Ring lithiation of 1,8-bis(dimethylamino)naphthalene: another side of the 'proton sponge coin'

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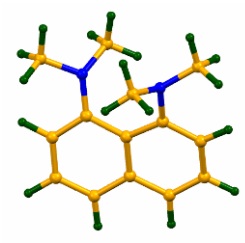
Supporting Information

SI-1. Crystal data and structure refinement for $(5a \cdot Et_2O)_2$

Parameter	Data
Empirical formula	$C_{18}H_{27}LiN_2O$
Formula weight	294.36
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	8.847(4)
b (Å)	23.449(9)
c (Å)	8.877(4)
α (°)	90
β (°)	108.188(6)
γ (°)	90
V (Å^3)	1749.4(12)
Z	4
d_{calc}, g·cm^{-3}	1.118
μ (mm^{-1})	0.068
F(000)	640
θ range, deg.	2.42 – 26.00
Reflections collected/unique	10889/3424
R(int)	0.2432
Refined parameters	205
Completeness to theta θ, %	99.9
GOF (F^2)	0.968
Reflections with $I > 2\sigma(I)$	1266
$R_1(F)$ ($I > 2\sigma(I)$)[a]	0.0847
$wR_2(F^2)$ (all data)[b]	0.1820
Largest diff. peak/hole, e·Å^{-3}	0.275/–0.242

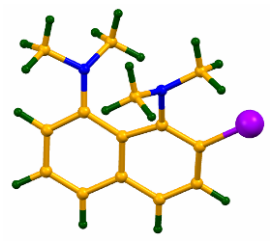
[a] $R_1 = \sum||F_o| - |F_c||/\sum(F_o)$; [b] $wR_2 = (\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]^{1/2}$

SI-2. Some quantum-chemical characteristics of structures 1, 5a–d (and their complexes with TMEDA) and 5a complex with THF [B3LYP/6-311G+(d,p)]



1

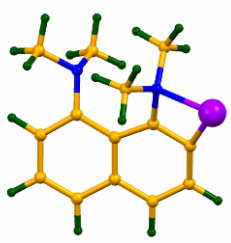
E = –653.975466 a.u.



5a(*in*,*in*)

E = –660.873233 a.u.

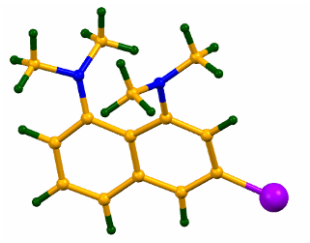
C…Li = 1.954 Å



5a(*in*,*out*)

E = –660.880958 a.u.

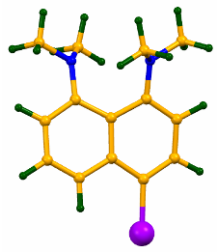
C…Li = 1.934 Å



5b

E = –660.867354 a.u.

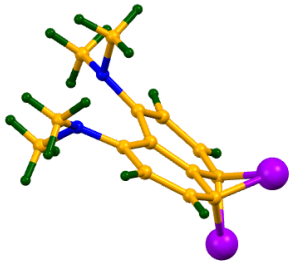
C…Li = 1.959 Å



5c

E = –660.867941 a.u.

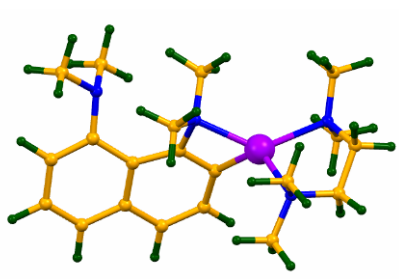
C…Li = 1.959 Å



5d

E = –667.802743 a.u.

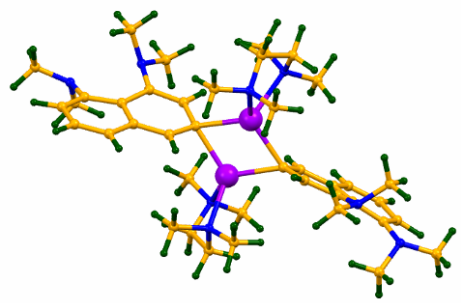
C…Li = 2.025(9) Å



5a·TMEDA

E = –1008.765508 a.u.

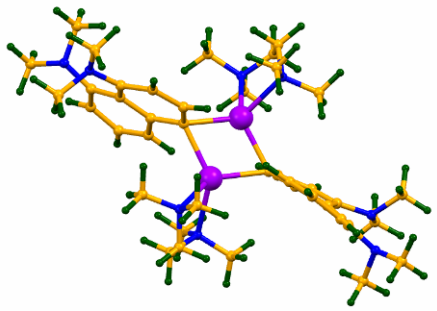
C…Li = 2.029 Å



(5b·TMEDA)$_2$

E = –2017.559526 a.u.

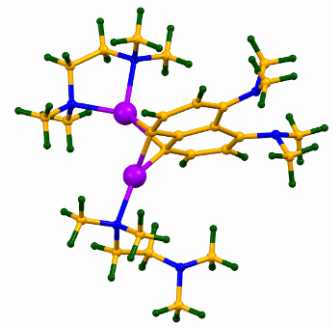
C…Li = 2.233(41)/2.240(9) Å



(5c·TMEDA)$_2$

E = –2017.560870 a.u.

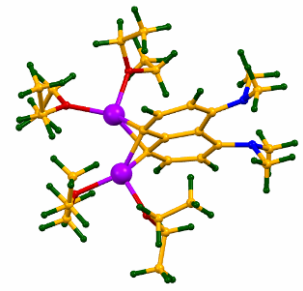
C…Li = 2.226(49)/2.230(57) Å



5d·(TMEDA)$_2$

E = –1363.559376 a.u.

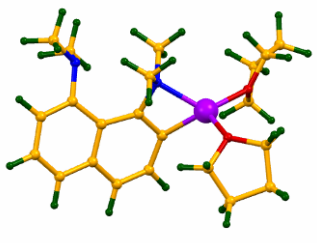
C…Li = 2.058(67)/2.150(7) Å



5d·(Et$_2$O)$_4$

E = –1602.802528 a.u.

C…Li = 2.118(60)/2.148(91) Å

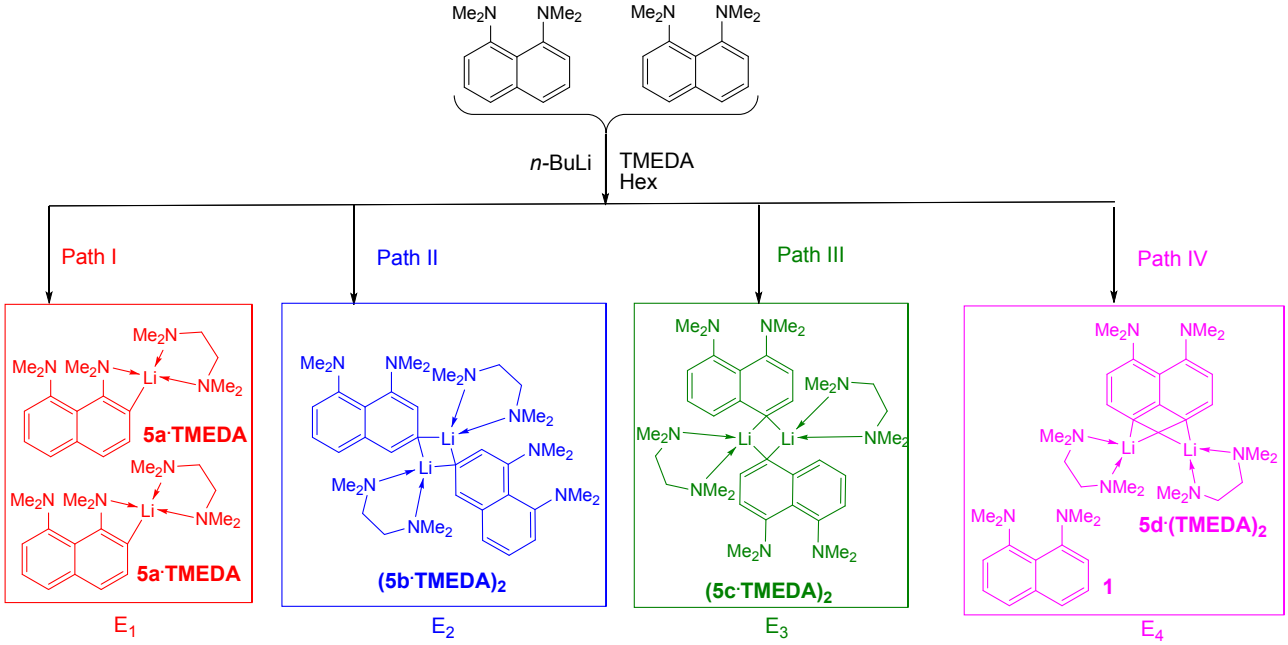


11c ≡ 5a·THF$_2$

E = –1125.961892 a.u.

C…Li = 2.051 Å

SI-3. Relative energies of complexes 5a-d with TMEDA [B3LYP/6-311G+(d,p)]

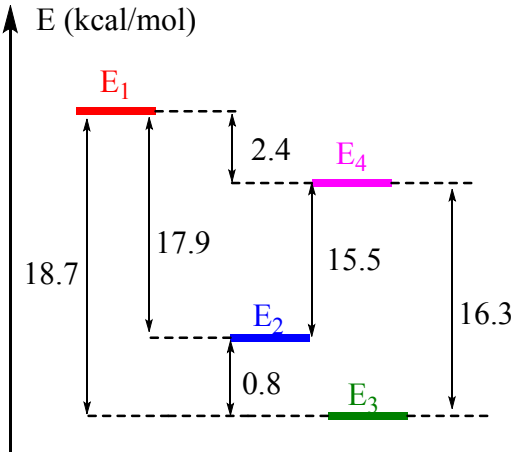


E_1 = 2E[**5a·TMEDA**] = –2017.531016 a.u.

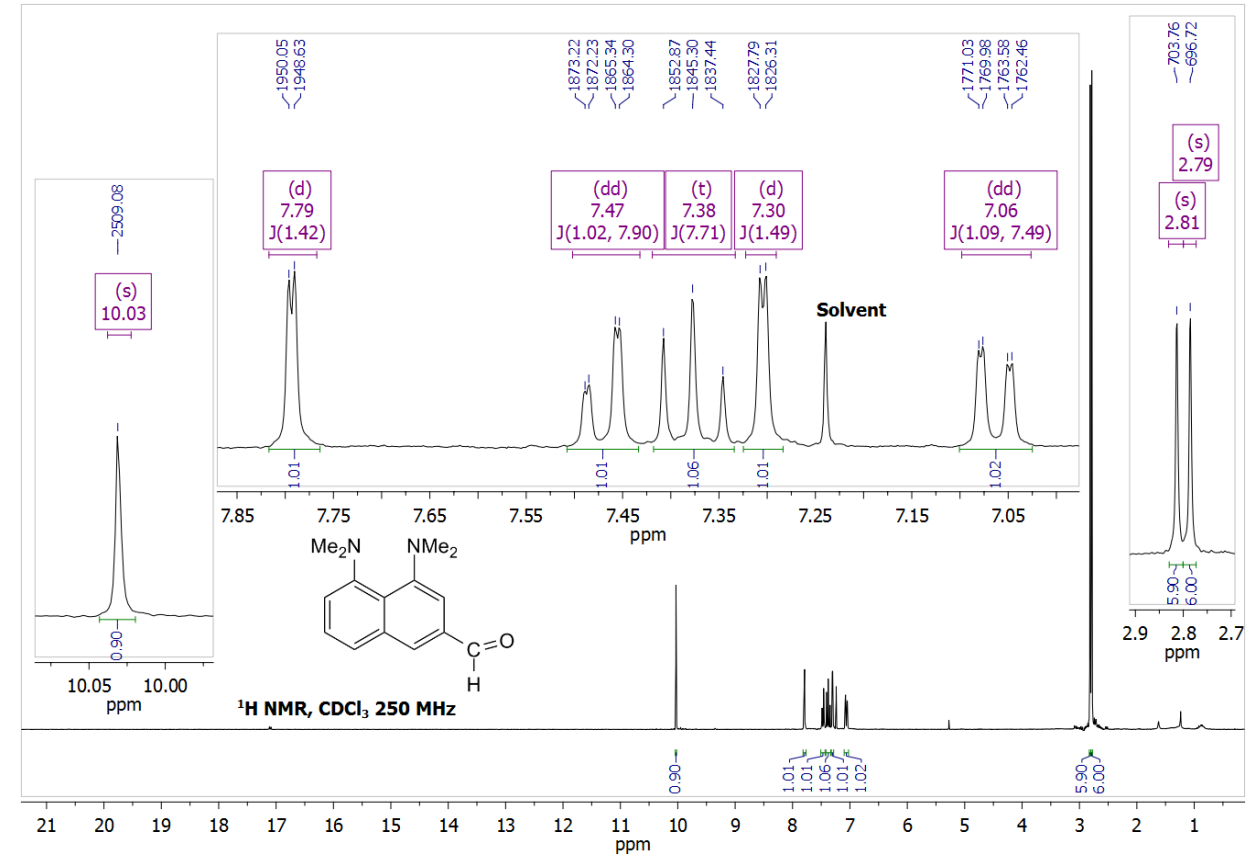
E_2 = E[**(5b·TMEDA)$_2$**] = –2017.559526 a.u.

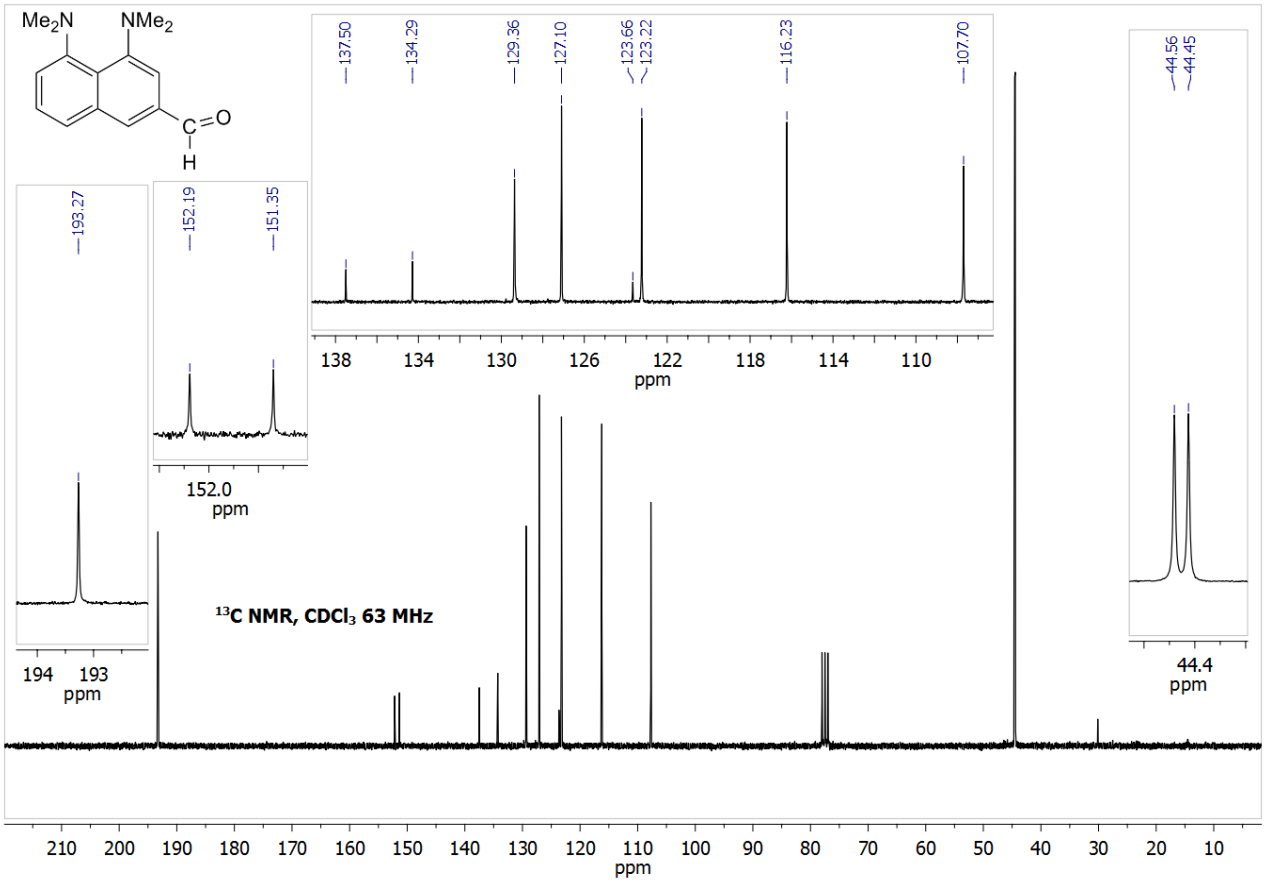
E_3 = E[**(5c·TMEDA)$_2$**] = –2017.560870 a.u.

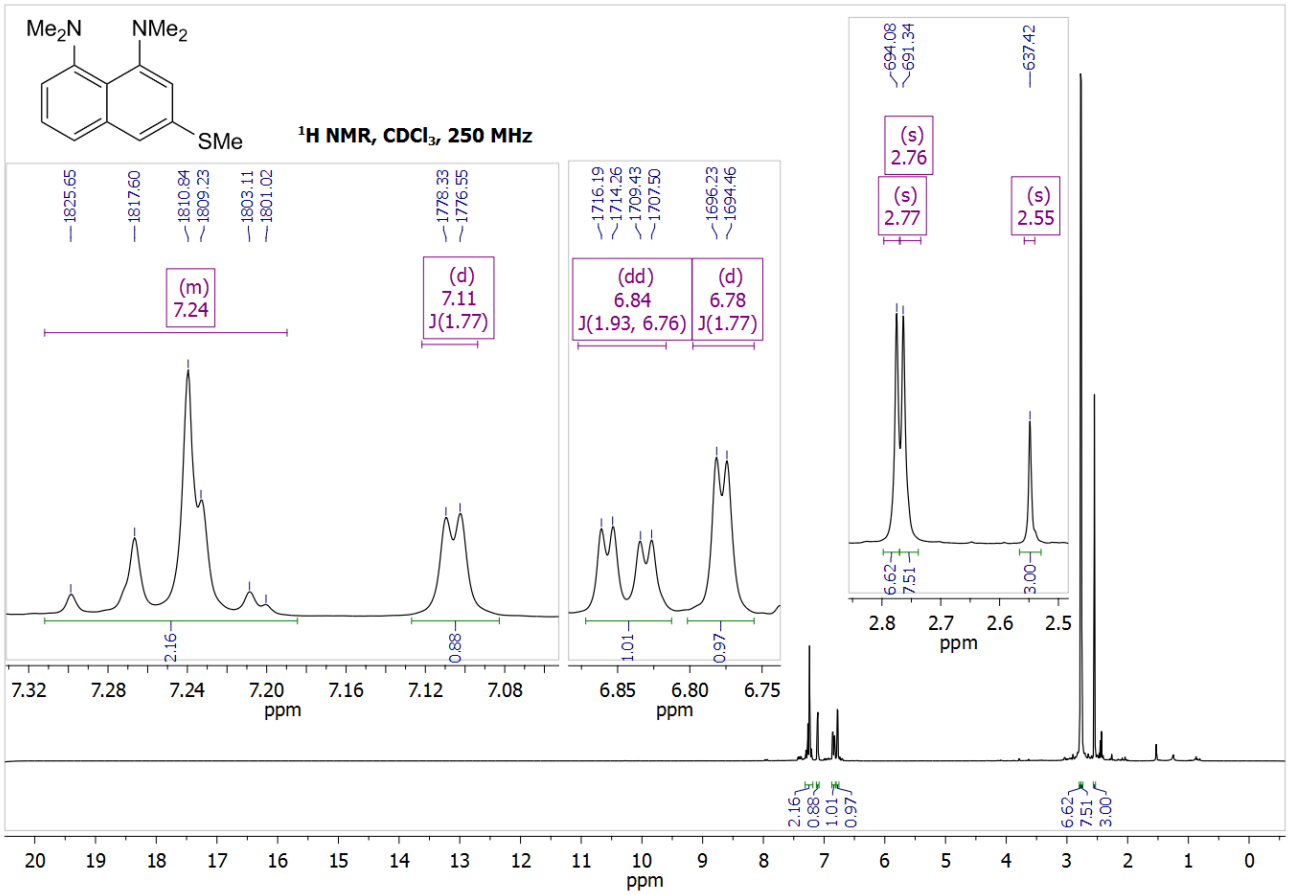
E_4 = E[**5d·(TMEDA)$_2$**] + E[**1**] = –2017.534842 a.u.

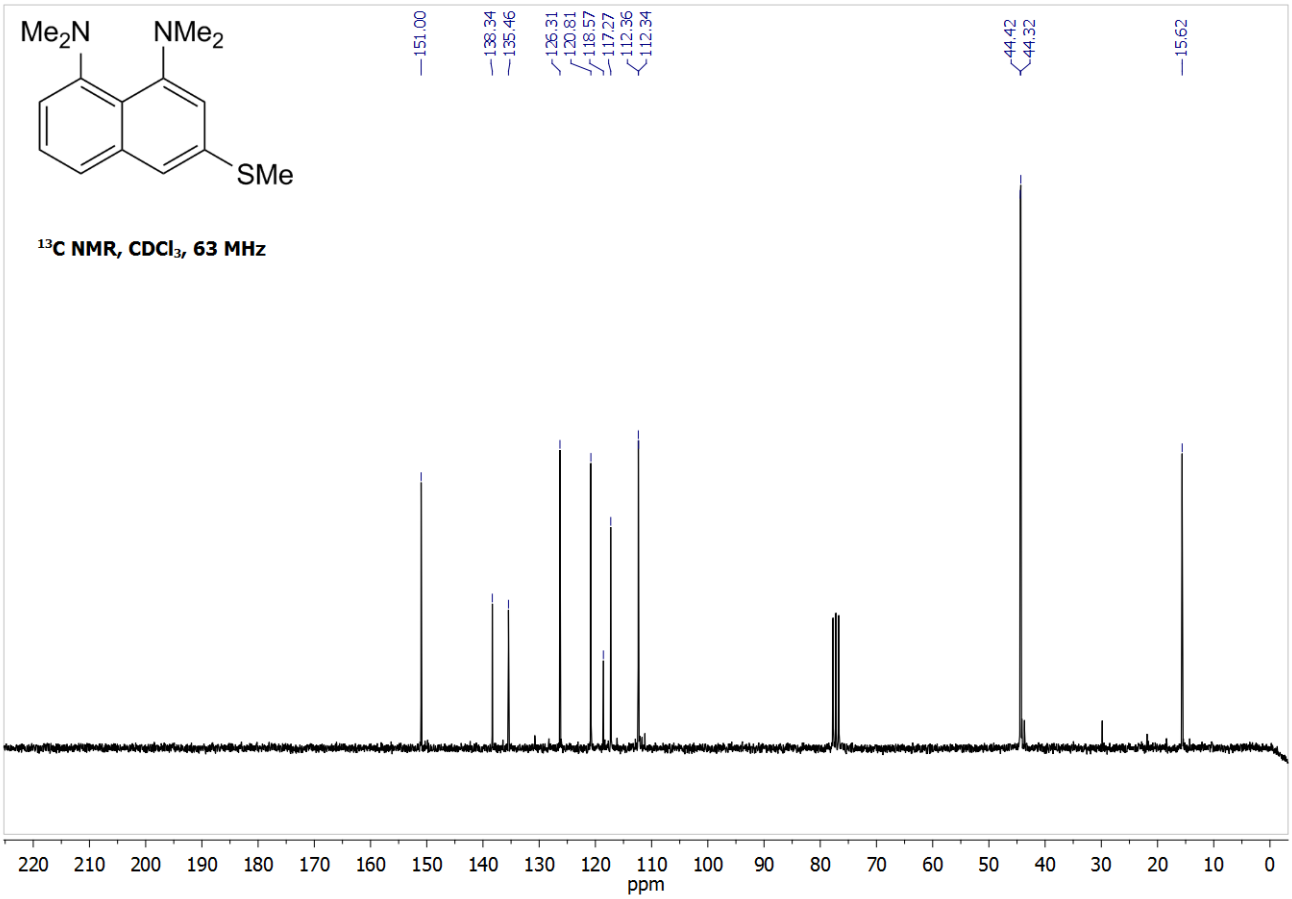


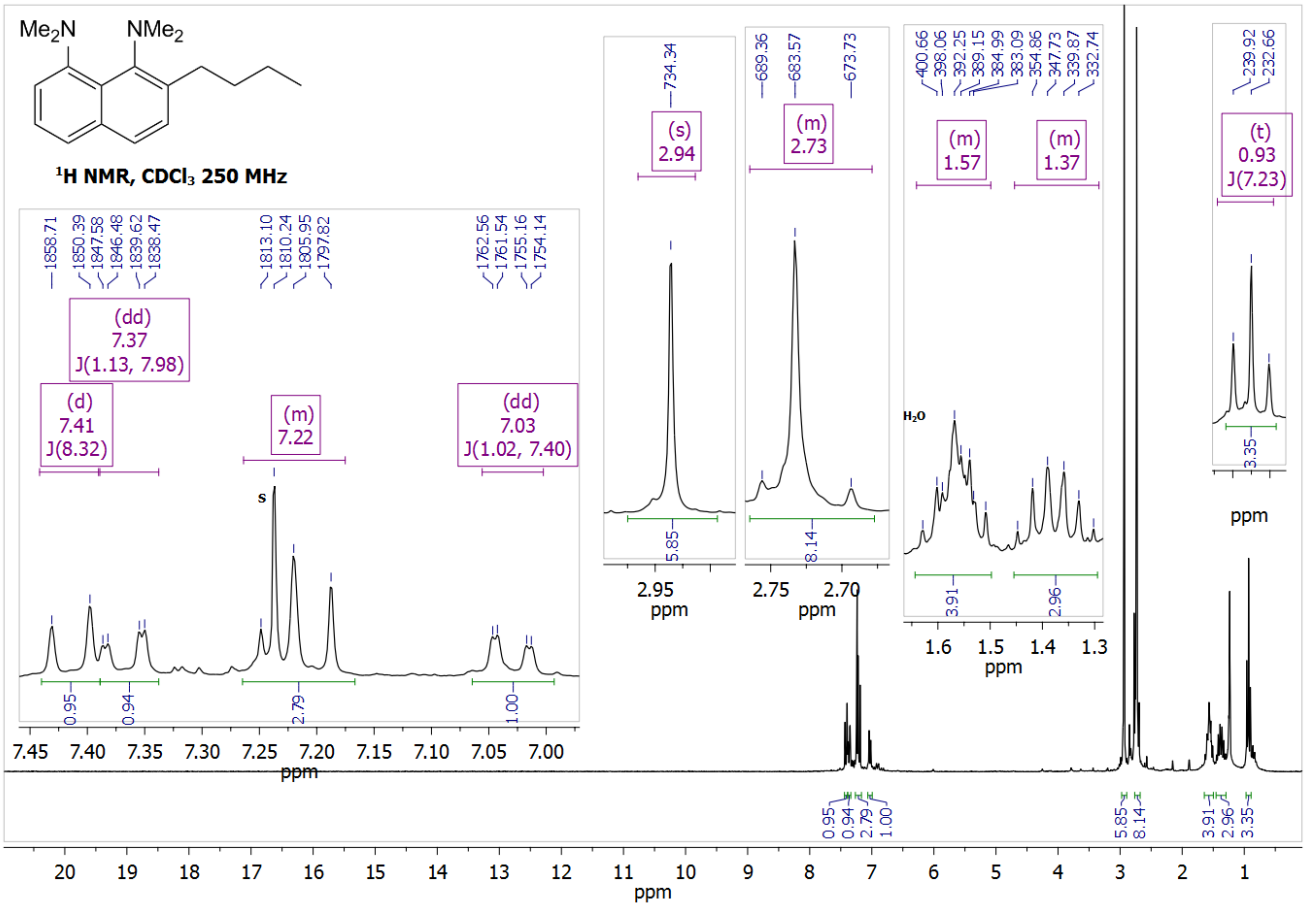
SI-4. ^{1}H and ^{13}C NMR spectra for new products






Me2N
NMe2
SMe
1H NMR, CDCl3, 250 MHz
(m)
7.24
(d)
7.11
J(1.77)
(dd)
6.84
J(1.93, 6.76)
(d)
6.78
J(1.77)
(s)
2.76
(s)
2.77
(s)
2.55
ppm


Me2N
NMe2
SMe
13C NMR, CDCl3, 63 MHz
ppm


Me2N
NMe2
1H NMR, CDCl3 250 MHz
(dd)
7.37
J(1.13, 7.98)
(d)
7.41
J(8.32)
(m)
7.22
(dd)
7.03
J(1.02, 7.40)
(s)
2.94
(m)
2.73
(m)
1.57
(m)
1.37
(t)
0.93
J(7.23)
H2O
ppm

SI-5. **Thermochemical data and Cartesian Coordinates for structures 1, 5a–d and their ligated complexes [B3LYP/6-311G+(d,p)]**

Compound **1**

Zero-point correction= 0.291866 (Hartree/Particle)
Thermal correction to Energy= 0.306876
Thermal correction to Enthalpy= 0.307820
Thermal correction to Gibbs Free Energy= 0.251106
Sum of electronic and zero-point Energies= -653.683600
Sum of electronic and thermal Energies= -653.668590
Sum of electronic and thermal Enthalpies= -653.667646
Sum of electronic and thermal Free Energies= -653.724360

HF=-653.9754662

C	-0.059163	0.175678	0.014126
C	-0.087583	-0.031127	1.418262
C	1.136113	-0.072803	2.173786
C	2.375603	-0.123100	1.421557
C	2.343028	0.112249	0.053545
C	1.134856	0.296346	-0.644537
C	1.020411	-0.060804	3.619878
C	-0.227753	-0.252621	4.197168
C	-1.400192	-0.355619	3.425389
C	-1.339356	-0.196285	2.067076
N	2.151412	0.162218	4.437022
C	2.067417	-0.220035	5.835856
N	3.599916	-0.426369	2.058702
C	3.685413	-1.740932	2.694382
C	4.830763	-0.083158	1.367893
C	2.822959	1.450601	4.268148
H	5.056072	-0.739680	0.509453
H	4.794155	0.948761	1.014207
H	5.660399	-0.172375	2.074291
H	4.462652	-1.729666	3.463547
H	2.743450	-2.000229	3.168244
H	3.934003	-2.523485	1.957833
H	2.836123	1.742515	3.222356
H	3.857395	1.376679	4.615001
H	2.316290	2.241813	4.846049
H	3.073542	-0.193562	6.262814
H	1.433841	0.450605	6.442090
H	1.684070	-1.237571	5.930450
H	-0.320902	-0.262525	5.274509
H	-2.353020	-0.500372	3.922763

H	-2.240468	-0.197146	1.463959
H	-1.000490	0.239263	-0.520299
H	1.160598	0.472691	-1.714328
H	3.264275	0.093977	-0.512486

Compound **5a(*in*,*in*)**

Zero-point correction= 0.280274 (Hartree/Particle)
Thermal correction to Energy= 0.296379
Thermal correction to Enthalpy= 0.297323
Thermal correction to Gibbs Free Energy= 0.238401
Sum of electronic and zero-point Energies= -660.592960
Sum of electronic and thermal Energies= -660.576854
Sum of electronic and thermal Enthalpies= -660.575910
Sum of electronic and thermal Free Energies= -660.634832

HF=-660.8732332

C	-0.045569	-0.019451	0.079060
C	-0.020483	0.078311	1.463502
C	1.185950	0.185116	2.182875
C	2.380947	0.121854	1.517389
C	2.413518	0.044048	0.100454
C	1.196616	0.082905	-0.664265
C	1.346525	0.220498	-2.100074
C	2.563697	0.051512	-2.761833
C	3.707011	-0.153358	-1.936755
C	3.657830	-0.080569	-0.567780
N	0.179067	0.589383	-2.863871
N	-1.276868	-0.235975	-0.591510
C	0.203288	0.354508	-4.276344
C	-1.376036	-1.486724	-1.339795
C	-2.503268	0.053782	0.128686
C	-0.383205	1.901593	-2.557231
H	0.831640	1.089447	-4.859595
H	0.529853	-0.670111	-4.490432
H	-0.800592	0.478266	-4.692878
H	-1.407642	1.968243	-2.936172
H	-0.408076	2.059594	-1.483115
H	0.213978	2.712288	-3.013921
H	-0.438420	-1.704876	-1.843597
H	-2.162956	-1.404002	-2.095761
H	-1.620314	-2.334072	-0.675774
H	-3.333930	0.047158	-0.582936
H	-2.740786	-0.680671	0.919032
H	-2.452377	1.044579	0.584121

H	-0.945460	0.016590	2.020981
H	1.156664	0.259391	3.264699
H	3.321475	0.129943	2.058005
H	4.562038	-0.135377	0.032259
H	4.678839	-0.312921	-2.402918
Li	2.522721	0.185461	-4.710766

Compound **5a(*in,out*)**

Zero-point correction= 0.281055 (Hartree/Particle)
Thermal correction to Energy= 0.297050
Thermal correction to Enthalpy= 0.297994
Thermal correction to Gibbs Free Energy= 0.239460
Sum of electronic and zero-point Energies= -660.599903
Sum of electronic and thermal Energies= -660.583908
Sum of electronic and thermal Enthalpies= -660.582964
Sum of electronic and thermal Free Energies= -660.641498

HF=-660.8809581

C	0.042411	0.105067	0.018796
C	0.023328	0.045746	1.437693
C	1.262753	0.053532	2.174424
C	2.458242	-0.151605	1.380958
C	2.467976	-0.099690	-0.006943
C	1.230538	0.126604	-0.665652
C	1.155674	0.252602	3.597738
C	-0.075685	0.161700	4.223398
C	-1.266253	-0.018123	3.492342
C	-1.217439	-0.017296	2.122469
N	2.314468	0.657962	4.344384
C	2.345135	0.281370	5.753030
N	3.755706	-0.643512	1.937178
C	3.662611	-1.795673	2.842698
C	4.738925	0.348575	2.401328
C	2.569877	2.095652	4.185520
Li	4.200795	-0.958046	0.020926
H	4.720203	1.213751	1.735465
H	4.551112	0.683095	3.424034
H	5.743037	-0.093988	2.369188
H	4.647207	-2.271255	2.922233
H	3.336714	-1.518735	3.849480
H	2.958827	-2.522992	2.433103
H	2.592124	2.358991	3.128198
H	3.536860	2.351867	4.628562
H	1.793673	2.704935	4.677289

H	3.352151	0.457752	6.143158
H	1.644719	0.855626	6.382605
H	2.114413	-0.779649	5.863786
H	-0.140856	0.288379	5.296861
H	-2.213617	-0.090435	4.015098
H	-2.128601	-0.068304	1.535480
H	-0.909887	0.135830	-0.504349
H	1.209670	0.231116	-1.748576

Compound **5b**

Zero-point correction= 0.280406 (Hartree/Particle)
Thermal correction to Energy= 0.296948
Thermal correction to Enthalpy= 0.297892
Thermal correction to Gibbs Free Energy= 0.237623
Sum of electronic and zero-point Energies= -660.586948
Sum of electronic and thermal Energies= -660.570405
Sum of electronic and thermal Enthalpies= -660.569461
Sum of electronic and thermal Free Energies= -660.629731

HF=-660.8673537

C	-0.067000	-0.008284	0.090499
C	-0.021115	0.062237	1.475890
C	1.197361	0.137884	2.178916
C	2.381599	0.074832	1.495046
C	2.397675	0.028917	0.075069
C	1.166755	0.090560	-0.664357
C	1.290328	0.243966	-2.097876
C	2.540427	0.108663	-2.688785
C	3.769385	-0.088918	-1.988931
C	3.641783	-0.072665	-0.608137
N	0.148495	0.555823	-2.889654
N	-1.309482	-0.198081	-0.566106
C	0.213207	0.281523	-4.312835
C	-1.443480	-1.446513	-1.313737
C	-2.520571	0.114714	0.170470
C	-0.455081	1.859156	-2.624723
H	0.851520	0.985564	-4.877381
H	0.581854	-0.730910	-4.488447
H	-0.797033	0.355243	-4.727104
H	-1.475798	1.880263	-3.018686
H	-0.501690	2.047899	-1.555712
H	0.118176	2.674940	-3.100451
H	-0.522710	-1.675944	-1.841799
H	-2.245135	-1.350359	-2.051808

H	-1.685620	-2.290364	-0.644055
H	-3.358606	0.131873	-0.532147
H	-2.766504	-0.619883	0.958348
H	-2.441476	1.100847	0.631846
H	-0.939220	0.000787	2.044544
H	1.184396	0.190872	3.262577
H	3.329713	0.065139	2.022946
H	4.520512	-0.139149	0.036053
Li	5.546661	-0.295627	-2.785502
H	2.580081	0.209682	-3.768985

Compound **5c**

Zero-point correction= 0.280102 (Hartree/Particle)
Thermal correction to Energy= 0.296711
Thermal correction to Enthalpy= 0.297655
Thermal correction to Gibbs Free Energy= 0.237140
Sum of electronic and zero-point Energies= -660.587839
Sum of electronic and thermal Energies= -660.571230
Sum of electronic and thermal Enthalpies= -660.570286
Sum of electronic and thermal Free Energies= -660.630801

HF=-660.8679409

C	-0.058552	-0.005325	0.074510
C	-0.020641	0.106251	1.457452
C	1.196484	0.209249	2.156223
C	2.377849	0.116965	1.469397
C	2.423624	0.018426	0.050031
C	1.177548	0.083624	-0.680214
C	1.270588	0.238967	-2.116096
C	2.506530	0.075425	-2.718527
C	3.678583	-0.162861	-1.968826
C	3.708254	-0.140782	-0.584053
N	0.130923	0.579049	-2.893524
N	-1.296106	-0.222087	-0.580455
C	0.189632	0.329001	-4.321657
C	-1.410613	-1.468818	-1.333532
C	-2.514432	0.076063	0.149086
C	-0.464238	1.880481	-2.600754
H	0.843501	1.029389	-4.872158
H	0.536624	-0.687846	-4.515334
H	-0.818223	0.431377	-4.734656
H	-1.489416	1.911149	-2.981871
H	-0.496815	2.053722	-1.528546

H	0.106120	2.701246	-3.070600
H	-0.480794	-1.691367	-1.848494
H	-2.202291	-1.376680	-2.082664
H	-1.655759	-2.316134	-0.669447
H	-3.351451	0.067709	-0.554767
H	-2.746762	-0.653115	0.946161
H	-2.456896	1.069625	0.597806
H	-0.939551	0.056757	2.025875
H	1.186318	0.301188	3.237341
H	3.320950	0.125770	2.012358
Li	5.359239	-0.358220	0.448059
H	4.596389	-0.309230	-2.539891
H	2.592552	0.181583	-3.793409

Compound **5d**

Zero-point correction= 0.271160 (Hartree/Particle)
Thermal correction to Energy= 0.288222
Thermal correction to Enthalpy= 0.289166
Thermal correction to Gibbs Free Energy= 0.228488
Sum of electronic and zero-point Energies= -667.531604
Sum of electronic and thermal Energies= -667.514543
Sum of electronic and thermal Enthalpies= -667.513598
Sum of electronic and thermal Free Energies= -667.574276

-667.8027641

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.456436
C	1.214598	0.000000	2.240842
C	2.446840	-0.256352	1.529038
C	2.429312	-0.247604	0.138994
C	1.241860	-0.073111	-0.602330
C	1.072625	0.256377	3.656772
C	-0.201572	0.247506	4.212603
C	-1.365691	0.072792	3.435223
C	-1.327493	-0.000187	2.055537
N	2.203515	0.524560	4.468442
C	2.060443	0.378867	5.905451
N	3.651833	-0.524238	2.225937
C	3.651874	-1.717842	3.067761
C	4.902790	-0.378713	1.504412
C	2.970032	1.718690	4.122272
Li	-1.543972	-1.229059	0.456147
Li	-1.547489	1.228615	0.460464
H	5.092624	-1.182835	0.771239

H	4.929243	0.577614	0.979063
H	5.724083	-0.394642	2.226534
H	4.439315	-1.638483	3.823009
H	2.701137	-1.820994	3.581905
H	3.832456	-2.630182	2.472692
H	3.048903	1.821070	3.044222
H	3.981883	1.640577	4.530712
H	2.500577	2.630913	4.530381
H	3.056471	0.394832	6.357024
H	1.470159	1.182863	6.380167
H	1.592578	-0.577537	6.145521
H	-0.314073	0.428701	5.274668
H	-2.319319	0.052333	3.961044
H	1.328910	-0.052851	-1.687840
H	3.351082	-0.428772	-0.400439

Compound **5a·TMEDA**

Zero-point correction= 0.504403 (Hartree/Particle)
Thermal correction to Energy= 0.532394
Thermal correction to Enthalpy= 0.533338
Thermal correction to Gibbs Free Energy= 0.446424
Sum of electronic and zero-point Energies= -1008.261105
Sum of electronic and thermal Energies= -1008.233114
Sum of electronic and thermal Enthalpies= -1008.232169
Sum of electronic and thermal Free Energies= -1008.319084

HF=-1008.765508

C	3.611826	2.478022	-0.284927
C	2.368205	1.890125	-0.635333
C	2.082571	0.525305	-0.269479
C	3.202318	-0.259204	0.188543
C	4.391715	0.359787	0.533470
C	4.584766	1.743734	0.342775
C	0.699945	0.116549	-0.406907
C	-0.242261	0.842779	-1.120695
C	0.188534	2.076498	-1.680890
C	1.401683	2.636891	-1.357855
N	0.096029	-0.995870	0.368272
C	0.024377	-2.319263	-0.258178
N	3.103296	-1.690735	0.175913
C	3.213312	-2.225516	-1.186604
C	3.978757	-2.414477	1.087629
C	0.463280	-1.077338	1.782315
Li	-1.757744	-0.079947	-0.136988

N	-2.979456	0.946306	1.330721
C	-3.090787	0.250722	2.618671
C	-4.270639	0.992452	0.621777
C	-4.650610	-0.353967	0.001960
N	-3.639058	-0.844163	-0.951129
C	-3.719278	-0.139451	-2.241260
C	-2.446543	2.301978	1.535759
C	-3.776107	-2.289354	-1.165275
H	-0.190931	-2.201402	-1.321641
H	0.948475	-2.895247	-0.142706
H	-0.789931	-2.896401	0.198760
H	-0.290945	-1.669082	2.315507
H	1.439452	-1.545205	1.950650
H	0.482216	-0.073756	2.212495
H	2.521741	-1.707498	-1.850146
H	2.964663	-3.290962	-1.187373
H	4.233706	-2.109287	-1.588982
H	3.661521	-3.461120	1.123945
H	5.040823	-2.403319	0.787633
H	3.902293	-1.997426	2.093543
H	5.219912	-0.232600	0.901961
H	5.526338	2.199323	0.629822
H	3.775725	3.523434	-0.526373
H	1.654441	3.652018	-1.655528
H	-0.492771	2.649418	-2.310617
H	-1.476892	2.240980	2.031627
H	-2.292515	2.787111	0.571681
H	-3.119062	2.920295	2.152711
H	-2.992012	-2.633630	-1.841738
H	-3.667439	-2.820705	-0.217265
H	-4.751921	-2.555949	-1.603666
H	-2.919884	-0.488791	-2.894666
H	-4.692299	-0.306953	-2.732848
H	-3.569281	0.930953	-2.104279
H	-2.111706	0.214563	3.098029
H	-3.794622	0.757200	3.299965
H	-3.430260	-0.776830	2.477884
H	-5.640124	-0.260336	-0.476403
H	-5.084006	1.319574	1.291852
H	-4.189535	1.748536	-0.162286
H	-4.758013	-1.103443	0.790008

Compound **(5b·TMEDA)$_2$**
scf done: -2017.559526

C	6.169295	0.455559	0.563603
C	4.776342	0.107506	0.357063
C	3.904590	0.173660	1.498130
C	4.443689	0.371983	2.797863
C	5.790146	0.544990	2.978602
C	6.641151	0.620407	1.858792
C	4.160092	-0.306277	-0.885078
C	2.773889	-0.394926	-0.956827
C	1.857425	-0.211818	0.126860
C	2.497495	0.021046	1.335308
N	4.968533	-0.637516	-2.011677
C	5.805520	-1.822421	-1.849846
N	7.045270	0.652142	-0.535188
C	6.712607	1.769104	-1.416383
C	8.474056	0.580615	-0.285423
C	4.356400	-0.598398	-3.326179
Li	-0.012673	-1.432459	0.106610
Li	0.014902	1.072411	0.247401
C	-1.849950	-0.153202	0.041525
C	-2.297096	0.226022	-1.215259
C	-3.662332	0.412740	-1.574818
C	-4.698511	0.225207	-0.596398
C	-4.278852	-0.334883	0.670981
C	-2.919724	-0.446962	0.945911
C	-3.996590	0.768925	-2.909074
C	-5.299998	0.980301	-3.272150
C	-6.313597	0.934506	-2.295300
C	-6.044535	0.611825	-0.972127
N	-7.080637	0.685184	-0.006356
C	-6.891036	1.677754	1.048932
N	-5.249375	-0.786426	1.611751
C	-6.051662	-1.926997	1.179084
C	-4.840630	-0.922877	2.996841
C	-8.452293	0.671176	-0.482858
N	0.214302	-3.174948	1.583083
C	1.366977	-3.034140	2.483662
C	0.427959	-4.313507	0.674278
C	-0.512705	-4.306219	-0.527029
N	-0.319271	-3.142752	-1.410911
C	-1.492102	-2.974590	-2.280997
C	0.885542	-3.298753	-2.236650
C	-1.008200	-3.347199	2.375951

N	0.393247	2.941771	-1.068560
C	1.639690	2.819393	-1.840174
C	0.521648	3.989669	-0.036437
C	-0.514190	3.843327	1.076426
N	-0.318579	2.629010	1.888594
C	-1.527271	2.360180	2.680243
C	-0.722012	3.242459	-1.978586
C	0.827950	2.776669	2.795585
H	-1.581398	0.397092	-2.023806
H	-7.318124	1.213914	-2.583084
H	-5.557272	1.234872	-4.295126
H	-3.195594	0.860815	-3.635825
H	1.919984	0.082565	2.259125
H	-9.114421	0.506916	0.371908
H	-8.767078	1.613110	-0.966797
H	-8.600390	-0.145715	-1.191617
H	-7.527284	1.432522	1.904212
H	-5.858888	1.682064	1.386382
H	-7.153996	2.691366	0.698397
H	7.681493	0.867970	2.020684
H	6.204789	0.679019	3.972399
H	3.764575	0.373612	3.644522
H	8.991099	0.527514	-1.247741
H	8.877278	1.454579	0.256764
H	8.716686	-0.319233	0.282773
H	7.195337	1.629226	-2.387947
H	5.639880	1.820690	-1.576228
H	7.054370	2.729903	-0.992436
H	-5.735882	-1.051388	3.612987
H	-4.183129	-1.790332	3.188112
H	-4.322483	-0.022056	3.331349
H	-6.957616	-1.995778	1.788940
H	-6.351887	-1.810897	0.141352
H	-5.494712	-2.876448	1.279571
H	6.610571	-1.813004	-2.591064
H	6.257015	-1.838886	-0.861549
H	5.222895	-2.752115	-1.984581
H	5.148382	-0.641612	-4.080369
H	3.667013	-1.438233	-3.527587
H	3.806446	0.334449	-3.463427
H	2.360568	-0.670106	-1.922478
H	-2.657520	-0.831107	1.927080
H	1.527433	3.929398	0.383697
H	0.430543	4.992822	-0.484006
H	-0.493662	4.745539	1.712588

H	-1.514339	3.791700	0.639284
H	0.922576	1.883963	3.413999
H	1.760974	2.886984	2.245239
H	0.702753	3.647709	3.461421
H	-1.379421	1.454305	3.271044
H	-1.758123	3.189529	3.369995
H	-2.379744	2.191489	2.022207
H	1.522135	2.043110	-2.596984
H	1.905089	3.764416	-2.343757
H	2.454958	2.518941	-1.182499
H	-0.802515	2.453404	-2.727057
H	-1.667616	3.274944	-1.436720
H	-0.575441	4.204011	-2.497721
H	0.836951	-4.207029	-2.861390
H	0.988220	-2.434274	-2.893807
H	1.780490	-3.345422	-1.616498
H	-0.383618	-5.249616	-1.086124
H	-1.548796	-4.291861	-0.181453
H	0.309018	-5.271625	1.210451
H	1.464986	-4.276334	0.333774
H	-1.663155	-3.861952	-2.913340
H	-2.379533	-2.786866	-1.676487
H	-1.345752	-2.109460	-2.928090
H	-1.134797	-2.487960	3.035867
H	-1.885517	-3.399278	1.731680
H	-0.968494	-4.259562	2.995551
H	1.204862	-2.194879	3.160987
H	1.524306	-3.942789	3.089339
H	2.268351	-2.824886	1.908451

Compound **(5c·TMEDA)$_2$**
scf done: -2017.560870

C	5.283589	0.677624	-1.095217
C	4.303994	0.044412	-0.231402
C	2.907214	0.142169	-0.599416
C	2.586725	0.622165	-1.901917
C	3.552793	1.049423	-2.775851
C	4.894039	1.117461	-2.352925
C	1.813435	-0.219097	0.271553
C	2.219038	-0.752400	1.485723
C	3.563853	-1.048612	1.808855
C	4.610356	-0.699187	0.971779
N	5.942552	-1.090763	1.278607

C	6.563433	-2.006307	0.324865
N	6.621487	0.862827	-0.666361
C	6.804308	1.687327	0.525392
C	7.626412	1.149804	-1.673309
C	6.232044	-1.474846	2.647914
Li	-0.041303	-1.372411	-0.178706
C	-1.805065	-0.021958	-0.314343
C	-2.938090	0.070776	0.577217
C	-4.319039	0.101097	0.141712
C	-4.551607	0.262310	-1.278397
C	-3.470151	0.148444	-2.135213
C	-2.152077	-0.036622	-1.656794
C	-5.355106	-0.030769	1.149214
C	-5.013983	0.055813	2.492023
C	-3.674663	0.172946	2.907275
C	-2.670329	0.131709	1.974732
N	-6.704508	-0.266624	0.782098
C	-7.736135	0.009540	1.764735
N	-5.846761	0.553537	-1.789211
C	-6.086298	0.301350	-3.198174
C	-6.962227	-1.514128	0.067222
C	-6.414670	1.832514	-1.371652
Li	0.039102	1.162246	0.226232
H	-1.630350	0.131089	2.281650
H	-3.448762	0.232010	3.967406
H	-5.784018	-0.027786	3.247239
H	-3.625342	0.257585	-3.202689
H	-1.376689	-0.122914	-2.420756
H	1.477133	-1.015445	2.242451
H	3.771534	-1.600281	2.718892
H	1.539554	0.632067	-2.183973
H	3.290591	1.392652	-3.771729
H	5.620217	1.574910	-3.011426
H	-7.499175	1.820140	-1.516042
H	-6.216936	2.012443	-0.318612
H	-5.996902	2.671597	-1.956366
H	-7.162552	0.361446	-3.384742
H	-5.594561	1.025954	-3.872379
H	-5.747906	-0.700943	-3.467978
H	-8.707206	-0.003311	1.261634
H	-7.781403	-0.728874	2.585485
H	-7.591515	0.999848	2.200781
H	-7.900905	-1.435048	-0.488740
H	-6.165980	-1.719007	-0.642508
H	-7.041233	-2.366651	0.764673

H	7.650260	-1.987985	0.449377
H	6.215104	-3.044052	0.474171
H	6.335435	-1.708537	-0.694896
H	7.317213	-1.538516	2.769908
H	5.853834	-0.722184	3.342477
H	5.810252	-2.454961	2.935723
H	8.614637	1.048358	-1.216192
H	7.556608	0.435941	-2.496219
H	7.559169	2.170360	-2.091229
H	7.774171	1.468458	0.981125
H	6.771010	2.762859	0.277431
H	6.031584	1.476098	1.258489
N	-0.720531	-3.300329	0.941883
C	-0.077051	-4.375173	0.169196
C	-0.159912	-4.158885	-1.339742
H	0.969881	-4.428586	0.475921
H	-0.526419	-5.355055	0.409240
N	0.533683	-2.940348	-1.787768
H	0.247943	-5.051535	-1.846257
H	-1.206233	-4.080136	-1.643537
C	1.994199	-3.115745	-1.744696
C	0.124588	-2.604817	-3.157314
H	0.631280	-1.691990	-3.475310
H	0.378926	-3.405824	-3.872215
H	-0.952270	-2.432856	-3.192968
H	2.479721	-2.213046	-2.112024
H	2.337465	-3.272380	-0.722376
H	2.312637	-3.972023	-2.363619
C	-2.186664	-3.388799	0.853815
C	-0.315000	-3.380740	2.350220
H	-2.635637	-2.596021	1.450013
H	-2.522812	-3.250483	-0.173283
H	-2.551403	-4.364168	1.219138
H	-0.774991	-2.563658	2.909026
H	-0.624507	-4.332203	2.815377
H	0.769066	-3.289192	2.431093
N	-0.457959	3.226124	-0.740859
C	-0.008244	3.331536	-2.134648
C	-1.916786	3.410818	-0.685862
C	0.231969	4.224227	0.091621
C	0.087496	3.955027	1.587793
H	1.289090	4.219090	-0.183505
H	-0.143236	5.240903	-0.121290
N	0.675618	2.670340	1.996469
H	0.544951	4.793541	2.142512

H	-0.970187	3.944317	1.860463
C	2.143995	2.746228	2.017847
C	0.190786	2.285437	3.326189
H	0.607673	1.313279	3.596954
H	0.484905	3.012970	4.102396
H	-0.897610	2.206945	3.318969
H	2.555001	1.781526	2.310704
H	2.535608	2.975070	1.027203
H	2.493328	3.520337	2.723078
H	-2.203344	4.423078	-1.019008
H	-2.401459	2.673803	-1.323642
H	-2.290117	3.256899	0.326178
H	-0.235817	4.320347	-2.568300
H	1.068119	3.162461	-2.194636
H	-0.511883	2.571955	-2.735446

Compound **5d·(TMEDA)$_2$**

scf done: -1363.559376

C	0.116471	0.702705	1.410325
C	0.451646	-0.059692	0.220008
C	1.527620	-1.033672	0.180567
C	2.417228	-1.067608	1.319114
C	2.081444	-0.333789	2.449538
C	0.933114	0.487559	2.506181
C	1.614005	-1.862208	-1.002025
C	0.832877	-1.534072	-2.102512
C	-0.097160	-0.469295	-2.080215
C	-0.371696	0.257436	-0.935725
N	2.468085	-3.000822	-1.044141
C	2.809435	-3.542269	-2.345947
N	3.633086	-1.814678	1.287720
C	4.624213	-1.346971	0.324934
C	4.246960	-2.152689	2.558640
C	2.149141	-4.061082	-0.092306
Li	-0.018181	2.215849	-0.121153
N	-0.903563	4.197767	-0.397487
C	-1.797217	4.608722	0.691236
C	0.281239	5.074462	-0.458490
C	1.434610	4.451235	-1.247183
N	1.847743	3.151858	-0.696301
C	2.670348	3.302634	0.513064
C	-1.635224	4.179680	-1.671369
C	2.571018	2.353131	-1.696154

Li	-1.753794	0.450231	0.589005
N	-3.638397	-0.118505	1.280980
C	-4.598134	-0.509996	0.222795
C	-4.025083	-1.406802	-0.880753
N	-3.792362	-2.802844	-0.507313
C	-5.027774	-3.565295	-0.386866
C	-3.353886	-1.228901	2.214553
C	-4.170960	1.023887	2.040024
C	-2.863502	-3.450925	-1.429961
H	4.722677	-1.295595	3.070083
H	3.506101	-2.584117	3.234496
H	5.026669	-2.899782	2.381629
H	5.378538	-2.123473	0.164536
H	4.153384	-1.135545	-0.631408
H	5.139030	-0.434673	0.679454
H	1.889213	-3.638540	0.873980
H	3.019918	-4.709835	0.043467
H	1.305771	-4.682234	-0.444938
H	3.627281	-4.258532	-2.222115
H	1.977241	-4.074942	-2.841918
H	3.149837	-2.746920	-3.012098
H	0.900716	-2.141730	-2.997937
H	-0.643712	-0.273856	-3.004557
H	0.738315	0.998453	3.450363
H	2.741059	-0.360694	3.309798
H	0.029733	6.054537	-0.898652
H	0.601768	5.266848	0.568179
H	2.274531	5.166431	-1.275680
H	1.128376	4.292814	-2.283988
H	-2.019458	5.179000	-1.936558
H	-0.994092	3.825787	-2.478833
H	-2.474395	3.486550	-1.597827
H	-2.174283	5.636239	0.556326
H	-2.653776	3.933348	0.734957
H	-1.271958	4.548175	1.645931
H	2.814223	1.378902	-1.271618
H	1.935827	2.185684	-2.566995
H	3.503795	2.844927	-2.018849
H	2.888288	2.318067	0.927470
H	3.618427	3.822656	0.295520
H	2.133152	3.865938	1.277155
H	-5.496603	-0.959433	0.675787
H	-4.926652	0.413100	-0.264104
H	-4.258411	-1.516223	2.775440
H	-3.002239	-2.093851	1.656005

H	-2.585536	-0.913919	2.923654
H	-5.120495	0.777810	2.542534
H	-3.446779	1.326021	2.799214
H	-4.346685	1.870497	1.371593
H	-4.712782	-1.342960	-1.747761
H	-3.072084	-0.978854	-1.206430
H	-4.800639	-4.583387	-0.061804
H	-5.689054	-3.119925	0.359028
H	-5.582456	-3.625594	-1.343020
H	-2.656210	-4.467082	-1.085257
H	-3.263897	-3.515325	-2.459221
H	-1.922296	-2.899556	-1.461631

Compound **5d·$(Et_2O)_4$**

Zero-point correction= 0.820762 (Hartree/Particle)
Thermal correction to Energy= 0.871890
Thermal correction to Enthalpy= 0.872834
Thermal correction to Gibbs Free Energy= 0.731380
Sum of electronic and zero-point Energies= -1601.981765
Sum of electronic and thermal Energies= -1601.930638
Sum of electronic and thermal Enthalpies= -1601.929694
Sum of electronic and thermal Free Energies= -1602.071148

scf done: -1602.802528

C	0.128088	0.128002	-1.208026
C	-0.656093	0.028433	0.010055
C	-2.104788	-0.072108	0.014893
C	-2.779030	0.150342	-1.245698
C	-2.016330	0.236793	-2.402720
C	-0.603510	0.174647	-2.382879
C	-2.732395	-0.391979	1.278021
C	-1.955681	-0.380460	2.428313
C	-0.564559	-0.127203	2.399783
C	0.144399	0.030087	1.221130
N	-4.115883	-0.738800	1.352209
C	-4.768353	-0.631462	2.643430
N	-4.197016	0.299958	-1.311556
C	-4.730718	1.472650	-0.627118
C	-4.836099	0.103791	-2.598985
C	-4.482818	-1.976126	0.672860
Li	1.277135	1.407749	0.078799
O	0.409277	3.334104	0.033562
C	-0.233913	3.731693	-1.192548

C	0.181777	5.118186	-1.670687
C	-0.076997	3.974303	1.227044
C	-1.501172	3.593846	1.612930
O	3.294435	2.118869	0.199572
C	3.543789	2.961689	1.334194
C	3.225717	2.207298	2.612870
C	3.756634	2.704034	-1.027943
C	3.656471	1.687380	-2.149722
Li	1.329776	-1.271112	-0.083760
O	3.260850	-1.906108	-0.040524
C	4.225283	-1.317800	0.851373
C	4.232925	-2.006348	2.209358
C	3.762769	-2.961507	-0.874147
C	4.447798	-2.440777	-2.131710
O	0.525937	-3.179113	-0.278311
C	0.699065	-4.176607	0.739385
C	-0.303339	-4.054704	1.880638
C	-0.551632	-3.427335	-1.203856
C	-0.118040	-4.317929	-2.361920
H	5.217138	-1.352435	0.387060
H	-4.477604	-1.421011	3.360845
H	-4.553533	0.337523	3.098338
H	-5.850095	-0.708993	2.495687
H	-5.565070	-2.002966	0.511304
H	-3.996971	-2.032322	-0.297453
H	-4.200106	-2.866002	1.265872
H	-4.251141	1.597432	0.339571
H	-5.804767	1.346181	-0.458728
H	-4.581253	2.393823	-1.220971
H	-5.917043	0.029746	-2.444652
H	-4.662352	0.926820	-3.316715
H	-4.490631	-0.825099	-3.057126
H	-2.514579	0.397902	-3.352589
H	-0.097542	0.217366	-3.349970
H	-0.050215	-0.108587	3.363154
H	-2.419710	-0.614743	3.380408
H	0.657974	-5.174712	0.285033
H	1.714773	-4.028569	1.113259
H	-1.399729	-3.864942	-0.668227
H	-0.855402	-2.446119	-1.566617
H	3.940343	-0.269916	0.945254
H	4.441920	-3.595437	-0.290784
H	2.889913	-3.559126	-1.138332
H	-0.056301	-4.780508	2.662257
H	-0.277296	-3.050901	2.308500

H	-1.325304	-4.256944	1.552232
H	-0.957135	-4.464142	-3.048830
H	0.697171	-3.851535	-2.920688
H	0.210797	-5.305128	-2.024524
H	4.763200	-3.281965	-2.756798
H	3.760341	-1.819685	-2.709807
H	5.336935	-1.848717	-1.899132
H	0.049151	2.965808	-1.914640
H	-1.319500	3.668176	-1.077671
H	0.023587	5.061939	1.123386
H	0.611620	3.656758	2.011675
H	-0.284806	5.321134	-2.639399
H	-0.131729	5.909254	-0.984710
H	1.265826	5.183040	-1.797169
H	-1.737367	4.049726	2.579764
H	-2.238572	3.956173	0.893193
H	-1.600623	2.511546	1.708136
H	4.965901	-1.528841	2.867435
H	3.249782	-1.928622	2.678930
H	4.499562	-3.063803	2.126547
H	4.597781	3.269693	1.318822
H	2.930281	3.867276	1.246111
H	4.795778	3.031694	-0.890212
H	3.152538	3.594513	-1.245934
H	3.922368	2.161919	-3.098799
H	4.340745	0.853380	-1.979812
H	2.642885	1.283378	-2.227561
H	3.316260	2.881299	3.469518
H	2.212665	1.796848	2.591554
H	3.919230	1.376404	2.760020

Compound **11c**
scf done: -1125.961892

C	-3.783606	-2.747700	-1.749477
C	-4.571549	-3.025067	-0.458897
C	-3.877710	-2.116180	0.564684
O	-3.242381	-1.059198	-0.194017
C	-3.470239	-1.262680	-1.614701
Li	-1.574131	-0.011625	0.160458
O	-2.155522	1.577164	1.214588
C	-3.511181	1.991639	1.457667
C	-3.680839	3.359003	0.755548
C	-2.241287	3.748553	0.332341

C	-1.362453	2.777259	1.120145
C	-0.114680	0.333260	-1.238821
C	0.857483	-0.115925	-0.355093
C	2.249828	0.272046	-0.442577
C	2.529610	1.412487	-1.278356
C	1.531995	1.884733	-2.170186
C	0.298531	1.276789	-2.219122
C	3.384030	-0.340757	0.203326
C	4.598781	0.321706	0.250380
C	4.796439	1.546295	-0.421702
C	3.798686	2.046759	-1.217714
N	3.263959	-1.682471	0.694725
C	4.192417	-2.079934	1.743838
N	0.290134	-0.850469	0.798055
C	0.755025	-0.460626	2.129743
C	0.120004	-2.299163	0.674600
C	3.263369	-2.660897	-0.399242
H	-0.203512	-2.537031	-0.340009
H	1.036152	-2.856963	0.899214
H	-0.654842	-2.636722	1.374948
H	0.003642	-0.758289	2.870830
H	1.710031	-0.921225	2.405235
H	0.864177	0.624067	2.175875
H	2.529813	-2.380455	-1.154278
H	3.002158	-3.649594	-0.010575
H	4.251845	-2.731082	-0.883959
H	3.865384	-3.038041	2.158804
H	5.230450	-2.210861	1.392343
H	4.192240	-1.340180	2.546480
H	5.440265	-0.130540	0.760153
H	5.758630	2.043193	-0.359357
H	3.961803	2.936373	-1.817801
H	1.776341	2.724045	-2.817478
H	-0.409877	1.609275	-2.978508
H	-3.668272	2.076990	2.539733
H	-4.160944	1.209334	1.065553
H	-1.150566	3.147335	2.132132
H	-0.431249	2.515366	0.620667
H	-4.113941	4.091552	1.439741
H	-4.341871	3.286073	-0.109402
H	-2.004371	4.791124	0.551933
H	-2.094269	3.584947	-0.736688
H	-3.099863	-2.646593	1.121793
H	-4.573880	-1.667905	1.278767
H	-4.320523	-0.643955	-1.927027

H	-2.566411	-0.929425	-2.126453
H	-4.351337	-2.974753	-2.653647
H	-2.857398	-3.328612	-1.771318
H	-4.551086	-4.073545	-0.156703
H	-5.617692	-2.731776	-0.584701