 0,1.0721982,0.68897083,-0.01865676\C,0,-0.2325881,1.22778084,0.0081664
 4\C,0,-1.39530833,0.46787233,0.00533644\C,0,-1.26215376,-0.94775617,-0
 .06723312\H,0,0.12323334,-2.56567831,-0.04959617\H,0,-0.3270674,2.3018
 6665,0.03331694\O,0,-5.88498059,-4.12415218,-0.3162886\O,0,-3.37093658
 ,-5.24976191,-0.64581744\O,0,-4.32633614,4.38287746,0.44421951\O,0,-6.
 48160049,2.92766672,0.36744157\C,0,2.52246014,-1.3484794,0.07678387\C,
 0,2.25034974,1.5306577,-0.0733458\C,0,3.54468421,0.92670422,-0.0690237
 1\C,0,3.6800901,-0.52126041,0.05743009\C,0,2.68430374,-2.75366791,0.19
 067923\H,0,1.82386994,-3.4127847,0.21850808\C,0,3.92904019,-3.3545641,
 0.29326159\C,0,5.11306559,-2.510643,0.2925463\C,0,4.95489223,-1.138264
 1,0.17055895\H,0,5.85812233,-0.53947185,0.18258996\C,0,4.68101764,1.76
 686415,-0.18748456\H,0,5.6782472,1.34452588,-0.21728488\C,0,4.5832441,
 3.1481983,-0.29288893\C,0,2.15333666,2.94776385,-0.16277535\H,0,1.1866
 7086,3.43796212,-0.17065803\C,0,3.26399254,3.7638326,-0.26333843\O,0,4
 .15063286,-4.66454874,0.42026461\O,0,6.27662501,-3.15113149,0.42953482
 \O,0,5.60226579,3.99038456,-0.43425281\O,0,3.25050038,5.09543366,-0.36
 396304\Li,0,-5.95260966,4.45726219,-0.74885249\Li,0,-5.87202147,4.1779
 6697,1.75360953\Li,0,4.84004071,5.40864299,0.72852731\Li,0,4.64021782,
 5.14523498,-1.74160681\Li,0,5.77938594,-4.70231685,-0.66613805\Li,0,5.
 54282265,-4.37443751,1.81188163\\Version=EM64L-G09RevB.01\State=1-A\HF
 =-1797.2250524\RMSD=4.639e-09\Dipole=6.8349352,11.2945111,1.2951439\Qu
 adrupole=10.6210252,28.0120691,-38.6330942,-119.047304,-9.7659728,-12.

8246841\PG=C01 [X(C30H10Li6O8)]\@

6_8Li

1\1\GINC-C04\SP\RB3LYP\6-311+G(d)\C30H10Li8O8\ZHOU\22-Apr-2015\0\#p b

3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Required\\0,
1\C,0,-3.74246662,-3.56201948,-0.33415652\C,0,-2.55430304,-2.84892891,
-0.29648822\C,0,-2.51132051,-1.43689255,-0.13861789\C,0,-3.73218827,-0
.72333983,-0.03201064\C,0,-4.9479091,-1.45766373,-0.05468093\C,0,-4.98
847467,-2.83774838,-0.1909989\C,0,-3.72551743,0.73895414,0.08335549\C,
0,-2.50076885,1.45375362,0.04344397\C,0,-2.53380237,2.87245459,0.12673
084\H,0,-1.6149963,3.44817927,0.09939084\C,0,-3.71367355,3.5882373,0.2
5695317\C,0,-4.96258462,2.85761228,0.31668841\C,0,-4.93265688,1.473806
25,0.2250445\H,0,-1.63843169,-3.4179976,-0.41471619\H,0,-5.90184214,-0
.94881705,0.02569023\H,0,-5.88742906,0.96265543,0.27387333\C,0,-0.0050
5121,-1.36707659,-0.07299759\C,0,1.23744648,-0.71916407,-0.04960276\C,
0,1.24209048,0.70861019,-0.09355096\C,0,0.00505121,1.36707659,-0.07299
759\C,0,-1.23744648,0.71916407,-0.04960276\C,0,-1.24209048,-0.70861019
,-0.09355096\H,0,-0.01148088,-2.44667561,-0.05566971\H,0,0.01148088,2.
44667561,-0.05566971\O,0,-6.10326414,-3.58400699,-0.22248145\O,0,-3.85
610713,-4.89119786,-0.50107945\O,0,-3.81455349,4.92610785,0.34946586\O
,0,-6.06791701,3.6042246,0.46805171\C,0,2.50076885,-1.45375362,0.04344
397\C,0,2.51132051,1.43689255,-0.13861789\C,0,3.73218827,0.72333983,-0
.03201064\C,0,3.72551743,-0.73895414,0.08335549\C,0,2.53380237,-2.8724
5459,0.12673084\H,0,1.6149963,-3.44817927,0.09939084\C,0,3.71367355,-3
.5882373,0.25695317\C,0,4.96258462,-2.85761228,0.31668841\C,0,4.932656
88,-1.47380625,0.2250445\H,0,5.88742906,-0.96265543,0.27387333\C,0,4.9
479091,1.45766373,-0.05468093\H,0,5.90184214,0.94881705,0.02569023\C,0
,4.98847467,2.83774838,-0.1909989\C,0,2.55430304,2.84892891,-0.2964882
2\H,0,1.63843169,3.4179976,-0.41471619\C,0,3.74246662,3.56201948,-0.33

415652\O,0,3.81455349,-4.92610785,0.34946586\O,0,6.06791701,-3.6042246
,0.46805171\O,0,6.10326414,3.58400699,-0.22248145\O,0,3.85610713,4.891
19786,-0.50107945\Li,0,-5.44823485,5.00948904,-0.73022248\Li,0,-5.1795
9625,4.8127664,1.74407496\Li,0,5.28251176,5.02673781,0.83399373\Li,0,5
.43398323,4.74665913,-1.65115903\Li,0,5.44823485,-5.00948904,-0.730222
48\Li,0,5.17959625,-4.8127664,1.74407496\Li,0,-5.28251176,-5.02673781,
0.83399373\Li,0,-5.43398323,-4.74665913,-1.65115903\\Version=EM64L-G09
RevB.01\State=1-A\HF=-1812.4861973\RMSD=4.003e-09\Dipole=0.,0.,0.38610
55\Quadrupole=2.1235709,68.5429599,-70.6665308,0.3945152,0.,0.\PG=C02
[X(C30H10Li8O8)]\@

9

1\1\GINC-C08\FOpt\RB3LYP\6-311+G(d)\C14H6O4\ZHOU\20-Apr-2015\0\#p opt
freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\d\0,1\C,-0.0959
986951,3.6041136607,0.2863049798\C,0.0959986951,-3.6041136607,0.286304
9798\C,-0.058975396,2.8906930333,-1.0060691521\C,0.058975396,-2.890693
0333,-1.0060691521\C,0.0074123191,1.3925956057,-0.9714956121\C,-0.0074
123191,-1.3925956057,-0.9714956121\C,0.0483077129,0.7029249398,0.25318
4\C,-0.0483077129,-0.7029249398,0.253184\C,0.3622167881,1.5007579936,1
.4864956873\C,-0.3622167881,-1.5007579936,1.4864956873\C,0.0732911405,
2.9541712491,1.4450854979\C,-0.0732911405,-2.9541712491,1.4450854979\C
,-0.0175329412,0.6920476896,-2.1813027953\C,0.0175329412,-0.6920476896
,-2.1813027953\H,-0.0453260493,1.249055202,-3.1097167188\H,0.045326049
3,-1.249055202,-3.1097167188\H,-0.225748111,4.6799612912,0.2390444868\
H,0.225748111,-4.6799612912,0.2390444868\H,0.1086459924,3.4717824055,2
.3977712945\H,-0.1086459924,-3.4717824055,2.3977712945\O,-0.9412525092
,-1.0233794682,2.4455471472\O,0.9412525092,1.0233794682,2.4455471472\O
,0.1081097741,-3.5005588526,-2.0629448252\O,-0.1081097741,3.5005588526
,-2.0629448252\\Version=EM64L-G09RevB.01\State=1-A\HF=-838.1857021\RMS

D=5.941e-09\RMSF=6.496e-05\Dipole=0.,0.,-0.046475\Quadrupole=0.6215504
,8.1783101,-8.7998605,-1.3053424,0.,0.\PG=C02 [X(C14H6O4)]\ \@

9_4Li

1\1\GINC-C04\FOpt\RB3LYP\6-311+G(d)\C14H6Li4O4\ZHOU\20-Apr-2015\0\#p
opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card Re
quired\\0,1\C,0.091878556,3.5850149725,-0.2055174561\C,-0.1173762985,2
.8661768581,0.9770341839\C,-0.0732943671,1.4303156988,0.8760054885\C,0
.0703070394,0.7364265511,-0.3806394367\C,0.4310923855,1.5312235234,-1.
5327686217\C,0.381182921,2.9295668564,-1.403591254\C,-0.0792212357,0.6
753014428,2.0897407385\C,-0.0703070394,-0.7364265511,-0.3806394367\C,0
.0732943671,-1.4303156988,0.8760054885\C,0.0792212357,-0.6753014428,2.
0897407385\C,0.1173762985,-2.8661768581,0.9770341839\C,-0.091878556,-3
.5850149725,-0.2055174561\C,-0.381182921,-2.9295668564,-1.403591254\C,
-0.4310923855,-1.5312235234,-1.5327686217\H,-0.1505794042,1.2257411956
,3.0210028197\H,0.1505794042,-1.2257411956,3.0210028197\H,0.0780162167
,4.6721703012,-0.1668697498\H,0.6333948433,3.5120172508,-2.2872404738\
H,-0.6333948433,-3.5120172508,-2.2872404738\H,-0.0780162167,-4.6721703
012,-0.1668697498\O,-0.8368398604,-1.0196350092,-2.7069366299\O,0.3182
725026,-3.4690405396,2.1331262696\O,0.8368398604,1.0196350092,-2.70693
66299\O,-0.3182725026,3.4690405396,2.1331262696\Li,-0.9929160773,0.737
8612267,-3.1795147192\Li,0.650758704,-4.1316883606,3.6871670109\Li,0.9
929160773,-0.7378612267,-3.1795147192\Li,-0.650758704,4.1316883606,3.6
871670109\\Version=EM64L-G09RevB.01\State=1-A\HF=-868.6955083\RMSD=8.7
04e-09\RMSF=1.329e-05\Dipole=0.,0.,4.3759641\Quadrupole=-37.5818254,-3
.0111022,40.5929276,-19.5933935,0.,0.\PG=C02 [X(C14H6Li4O4)]\ \@

3 with electron-withdrawn group 1\1\GINC-C02\FOpt\RB3LYP\6-
311+G(d)\C16H2Cl2F6O4\ZHOU\01-May-2015\0\#

p opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Card
 Required\\0,1\\C,0.5580898141,3.5343350029,0.8822332081\\C,-0.0607776855
 ,2.8512818054,-0.2802403101\\C,0.0549332712,1.4845174395,-0.3854221534\\
 C,0.2283322957,0.6986333434,0.8625927166\\C,0.756419354,1.2368353795,1.
 9841646666\\C,1.0384966951,2.6640506109,2.0685185403\\C,0.0375117307,0.6
 895854857,-1.6041965731\\C,-0.2283322957,-0.6986333434,0.8625927166\\C,-
 0.0549332712,-1.4845174395,-0.3854221534\\C,-0.0375117307,-0.6895854857
 ,-1.6041965731\\C,0.0607776855,-2.8512818054,-0.2802403101\\C,-0.5580898
 141,-3.5343350029,0.8822332081\\C,-1.0384966951,-2.6640506109,2.0685185
 403\\C,-0.756419354,-1.2368353795,1.9841646666\\H,0.968342658,0.63541795
 49,2.8596291709\\H,-0.968342658,-0.6354179549,2.8596291709\\O,0.77363236
 4,4.7263594401,0.8961842105\\O,-0.773632364,-4.7263594401,0.8961842105\\
 O,1.5711810346,3.1891685189,3.0229818749\\O,-1.5711810346,-3.1891685189
 ,3.0229818749\\C,-0.7781899469,3.7768559659,-1.2520049845\\C,0.778189946
 9,-3.7768559659,-1.2520049845\\F,1.4632613829,-4.7098632555,-0.55718104
 97\\F,1.704813306,-3.123505908,-1.9852627297\\F,-0.038418229,-4.43361680
 69,-2.0985645001\\F,-1.704813306,3.123505908,-1.9852627297\\F,0.03841822
 9,4.4336168069,-2.0985645001\\F,-1.4632613829,4.7098632555,-0.557181049
 7\\Cl,0.3006852779,1.4887687136,-3.1121189143\\Cl,-0.3006852779,-1.48876
 87136,-3.1121189143\\Version=EM64L-G09RevB.01\\State=1-A\\HF=-2431.61277
 19\\RMSD=5.147e-09\\RMSF=2.314e-05\\Dipole=0.,0.,-1.0289699\\Quadrupole=18
 .7750409,-33.3111136,14.5360726,-8.3542616,0.,0.\\PG=C02 [X(C16H2Cl2F6O
 4)]\\@

3_4Li with electron-withdrawn group

1\\I\\GINC-C04\\FOpt\\RB3LYP\\6-311+G(d)\\C16H2Cl2F6Li4O4\\ZHOU\\01-May-2015\\0
 \\#p opt freq b3lyp/6-311+g(d) scrf=(solvent=thf) symm=loose\\Title Ca
 rd Required\\0,1\\C,0.4242604803,3.5514436604,1.1652036549\\C,0.01177715
 28,2.9189569819,-0.0134477641\\C,0.0284273644,1.4645023179,-0.104939228
 1\\C,0.0853093481,0.7178560717,1.1094010317\\C,0.3763113386,1.3982564443

,2.3283130122\C,0.6372490805,2.7466728145,2.373497748\C,0.0431448746,0.6927479191,-1.305267514\C,-0.0853093481,-0.7178560717,1.1094010317\C,-0.0284273644,-1.4645023179,-0.1049392281\C,-0.0431448746,-0.6927479191,-1.305267514\C,-0.0117771528,-2.9189569819,-0.0134477641\C,-0.4242604803,-3.5514436604,1.1652036549\C,-0.6372490805,-2.7466728145,2.373497748\C,-0.3763113386,-1.3982564443,2.3283130122\H,0.4894961167,0.8397852866,3.2489938175\H,-0.4894961167,-0.8397852866,3.2489938175\O,0.5905939978,4.844360219,1.3383095312\O,-0.5905939978,-4.844360219,1.3383095312\O,1.0042297888,3.4361244415,3.4474619672\O,-1.0042297888,-3.4361244415,3.4474619672\Li,2.1762706677,4.7124732671,2.5399410875\Li,-0.2711372842,4.9208315311,3.1257054933\Li,0.2711372842,-4.9208315311,3.1257054933\Li,-2.1762706677,-4.7124732671,2.5399410875\C,-0.6503537055,3.8069705614,-1.0255763627\C,0.6503537055,-3.8069705614,-1.0255763627\F,0.1886507469,4.4473070924,-1.9018422517\F,-1.5754918427,3.1594625676,-1.7842339232\F,-1.3646194057,4.8162347335,-0.4419047405\F,1.5754918427,-3.1594625676,-1.7842339232\F,-0.1886507469,-4.4473070924,-1.9018422517\F,1.3646194057,-4.8162347335,-0.4419047405\Cl,0.3967026643,1.478506329,-2.8494271784\Cl,-0.3967026643,-1.478506329,-2.8494271784\\Version=EM64L-G09RevB.01\State=1-A\HF=-2462.2351317\RMSD=7.483e-09\RMSF=1.769e-05\Dipole=0.,0.,9.0176921\Quadrupole=-20.409972,40.5011876,-20.0912156,30.7307958,0.,0.\PG=C02 [X(C16H2Cl2F6Li4O4)]\\@