Electronic Supplementary Information

In Silico Design of Adamantane Derived Organic Superbases with Extended Hydrogen Bond Network and their Use as Molecular Containers for the Storage of H_2 and CO_2

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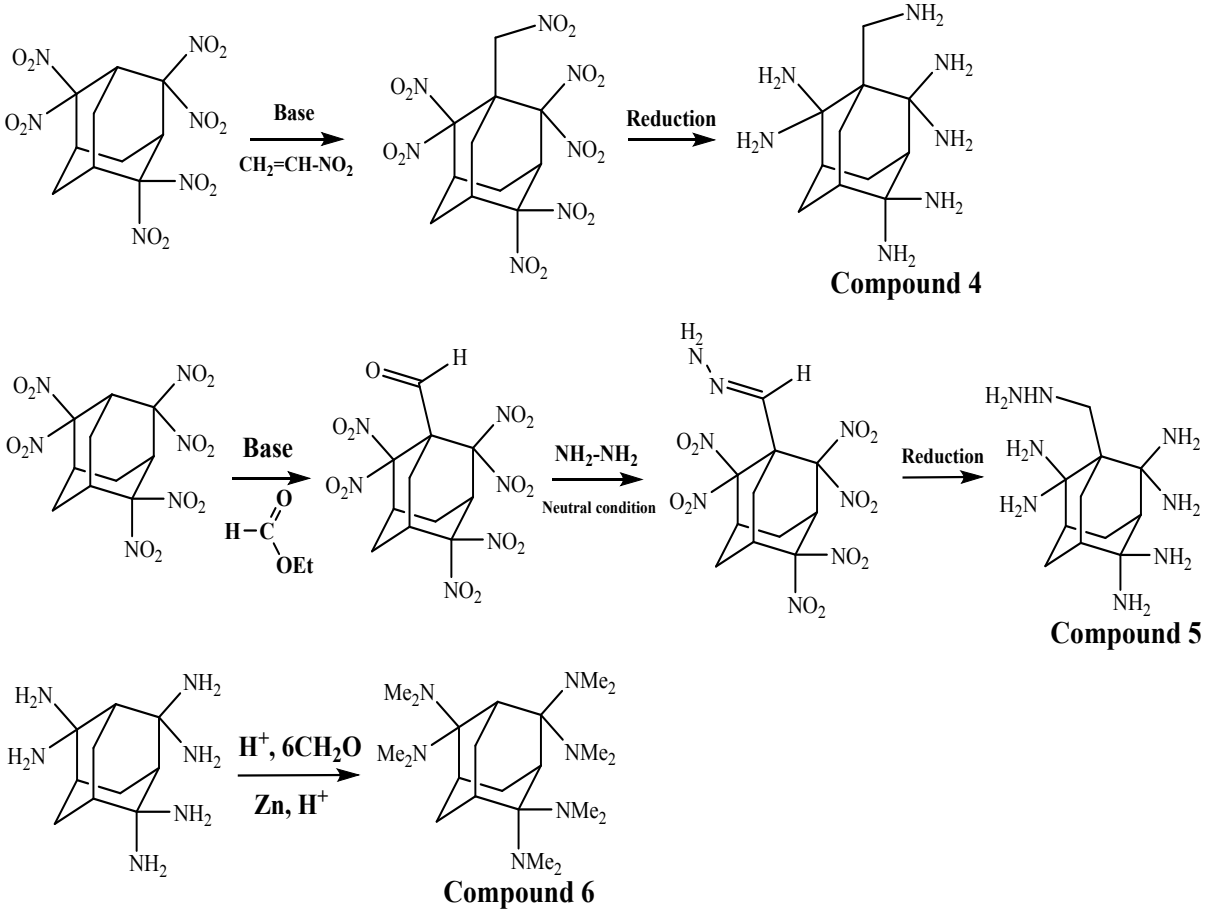

Scheme S1: Proposed reaction pathways for the synthesis of compound **4**-**6**.

Table S1: Calculated hydrogen bond energies (E_{HB}) and potential energies densities (V(r)) at corresponding bond critical point (BCP) at B3LYP/6-311+G(d,p) level of theory.

Compound	Bond critical point	V(r) at BCP	V(r)/2	E_{HB}=(V(r)/2)*627.5095(kcal/mol)
$2H^+$	87	-0.0750	-0.0375	-23.5
$3H^+$	51, 76	-0.0093, -0.0757	-0.0425	-26.7
$4H^+$	67, 85	-0.0471, -0.0408	-0.0439	-27.6
$5H^+$	51, 67, 84	-0.0101, -0.0617, -0.0279	-0.0498	-31.3

Table S2: Calculated interaction energies (ΔE) of **2** with metal ions (Li^+, Na^+) using M06-2X/6-31+G(d) and M062X/6311+G(d,p)//MO6-2X/6-31+G(d) levels of theory in the gas phase. Energies are given in kcal mol^{-1}.

System	Li^+		Na^+	
	M06-2X/631+G(d)	**M062X/6311+G(d,p)// MO62X/631+G(d)**	**M06-2X/631+G(d)**	**M062X/6311+G(d,p)// MO62X/631+G(d)**
7	-75.7	-74.9	-49.3	-47.6
8	-4.2	-3.2	12.2	13.8

Table S3: Calculated Interaction energy (ΔE) and desorption energy (ΔDE) per hydrogen molecule using M06-2X/6-31+G(d) and M06-2X/6-311+G(d,p)//MO6-2X/6-31+G(d) levels of theory in the gas phase. Energies are given in kcal mol^{-1}.

System	ΔE		ΔE_{DE}	
	M06-2X/631+G(d)	**M062X/6311+G(d,p)// MO62X/631+G(d)**	**M06-2X/631+G(d)**	**M062X/6311+G(d,p)// MO62X/631+G(d)**
$9.(Li^+)_2$-(H_2)	-4.2	-4.6	4.2	4.6
$9.(Li^+)_2$-$(H_2)_2$	-4.1	-4.4	4.0	4.2
$9.(Li^+)_2$-$(H_2)_3$	-3.7	-4.0	2.9	3.1
$9.(Li^+)_2$-$(H_2)_4$	-3.5	-3.8	3.0	3.1

$9.(Li^+)_2$-$(H_2)_5$	-3.3	-3.5	2.7	2.4
$9.(Li^+)_2$-$(H_2)_6$	-3.2	-3.3	2.6	2.4

Table S4: Calculated Interaction energy (ΔE) and desorption energy (ΔDE) per carbon dioxide and carbon monoxide molecule using M06-2X/6-31+G(d) and M06-2X/6-311+G(d,p)//MO6-2X/6-31+G(d) levels of theory in the gas phase. Energies are given in kcal mol^{-1}.

System	**ΔE**		**ΔE_{DE}**	
	M06-2X/631+G(d)	**M062X/6311+G(d,p)//MO62X/631+G(d)**	**M06-2X/631+G(d)**	**M062X/6311+G(d,p)//MO62X/631+G(d)**
$10.(Li^+)_2$-(CO_2)	-15.6	-15.6	15.6	15.6
$11.(Li^+)_2$-(CO)	-10.5	-10.0	10.5	10.0
$10.(Li^+)_2$-$(CO_2)_2$	-15.1	-15.1	14.6	14.6
$11.(Li^+)_2$-$(CO)_2$	-9.9	-9.5	9.3	8.9
$10.(Li^+)_2$-$(CO_2)_3$	-13.4	-13.4	10.0	10.0
$11.(Li^+)_2$-$(CO)_3$	-9.0	-8.6	7.1	6.8
$10.(Li^+)_2$-$(CO_2)_4$	-12.5	-12.5	9.9	9.9
$11.(Li^+)_2$-$(CO)_4$	-8.4	-8.0	6.8	6.5
$10.(Li^+)_2$-$(CO_2)_5$	-11.3	-11.1	6.3	5.6
$11.(Li^+)_2$-$(CO)_5$	-7.8	-7.3	5.4	4.6
$10.(Li^+)_2$-$(CO_2)_6$	-10.5	-10.3	6.6	5.9

11.$(Li^+)_2$-$(CO)_6$	-7.4	-6.9	5.6	4.7

Electronic energies in gas phase (E) with different levels of theory of adamantane-1-amine, zero point vibrational energies (ZPVE), and Cartesian coordinates for 1 and $1H^+$ (All energies are given in Hartee).

B3LYP/6-31+G(d)

1

E= -446.08577614, ZPE=0.260229

C	-1.33052700	-1.25432700	0.74404000
H	-0.98447800	-2.15419900	1.27301600
H	-2.42954400	-1.27754900	0.76026100
C	-0.82123300	-1.26671900	-0.71343400
H	-1.18414100	-2.16958100	-1.22342900
C	-0.81644200	0.01211900	1.46098600
H	-1.17273100	0.02069700	2.50045300
C	0.72738800	0.01203500	1.44362000
C	0.72189800	-1.26040000	-0.72366400
H	1.10471900	-1.28150900	-1.75237300
H	1.10591500	-2.16025800	-0.21866800
C	1.26126500	-0.00012500	-0.01314400
C	0.72190900	1.24818400	-0.74442600
C	-1.34011200	-0.01200400	-1.44755700
C	-1.33044700	1.26657800	0.72337200
H	-2.42946300	1.29018100	0.73934500
H	-0.98421500	2.17500500	1.23740500
C	-0.82121100	1.25466600	-0.73414100
H	-1.18410500	2.14896900	-1.25899600
H	1.11391400	-0.86747400	1.98088100
H	1.11394300	0.90029500	1.96629400
H	1.10469200	1.25221300	-1.77333900
H	1.10600100	2.15627300	-0.25443000
H	-1.00329000	-0.02066700	-2.49395400
H	-2.43945300	-0.01218600	-1.46536400
N	2.72880900	-0.00087400	-0.10443200
H	3.11284300	0.82101300	0.36343100
H	3.11279700	-0.81514800	0.37658800

$1H^+$

E=-446.46055624, ZPE= 0.275554

C	1.36502600	0.92399200	1.12917400
H	1.02723000	1.58574500	1.93819300
H	2.46128300	0.93926900	1.14756400
C	0.85891600	1.43783500	-0.23512300
H	1.20572700	2.46349100	-0.40281400
C	0.85887400	-0.51544100	1.36275300
H	1.20554700	-0.88303100	2.33490600
C	-0.69099500	-0.51658900	1.36566100
C	-0.69082500	1.44134200	-0.23557600
H	-1.06723000	1.81935700	-1.19696600
H	-1.06692100	2.10568300	0.55569700
C	-1.16653500	0.00006900	-0.00004300
C	-0.69108400	-0.92452300	-1.13021900
C	1.36504500	0.51603700	-1.36462500
C	1.36500000	-1.44000300	0.23547600
H	2.46125300	-1.46365800	0.23925000
H	1.02720500	-2.47147400	0.40416700
C	0.85878300	-0.92281400	-1.12759500
H	1.20547400	-1.58087500	-1.93204200
H	-1.06744100	0.12709700	2.17355600
H	-1.06709600	-1.53408900	1.54456000
H	-1.06733000	-0.57133600	-2.10102700
H	-1.06756900	-1.94597400	-0.97625900
H	1.02733800	0.88568100	-2.34230700
H	2.46129000	0.52450900	-1.38682800
N	-2.71580900	0.00002500	0.00008600
H	-3.08702900	-0.94570500	0.15361000
H	-3.08700200	0.60575600	0.74243200
H	-3.08730200	0.33995300	-0.89559100

B3LYP/6-311+G(d,p)

1

E=-446.19520809, ZPE=0.258751

C	1.32959600	-1.26056900	-0.73051800
H	0.98434100	-2.16279400	-1.24915600
H	2.42540800	-1.28363100	-0.74597700
C	0.82002900	-1.25803200	0.72508700
H	1.18173200	-2.15298000	1.24278500
C	0.81617600	-0.00245200	-1.45882400
H	1.17198400	-0.00419100	-2.49502900
C	-0.72588200	-0.00233000	-1.44277000
C	-0.72129600	-1.25192800	0.73487200
H	-1.10343600	-1.26185800	1.76075600
H	-1.10524400	-2.15319600	0.23948000
C	-1.25988000	0.00013000	0.01264200
C	-0.72106900	1.25448500	0.73079700
C	1.33810300	0.00231900	1.44669000

C	1.32988000	1.25793400	-0.73461900
H	2.42569100	1.28063000	-0.75004700
H	0.98490100	2.15851900	-1.25624600
C	0.82026000	1.26038900	0.72097700
H	1.18209700	2.15700100	1.23569100
H	-1.11130300	-0.88484800	-1.96902800
H	-1.11115400	0.87855600	-1.97189200
H	-1.10317300	1.26772400	1.75664500
H	-1.10508800	2.15414800	0.23260300
H	1.00116300	0.00411900	2.48967000
H	2.43418200	0.00226800	1.46494000
N	-2.72630700	0.00044900	0.10260400
H	-3.11175800	0.81564200	-0.36746600
H	-3.11169800	-0.81792200	-0.36196200

1H+

E= -446.57066765, ZPE=- 0.27364

C	-1.36413400	-0.77607800	1.23314400
H	-1.02872600	-1.33145700	2.11561200
H	-2.45736200	-0.78806300	1.25207800
C	-0.85792500	-1.45377400	-0.05515500
H	-1.20447400	-2.48911100	-0.09455400
C	-0.85789600	0.67919100	1.28659500
H	-1.20436600	1.16279500	2.20293900
C	0.69038700	0.68089000	1.28957900
C	0.69022100	-1.45742900	-0.05528400
H	1.06462100	-1.95036600	-0.96059500
H	1.06467900	-2.01764100	0.81000600
C	1.16616500	-0.00003100	0.00011000
C	0.69052400	0.77676800	-1.23411000
C	-1.36395700	-0.68032700	-1.28855900
C	-1.36371100	1.45640700	0.05516700
H	-2.45689900	1.47964100	0.05616400
H	-1.02711000	2.49790900	0.09487700
C	-0.85775600	0.77479700	-1.23145700
H	-1.20417400	1.32652300	-2.10853000
H	1.06551200	0.14374700	2.16895000
H	1.06470100	1.71038300	1.34066800
H	1.06580700	0.30803700	-2.15170700
H	1.06482100	1.80720800	-1.20686100
H	-1.02843900	-1.16717100	-2.21055400
H	-2.45719800	-0.69082000	-1.30851300
N	2.71497600	-0.00039700	0.00001600
H	3.08096600	0.95583700	0.03649000
H	3.08092400	-0.51025800	0.80983000
H	3.08038000	-0.44690200	-0.84659400

B3LYP/6-311+G(2d,p)

1

E= -446.20382319, ZPE= 0.258890

C	-1.32747200	-1.25439200	0.73699300
H	-0.98230700	-2.15286000	1.26005200
H	-2.42227800	-1.27695700	0.75285200
C	-0.81929300	-1.26018100	-0.71670200
H	-1.18104700	-2.15732600	-1.22860300
C	-0.81433100	0.00584900	1.45691500
H	-1.16951200	0.00998400	2.49236000
C	0.72539300	0.00588900	1.44016000
C	0.71977200	-1.25401900	-0.72718600
H	1.10074900	-1.26989500	-1.75237200
H	1.10349400	-2.15166800	-0.22737900
C	1.25809900	0.00001700	-0.01310900
C	0.71961000	1.24819100	-0.73729400
C	-1.33714700	-0.00588500	-1.44396400
C	-1.32759600	1.26020900	0.72694500
H	-2.42240300	1.28280200	0.74266500
H	-0.98246900	2.16287000	1.24276200
C	-0.81944500	1.25429100	-0.72677000
H	-1.18130800	2.14724300	-1.24586900
H	1.11065800	-0.87288000	1.97060000
H	1.11054800	0.88897600	1.96347900
H	1.10056800	1.25577100	-1.76257200
H	1.10333500	2.14987200	-0.24481100
H	-1.00118800	-0.01005800	-2.48622100
H	-2.43226600	-0.00604300	-1.46103800
N	2.72353700	-0.00026200	-0.10355100
H	3.10759000	0.81669300	0.36414100
H	3.10752700	-0.81451000	0.36888600

1H$^+$

E= - 446.57917367, ZPE= 0.273903

C	1.36218400	0.52508600	1.35688300
H	1.02585400	0.90069400	2.32824000
H	2.45441200	0.53379800	1.37851200
C	0.85647400	1.43594800	0.22349700
H	1.20336100	2.45875600	0.38271800
C	0.85707500	-0.91172700	1.13137300
H	1.20402100	-1.56101900	1.93751800
C	-0.68832800	-0.91373000	1.13439100
C	-0.68888000	1.43913000	0.22418200
H	-1.06413100	2.09445600	-0.56981400
H	-1.06429500	1.82281100	1.17940500
C	-1.16411600	-0.00004500	0.00040400
C	-0.68989600	-0.52552100	-1.35789600
C	1.36097800	0.91309100	-1.13356300
C	1.36135300	-1.43813200	-0.22451000

H	2.45356600	-1.46194000	-0.22877900
H	1.02412500	-2.46693900	-0.38434000
C	0.85557100	-0.52429500	-1.35557300
H	1.20211300	-0.89768300	-2.32114600
H	-1.06357500	-0.55420900	2.09902400
H	-1.06392300	-1.93267000	0.98851100
H	-1.06573300	0.11021200	-2.16729100
H	-1.06548600	-1.54065700	-1.52823300
H	1.02398500	1.56638800	-1.94434900
H	2.45319500	0.92792200	-1.15239800
N	-2.70954500	0.00010400	0.00077500
H	-3.07525600	-0.94528800	-0.14591100
H	-3.07521300	0.34607400	0.89271900
H	-3.07470200	0.59974700	-0.74493900

M062x/6-311+G(2d,p)

1

E= -446.00878422, ZPE= 0.261017

C	-1.32060900	-1.24407400	0.74571500
H	-0.97129800	-2.13683100	1.27437800
H	-2.41475300	-1.26324700	0.76163400
C	-0.81661300	-1.26196500	-0.70411800
H	-1.17912100	-2.16215900	-1.20742200
C	-0.80865100	0.01746100	1.45316600
H	-1.16231700	0.02985600	2.48764800
C	0.72500300	0.01747700	1.43315800
C	0.71675000	-1.25464400	-0.71593900
H	1.09759000	-1.27247100	-1.74102600
H	1.10245800	-2.14582000	-0.20668400
C	1.25016000	-0.00012800	-0.01455000
C	0.71668500	1.23700300	-0.74601900
C	-1.33368200	-0.01731600	-1.43737500
C	-1.32064300	1.26162800	0.71593700
H	-2.41478600	1.28117500	0.73151300
H	-0.97128100	2.16680600	1.22303400
C	-0.81668100	1.24459000	-0.73396300
H	-1.17928700	2.13239100	-1.25871800
H	1.11167400	-0.85910500	1.96583300
H	1.11145900	0.90684300	1.94443600
H	1.09738300	1.22994900	-1.77128000
H	1.10253200	2.14022800	-0.25854600
H	-0.99646300	-0.02981900	-2.47842300
H	-2.42817100	-0.01753400	-1.44818300
N	2.71024200	-0.00130200	-0.10551600
H	3.08633800	0.81886200	0.36245400

H	3.08604300	-0.81019200	0.38189200

$1H^+$

E=-446.38138530, ZPE= 0.276296

C	1.35362700	-1.34097500	-0.55275600
H	1.01353100	-2.30187600	-0.94975600
H	2.44555500	-1.35951500	-0.55979100
C	0.85014400	-1.14886100	0.88360000
H	1.19799700	-1.96832200	1.51405900
C	0.85160000	-0.19121800	-1.43610300
H	1.20022400	-0.32749800	-2.46068400
C	-0.68694200	-0.19122300	-1.43939500
C	-0.68842600	-1.15035000	0.88477400
H	-1.06419300	-1.02245200	1.90608600
H	-1.06411600	-2.10468300	0.49903200
C	-1.15920200	0.00060400	-0.00042500
C	-0.68681300	1.34243900	0.55372900
C	1.35352000	0.19054500	1.43780800
C	1.35444100	1.14932500	-0.88401100
H	2.44633900	1.16535900	-0.89627500
H	1.01389000	1.97322400	-1.51797600
C	0.85171100	1.33932500	0.55297400
H	1.20013200	2.29474900	0.94750100
H	-1.06267500	-1.13976900	-1.83911100
H	-1.06213500	0.61991800	-2.07342000
H	-1.06268600	1.48565200	1.57297800
H	-1.06219400	2.16337900	-0.06752200
H	1.01305800	0.32776000	2.46825300
H	2.44543800	0.19276500	1.45751600
N	-2.68711100	0.00046000	-0.00027100
H	-3.05088200	0.75991000	-0.58380000
H	-3.04965300	-0.88520900	-0.36601200
H	-3.04981600	0.12572300	0.94964400

wB97X-D/6-311+G(2d,P)

1

E= -446.08272317, ZPE= 0.261740

C	-1.32014800	-1.25474200	0.72867700
H	-0.97065200	-2.15575100	1.24391500
H	-2.41477800	-1.27659500	0.74681800
C	-0.81802800	-1.25108100	-0.72129300
H	-1.18133900	-2.14416100	-1.23729900
C	-0.80740200	-0.00359800	1.45285400
H	-1.16073100	-0.00613200	2.48807600
C	0.72639800	-0.00360300	1.43269400

C	0.71538500	-1.24457100	-0.73436800
H	1.09523400	-1.25190600	-1.76022000
H	1.09990200	-2.14469500	-0.23954500
C	1.25259500	0.00006600	-0.01600400
C	0.71536900	1.24827900	-0.72817400
C	-1.33503600	0.00354700	-1.43671000
C	-1.32016100	1.25108700	0.73477000
H	-2.41479400	1.27277900	0.75300000
H	-0.97073100	2.14952900	1.25450000
C	-0.81803500	1.25465700	-0.71518800
H	-1.18137700	2.15029400	-1.22672700
H	1.11294900	-0.88726800	1.95407400
H	1.11300500	0.87736900	1.95856200
H	1.09531500	1.26075900	-1.75393900
H	1.09984000	2.14588600	-0.22877200
H	-0.99848700	0.00609300	-2.47864000
H	-2.43003300	0.00357400	-1.45022700
N	2.71120400	0.00034800	-0.10572800
H	3.09133100	0.81313900	0.36918100
H	3.09129700	-0.81558500	0.36378600

1H^{+}

E= -446.46221863, ZPE= 0.276964

C	-1.35564700	0.06678600	1.44770000
H	-1.01731900	0.11639200	2.48718300
H	-2.44776300	0.06743800	1.46944900
C	-0.85114100	-1.21954600	0.78127600
H	-1.19979600	-2.09064400	1.33799900
C	-0.85198300	1.28597600	0.66470700
H	-1.20057000	2.20423100	1.13958600
C	0.68641600	1.28923300	0.66691400
C	0.68718400	-1.22165900	0.78369500
H	1.06368400	-2.14100100	0.32092100
H	1.06227800	-1.18347200	1.81273700
C	1.16262900	0.00013000	0.00042500
C	0.68790100	-0.06678600	-1.44937400
C	-1.35362800	-1.28832700	-0.66653300
C	-1.35486200	1.22048000	-0.78282500
H	-2.44698200	1.23911800	-0.79475800
H	-1.01606700	2.09733100	-1.34305700
C	-0.85038600	-0.06715600	-1.44678600
H	-1.19802500	-0.11621900	-2.47969200
H	1.06073400	1.34819800	1.69527900
H	1.06238700	2.16257900	0.12179600
H	1.06430900	-0.97589300	-1.93201300
H	1.06374600	0.79472100	-2.01306100
H	-1.01398700	-2.21218500	-1.14443500

H	-2.44575200	-1.30839300	-0.67737200
N	2.68827200	0.00032000	0.00040200
H	3.05111600	0.80474800	-0.51509000
H	3.05062900	0.04457100	0.95499200
H	3.05057100	-0.84854000	-0.43847300

Optimized geometry at B3LYP/6-311+G(d,p) level of theory, gas phase electronic energies (E), zero point vibrational energies (ZPVE), and Cartesian coordinates for DMAN and DAN and their corresponding monoprotonated cations (All energies are given in Hartee).

DMAN

E= -653.97546678, ZPE= 0.291860

C	-0.38456400	2.38875700	2.08608500
C	-0.21562800	1.20479500	2.75232500
C	0.00000000	0.00000000	2.03328000
C	0.00000000	0.00000000	0.59444600
C	0.00000000	1.29160400	-0.06623000
C	-0.24172700	2.43303300	0.68665500
H	0.24696100	-1.16439800	3.83544700
H	-0.56783900	3.30828600	2.63115700
H	-0.24696100	1.16439800	3.83544700
C	0.21562800	-1.20479500	2.75232500
C	0.00000000	-1.29160400	-0.06623000
H	-0.26092600	3.39845200	0.19980900
C	0.24172700	-2.43303300	0.68665500
C	0.38456400	-2.38875700	2.08608500
H	0.26092600	-3.39845200	0.19980900
H	0.56783900	-3.30828600	2.63115700
N	-0.26097500	-1.39905400	-1.45077000
N	0.26097500	1.39905400	-1.45077000
C	-1.57460300	-0.93431600	-1.89567700
H	-2.34349700	-1.71042200	-1.74354900
H	-1.53808500	-0.68677500	-2.96020500
H	-1.87156400	-0.04342500	-1.35052300
C	0.13161800	-2.62424500	-2.12516000
H	-0.51144800	-3.48882900	-1.88507600
H	1.16334400	-2.88118900	-1.87853500
H	0.06964100	-2.46035200	-3.20430300
C	1.57460300	0.93431600	-1.89567700
H	1.53808500	0.68677500	-2.96020500
H	1.87156400	0.04342500	-1.35052300
H	2.34349700	1.71042200	-1.74354900
C	-0.13161800	2.62424500	-2.12516000
H	0.51144800	3.48882900	-1.88507600
H	-1.16334400	2.88118900	-1.87853500
H	-0.06964100	2.46035200	-3.20430300

DMANH$^+$

E= -654.37933343, ZPE= 0.305605

C	-2.07465100	-2.46820900	-0.00028400
C	-2.76822000	-1.28561500	-0.00015700
C	-2.08653200	-0.04251400	0.00003700
C	-0.64812000	-0.01878800	0.00014000
C	0.04207600	-1.27426900	0.00003800
C	-0.66507200	-2.45477800	-0.00020200
H	-3.89755800	1.12818800	0.00000300
H	-2.60032500	-3.41513000	-0.00044800
H	-3.85199100	-1.28295900	-0.00023900
C	-2.81467200	1.17471200	0.00009200
C	-0.03628600	1.27190300	0.00018800
H	-0.13146900	-3.39808300	-0.00029700
C	-0.76696800	2.43364700	0.00022800
C	-2.17550700	2.38822400	0.00020500
H	-0.26959800	3.39660700	0.00021300
H	-2.74025000	3.31188000	0.00022900
N	1.44535100	1.34666000	-0.00006900
N	1.50541000	-1.28502600	0.00019400
H	1.71567300	0.28016300	0.00014500
C	2.07231300	-1.90219600	-1.22242100
H	3.15477600	-1.75872800	-1.22524100
H	1.86584200	-2.97656600	-1.27444600
H	1.64695500	-1.42638200	-2.10678600
C	2.07192100	-1.90271900	1.22278900
H	1.86599100	-2.97724000	1.27391500
H	3.15430300	-1.75866400	1.22636500
H	1.64569700	-1.42775800	2.10717900
C	2.00385200	1.97075900	-1.24132300
H	1.73766000	3.02606800	-1.28052600
H	3.08891100	1.86664800	-1.22758500
H	1.59063700	1.45917900	-2.10863000
C	2.00429200	1.97116900	1.24075300
H	3.08955400	1.86944700	1.22536500
H	1.73583100	3.02585100	1.28108500
H	1.59348000	1.45809300	2.10832700

DAN

E= -496.73718561, ZPE= 0.181101

C	0.06732600	2.42182800	1.28629600
C	0.04522500	1.22833700	1.96223300
C	0.00000000	0.00000000	1.25296500
C	0.00000000	0.00000000	-0.18569200
C	-0.05701700	1.27192900	-0.85627100
C	0.00000000	2.44222700	-0.11743200
H	-0.06112900	-1.20286000	3.04582700
H	0.10907700	3.35959300	1.82927400

H	0.06112900	1.20286000	3.04582700
C	-0.04522500	-1.22833700	1.96223300
C	0.05701700	-1.27192900	-0.85627100
H	-0.03398800	3.39388200	-0.63879200
C	0.00000000	-2.44222700	-0.11743200
C	-0.06732600	-2.42182800	1.28629600
H	0.03398800	-3.39388200	-0.63879200
H	-0.10907700	-3.35959300	1.82927400
N	0.13787800	-1.35621500	-2.26015800
H	0.75879200	-0.67875200	-2.68431600
H	0.34542200	-2.29200300	-2.58166500
N	-0.13787800	1.35621500	-2.26015800
H	-0.75879200	0.67875200	-2.68431600
H	-0.34542200	2.29200300	-2.58166500

DANH$^+$

E= -497.10647603, ZPE= 0.194117

C	-2.53296900	-1.11828500	0.00000000
C	-1.39714500	-1.88715500	0.00000000
C	-0.11176400	-1.28843700	0.00000000
C	0.00000000	0.14468700	0.00000000
C	-1.20570400	0.91186800	0.00000000
C	-2.43085800	0.28846000	0.00000000
H	0.95137400	-3.16466600	0.00000000
H	-3.51157400	-1.58183600	0.00000000
H	-1.46601200	-2.96866800	0.00000000
C	1.06117300	-2.08640800	0.00000000
C	1.32334900	0.67148800	0.00000000
H	-3.33362200	0.89010900	0.00000000
C	2.44397000	-0.11837700	0.00000000
C	2.31223300	-1.52172000	0.00000000
H	3.43186000	0.33080300	0.00000000
H	3.19967400	-2.14152600	0.00000000
N	1.48903200	2.14666400	0.00000000
H	1.99292800	2.47444000	0.82654300
H	1.99292800	2.47444000	-0.82654300
N	-1.10925400	2.37247900	0.00000000
H	-1.57343800	2.76633700	-0.81644100
H	-1.57343800	2.76633700	0.81644100
H	0.45717100	2.54349800	0.00000000

B3LYP/6-311+G(d,p) level of theory optimized, gas phase electronic energies (E), zero point vibrational energies (ZPVE), and Cartesian coordinates for 2-6 and their corresponding monoprotonated cations (All energies are given in Hartee).

2

E= -723.03303545, ZPE= 0.345529

C	-0.00002000	-2.12922000	-0.00002500
H	-0.58363100	-2.76673300	0.66564800
H	0.58357900	-2.76672900	-0.66571100
C	0.93236100	-1.23412700	0.83857300
H	1.58507900	-1.86347100	1.45944800
C	-0.93238900	-1.23409600	-0.83860100
H	-1.58512100	-1.86341700	-1.45948300
C	-1.82078600	-0.37600100	0.09970500
C	0.08275300	-0.32370700	1.75479000
H	0.72302100	0.30872400	2.37046900
H	-0.50186300	-0.95107600	2.42826300
C	-0.86814500	0.56053400	0.90791400
H	-1.46053300	1.20313200	1.57172600
C	0.00001500	1.50271700	0.00000300
C	1.82077900	-0.37602400	-0.09970600
C	-0.08276800	-0.32367600	-1.75480500
H	0.50183300	-0.95104100	-2.42829400
H	-0.72303000	0.30877800	-2.37046700
C	0.86815300	0.56052800	-0.90791800
H	1.46055400	1.20312500	-1.57172000
N	2.76427700	0.40782100	0.73221100
H	3.35966000	-0.22939400	1.25608000
H	3.37781900	0.95506600	0.13309000
N	0.74558300	2.41656300	0.87650000
H	1.53794900	1.93674400	1.29374300
H	1.12314300	3.15715800	0.29035800
N	2.51939800	-1.25896300	-1.05540400
H	3.08748800	-0.70526800	-1.69136700
H	3.14956400	-1.88392600	-0.55921900
N	-0.74553100	2.41658400	-0.87648900
H	-1.53787600	1.93677000	-1.29377600
H	-1.12312100	3.15715800	-0.29033900
N	-2.76431100	0.40785100	-0.73217400
H	-3.35971600	-0.22936000	-1.25602300
H	-3.37782900	0.95509600	-0.13302800
N	-2.51937200	-1.25895800	1.05541100
H	-3.08744700	-0.70527400	1.69139700
H	-3.14955000	-1.88391700	0.55923500

$2H^+$

E= -723.43602263, ZPE= 0.358106

C	-0.09664600	-2.14826000	0.03184300
H	-0.68324400	-2.74916500	0.72634100
H	0.44968900	-2.82643200	-0.62462300
C	0.88421400	-1.27293400	0.83853600
H	1.53009600	-1.91533200	1.45148600
C	-1.01144000	-1.23804400	-0.80928400
H	-1.69492100	-1.85874500	-1.40030600
C	-1.85493700	-0.32182100	0.11931800

C	0.08025900	-0.31779300	1.75124600
H	0.73646800	0.28782700	2.38329400
H	-0.52832800	-0.91915200	2.42456700
C	-0.84417700	0.59017100	0.89901700
H	-1.41145700	1.25993400	1.56054800
C	0.03002200	1.46915000	-0.05617600
C	1.76208600	-0.47785600	-0.15590100
C	-0.15091100	-0.38685000	-1.76799000
H	0.40030800	-1.04651300	-2.43833900
H	-0.77287600	0.25291600	-2.39273500
C	0.84607600	0.48554500	-0.96582600
H	1.44866700	1.08742400	-1.65676500
N	2.75143200	0.40277900	0.69397000
H	3.10667400	-0.11410600	1.49884400
H	3.54780300	0.67114600	0.11627800
N	0.96322700	2.29110500	0.77502300
H	1.24662100	3.09184100	0.21036400
N	2.49957200	-1.33487800	-1.01559500
H	2.99733400	-0.89952700	-1.78102100
H	3.02917700	-2.07561700	-0.57547200
N	-0.66881700	2.41341200	-0.92235900
H	-1.47008700	1.95740900	-1.35769600
H	-1.04904400	3.17399400	-0.36417200
N	-2.75327400	0.49487800	-0.72222900
H	-3.34901400	-0.11369600	-1.27855200
H	-3.37577900	1.04952100	-0.13927400
N	-2.56059800	-1.14770500	1.10689400
H	-3.15355400	-0.57534500	1.70186700
H	-3.16439000	-1.82343200	0.64690300
H	0.48300400	2.66410400	1.59124000
H	2.18878800	1.29596800	0.97860000

2aH$^+$

E= -723.71665039, ZPE= 0.371884

C	0.00019800	2.16089200	-0.00004900
H	0.55223600	2.80392500	0.68447500
H	-0.55174700	2.80398600	-0.68459100
C	-0.96123300	1.26811500	0.81181500
H	-1.62909000	1.90386400	1.40413400
C	0.96150300	1.26795700	-0.81188100
H	1.62947200	1.90359400	-1.40419300
C	1.80450800	0.42615800	0.17819400
C	-0.14072400	0.36134300	1.75895700
H	-0.77741000	-0.26200500	2.38980900
H	0.42764500	0.99440300	2.43834400
C	0.83451900	-0.53334600	0.94717600
H	1.41475200	-1.15991900	1.63752400
C	-0.00016000	-1.46113600	-0.00002100
C	-1.80439700	0.42641800	-0.17821000
C	0.14085400	0.36132100	-1.75902500

H	-0.42738800	0.99447700	-2.43842800
H	0.77744000	-0.26214400	-2.38986100
C	-0.83457500	-0.53318400	-0.94726100
H	-1.41492300	-1.15964300	-1.63761600
N	-2.52862400	1.23593600	-1.08124000
H	-3.02246700	0.77913600	-1.83733600
H	-3.04466400	2.01622700	-0.69540100
N	-2.80716600	-0.44592100	0.67793700
H	-3.21919500	0.10560700	1.43391200
H	-3.57484200	-0.77045100	0.08636600
N	-0.89499600	-2.30116100	0.83403700
H	-1.22139200	-3.10705900	0.30297400
H	-0.41575300	-2.66973000	1.65350300
N	0.89433100	-2.30159400	-0.83401500
H	1.22049400	-3.10751900	-0.30285100
H	0.41488900	-2.67013500	-1.65337700
N	2.80734400	-0.44621700	-0.67783000
H	3.21925700	0.10521100	-1.43394100
H	3.57509900	-0.77050800	-0.08623000
N	2.52870300	1.23562000	1.08129100
H	3.02240400	0.77880600	1.83747000
H	3.04481000	2.01590100	0.69552800
H	-2.27253900	-1.28471500	1.04728100
H	2.27282200	-1.28518200	-1.04693600

3

E= -817.70125772, ZPE= 0.390510

C	-0.06678300	-0.41058100	1.41763300
C	0.22653200	1.08429800	1.08379800
H	0.57545400	1.56051400	2.00953800
C	-0.59189100	-1.08164700	0.09391900
H	-0.77863200	-2.14856900	0.29341100
C	-1.93518700	-0.41915300	-0.40315300
C	-1.10891900	1.73992900	0.64273100
H	-0.94379600	2.79921400	0.45131200
H	-1.85153500	1.66605500	1.43792300
C	-1.61998800	1.07917200	-0.65595800
H	-2.54740200	1.57766200	-0.97225900
C	-0.55073700	1.23896000	-1.75734200
H	-0.89091900	0.78476100	-2.69026600
H	-0.38308700	2.30127300	-1.93235400
C	1.29567000	1.30649100	-0.03941100
C	0.42419200	-0.94207100	-1.09184600
H	-0.19053300	-1.18029500	-1.96168100
C	0.76679400	0.56609200	-1.30312500
H	1.52009800	0.65719200	-2.09373200
N	1.33382300	2.76709200	-0.31414700
H	1.48069900	3.26014400	0.56472600
H	2.18181300	2.92726900	-0.85294400
N	2.66438600	0.89052900	0.25372200

H	2.93193100	1.13578100	1.20178800
H	2.83721800	-0.10219200	0.09707100
N	1.14135000	-1.13104000	1.85468300
H	1.56762300	-0.60679300	2.61528700
H	0.84668700	-2.01541300	2.26663400
N	-0.99430300	-0.42992700	2.57045000
H	-1.94470600	-0.22808900	2.26795900
H	-1.01383400	-1.36540600	2.96767900
N	-3.00626400	-0.51143500	0.61838800
H	-3.83406400	-0.03004000	0.27504700
H	-3.27131800	-1.48418300	0.75402200
N	-2.34903500	-1.05453100	-1.67033900
H	-2.66079000	-2.00722800	-1.50167800
H	-3.13357900	-0.54930100	-2.07305700
C	1.52234300	-2.01823300	-1.26282700
H	1.00040400	-2.98933500	-1.19755000
H	1.86340900	-1.93055700	-2.30045900
N	2.72386900	-1.97474300	-0.42744200
H	3.38944000	-2.68132900	-0.72001700
H	2.48050200	-2.10228400	0.54986900

$3H^+$

E= -818.11817249, ZPE= 0.404612

C	-0.11212400	-0.45535700	1.40922000
C	0.17674600	1.05228500	1.12035600
H	0.52684400	1.51057700	2.05398300
C	-0.62183900	-1.08734300	0.06418900
H	-0.81010100	-2.15769500	0.23169900
C	-1.96891000	-0.41140800	-0.42221400
C	-1.14710300	1.72779300	0.68011400
H	-0.98182000	2.79309600	0.52404700
H	-1.88403800	1.63129300	1.47583700
C	-1.65440300	1.09596900	-0.63292700
H	-2.57779700	1.60335300	-0.93714200
C	-0.58873500	1.28869900	-1.73076200
H	-0.92011900	0.85653700	-2.67524200
H	-0.42717300	2.35492300	-1.88967400
C	1.22111100	1.29408200	-0.00444500
C	0.39332100	-0.91693700	-1.11605800
H	-0.22014600	-1.14476700	-1.99023800
C	0.72645300	0.59499200	-1.29634400
H	1.48116000	0.71537500	-2.08467700
N	1.39014200	2.70233400	-0.21547200
H	1.64060500	3.24064600	0.60451500
H	1.94554000	2.96322100	-1.02085100
N	2.60853600	0.69551300	0.38910200
H	3.33173000	1.29908700	-0.00179100
H	2.72121000	0.67598400	1.40153600

N	1.12259000	-1.14833100	1.83441600
H	1.29500500	-0.86515800	2.79975800
H	0.91858700	-2.14514600	1.89891200
N	-1.02628300	-0.51139600	2.55491200
H	-1.98242200	-0.30709000	2.27004900
H	-1.03068200	-1.44851100	2.94723400
N	-3.02857800	-0.52934200	0.59811700
H	-3.85752900	-0.02778900	0.28840700
H	-3.30559100	-1.50143300	0.71174600
N	-2.35773800	-1.01071300	-1.70965500
H	-2.69937900	-1.95859600	-1.57567500
H	-3.11417300	-0.48212800	-2.13547400
C	1.52870800	-1.94633200	-1.31045000
H	1.09416800	-2.94793100	-1.21292600
H	1.84577300	-1.85279800	-2.35239400
N	2.76360900	-1.82107800	-0.49846400
H	2.66827400	-2.29173300	0.39476500
H	3.54942300	-2.23979700	-0.98735700
H	2.76734500	-0.33107400	0.02618400

4

E= -857.03713317, ZPE= 0.420319

C	-1.35446300	-2.01804900	-0.55826800
H	-0.87065800	-2.66998000	-1.28821200
H	-2.27541900	-2.49985400	-0.22590000
C	-1.65863000	-0.66097100	-1.21284600
H	-2.28642400	-0.81141600	-2.10293500
C	-0.43531300	-1.77895200	0.65095000
H	-0.22891900	-2.74011300	1.14365100
C	0.92552000	-1.18445000	0.20328800
C	-0.33358700	-0.00261700	-1.64085100
H	-0.52623200	0.95004300	-2.13848200
H	0.15692300	-0.65538300	-2.36452800
C	0.65326700	0.23425300	-0.45092300
C	-0.09553100	1.20657600	0.57752400
C	-2.41627100	0.25143700	-0.21959600
C	-1.13676400	-0.84063400	1.65366100
H	-2.06001800	-1.31010200	1.99482800
H	-0.51099100	-0.67031200	2.52965000
C	-1.45147600	0.51170000	0.97625500
H	-1.93617100	1.18044100	1.69905700
N	-2.76808700	1.51242900	-0.91525800
H	-3.36287500	1.30137600	-1.71337400
H	-3.31268500	2.10641100	-0.29443700
N	-0.25820900	2.53316800	-0.03681000

H	-1.01896600	2.51293400	-0.71116600
H	-0.54133600	3.17286900	0.70146300
N	-3.61044200	-0.45564900	0.28541300
H	-4.10491900	0.12665400	0.95634700
H	-4.25404500	-0.64142900	-0.47963500
N	0.61286800	1.49713000	1.83493300
H	1.13792800	0.67727800	2.13408400
H	1.27929900	2.24057400	1.65333700
N	1.78880200	-1.08488300	1.40567300
H	1.75506300	-1.97280400	1.90140500
H	2.75170800	-0.95801600	1.09517300
N	1.51628200	-2.07212800	-0.82371500
H	2.50632200	-1.85853700	-0.90171400
H	1.45451400	-3.03709500	-0.50784600
C	1.90269200	0.90296700	-1.09649000
H	2.16258100	0.32683200	-1.99374900
H	1.55426700	1.87430000	-1.45030500
C	3.20773500	1.15701200	-0.32163300
H	3.70378500	2.02286600	-0.78171500
H	3.00874400	1.42550800	0.71548100
N	4.09519400	-0.02856700	-0.30848800
H	4.40286700	-0.23864400	-1.25469300
H	4.93773600	0.16545500	0.22554700

$4H^+$

E= -857.45663816, ZPE= 0.433635

C	1.44496300	1.99842500	-0.55062900
H	1.01652400	2.66852100	-1.29710000
H	2.36403300	2.45152200	-0.17923300
C	1.72767100	0.62953000	-1.19132600
H	2.38904700	0.76157600	-2.05635100
C	0.47444600	1.79597600	0.62811100
H	0.27208200	2.76388300	1.10649600
C	-0.86816800	1.23212700	0.10055100
C	0.40396800	0.01078700	-1.67284400
H	0.58508700	-0.94734600	-2.16048300
H	-0.04096600	0.67007900	-2.41897300
C	-0.63511300	-0.19842200	-0.52295700
C	0.04830900	-1.17549900	0.54118200
C	2.42106800	-0.31400000	-0.17702200
C	1.12383200	0.84538300	1.65278200
H	2.06177000	1.28645500	1.98647400
H	0.50110400	0.72274600	2.54177400
C	1.40567800	-0.52542200	0.99286000
H	1.86010100	-1.20292500	1.73003200

N	2.71621300	-1.59390400	-0.85412700
H	3.30112000	-1.42317500	-1.66893300
H	3.25388900	-2.20053100	-0.23940700
N	0.14656400	-2.51208300	-0.04495100
H	0.90953800	-2.53619200	-0.72163700
H	0.39327600	-3.18148900	0.67934200
N	3.61236500	0.34804000	0.37008000
H	4.11506000	-0.26957800	1.00170400
H	4.25706600	0.60151600	-0.37377000
N	-0.77915600	-1.31538500	1.77700800
H	-1.44235000	-2.07276800	1.63403200
H	-0.18680700	-1.60158300	2.55362800
N	-1.83551500	1.09562200	1.29678600
H	-1.53302000	0.25573700	1.86070600
H	-1.85974600	1.95253600	1.84842600
N	-1.43013900	2.14379200	-0.85674900
H	-2.37580800	1.93267500	-1.14367800
H	-1.35509700	3.11791200	-0.58855700
C	-1.88770400	-0.81318300	-1.22389700
H	-2.15507800	-0.15167700	-2.05680300
H	-1.53357600	-1.73404100	-1.68811400
C	-3.18402600	-1.19273000	-0.49018000
H	-3.75878600	-1.83453200	-1.16632200
H	-2.98630500	-1.79404000	0.39729200
N	-3.99138400	-0.01965500	-0.06244600
H	-4.39320300	0.43946700	-0.87732000
H	-4.78757000	-0.32791500	0.49092100
H	-2.79355400	0.87035000	0.90685900

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E= -873.04439754, ZPE= 0.408108

C	-0.24857000	-1.05719000	0.52610100
C	-0.68327200	0.03457800	-0.55585600
C	1.19252000	-0.65945800	1.02133300
H	1.48024700	-1.41015400	1.76971600
C	2.27993300	-0.62562500	-0.09681900
C	0.42348700	0.05584400	-1.65913000
H	0.12693700	0.77951600	-2.42066900
H	0.46375200	-0.92620700	-2.13247300
C	1.81746700	0.43103200	-1.12993100
H	2.52728600	0.43803200	-1.96927400
C	1.75463100	1.82652700	-0.48917100
H	2.72575500	2.10441400	-0.07576900
H	1.48637600	2.56064600	-1.25138400
C	-0.71088100	1.49331300	0.07689700
C	1.12965600	0.73949900	1.67717500
H	2.11228000	1.00167600	2.06973800
C	0.70790700	1.79594100	0.63858700

H	0.66490200	2.77849500	1.12910200
N	-0.99106700	2.48526100	-0.99281600
H	-1.99036700	2.53754000	-1.16100400
H	-0.70554700	3.40925300	-0.67851600
N	-1.67501700	1.58284600	1.18693000
H	-1.76506800	2.55286800	1.47536200
H	-2.59467800	1.24553800	0.89827500
N	-1.18821400	-1.12031500	1.65888000
H	-0.86809700	-1.85269400	2.28532200
H	-1.24828100	-0.22962100	2.14076500
N	-0.25700400	-2.42882400	0.02255700
H	0.39739900	-2.55322800	-0.74104700
H	-1.20723900	-2.64749600	-0.26512000
N	2.38855100	-1.93275500	-0.77894900
H	3.14830800	-1.90066700	-1.45379500
H	2.61080300	-2.66390000	-0.10829000
N	3.55950100	-0.19630100	0.50653300
H	3.87675300	-0.89282600	1.17596200
H	4.27613300	-0.13056000	-0.21213100
H	0.43476000	0.73423400	2.51649300
C	-2.00524600	-0.31118200	-1.32929000
H	-2.49311900	0.62329100	-1.63648000
H	-1.71326900	-0.81842600	-2.25375500
N	-2.97122400	-1.22266000	-0.70554800
H	-3.63352000	-1.48587700	-1.42775500
N	-3.72881400	-0.56195200	0.35205400
H	-4.69132900	-0.88263500	0.29261200
H	-3.32394400	-0.94800700	1.20725500

$5H^+$

E= -873.47134525, ZPE= 0.422318

C	-0.00027800	-1.15681800	0.55057700
C	-0.63547400	-0.16622300	-0.53575100
C	1.36135700	-0.53786300	1.01115700
H	1.78099300	-1.21758400	1.76267900
C	2.39954300	-0.36608000	-0.14832100
C	0.41229300	-0.00251400	-1.67968500
H	-0.00342000	0.65642600	-2.44387400
H	0.57917800	-0.97582300	-2.14271100
C	1.74707700	0.58374100	-1.18660400
H	2.42325700	0.68449900	-2.04422000
C	1.49417900	1.96890600	-0.56977200
H	2.42114900	2.40169400	-0.19424500
H	1.09284400	2.63996200	-1.33094200
C	-0.84759000	1.27952300	0.06783900
C	1.10836900	0.84920700	1.64476000
H	2.05441300	1.26440400	1.98750800
C	0.50574800	1.81009300	0.59980700

H	0.32629100	2.78951000	1.06409500
N	-1.39031300	2.19092200	-0.90166300
H	-2.35079200	2.01235300	-1.16367500
H	-1.27396700	3.16666500	-0.65426200
N	-1.80674100	1.17766800	1.27200200
H	-1.80233000	2.03874800	1.81737700
H	-2.75950700	0.97648900	0.90459100
N	-0.89097700	-1.22657500	1.74637800
H	-1.72368300	-1.75084400	1.47981800
H	-0.41501100	-1.77046400	2.46331800
N	0.20133400	-2.52053200	0.09793900
H	0.92276500	-2.59127100	-0.61568700
H	-0.65657200	-2.97727300	-0.18668800
N	2.68055200	-1.65769600	-0.80635000
H	3.31016400	-1.51257600	-1.59176800
H	3.15734300	-2.28536400	-0.16337400
N	3.59675500	0.27658700	0.41125400
H	4.06315100	-0.34059100	1.07064300
H	4.26726000	0.48723500	-0.32311200
H	0.47016000	0.75114700	2.52493000
C	-1.89580300	-0.75673200	-1.22389800
H	-2.24320700	-0.05535000	-1.99568200
H	-1.56386500	-1.64420100	-1.76633100
N	-3.01021300	-1.20755100	-0.36927500
H	-3.50008300	-1.95562700	-0.85383800
N	-3.93656500	-0.14109000	-0.07306100
H	-4.49633700	0.10476400	-0.89300800
H	-4.58288700	-0.48232800	0.63431300
H	-1.50066300	0.31183000	1.83292000

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E= -1194.70048125, ZPE= 0.677400

C	0.00018900	2.38046600	-0.00003200
H	-0.60214500	3.01809000	-0.64751600
H	0.60260100	3.01800900	0.64746000
C	0.90509300	1.49551700	-0.87130800
H	1.46517100	2.14039000	-1.55007100
C	-0.90481600	1.49561800	0.87124300
H	-1.46481100	2.14054800	1.55002100
C	-1.88573500	0.67582500	-0.02738900
C	0.01811900	0.56444400	-1.72359400
H	0.64040200	-0.09489000	-2.32339600
H	-0.56284400	1.18718200	-2.40274500
C	-0.93171900	-0.29341200	-0.84231500
H	-1.55672000	-0.90658300	-1.48788700
C	-0.00007700	-1.26349100	-0.00002500
C	1.88590600	0.67561700	0.02733200
C	-0.01793600	0.56443300	1.72351600

H	0.56312800	1.18709100	2.40265500
H	-0.64028700	-0.09482900	2.32333200
C	0.93176600	-0.29354700	0.84221800
H	1.55668200	-0.90680500	1.48778600
N	2.86980100	-0.06576900	-0.79494700
N	0.77218900	-2.09302700	-0.96795100
N	2.52815400	1.62207700	1.00258200
N	-0.77258400	-2.09271300	0.96797600
N	-2.86961300	-0.06553500	0.79493400
N	-2.52798700	1.62232800	-1.00259400
C	1.68880200	-3.06324600	-0.39887000
H	1.21119600	-4.02978000	-0.16237700
H	2.49517300	-3.26486600	-1.11342500
H	2.14784500	-2.69205300	0.51322200
C	0.17109400	-2.64467500	-2.17356100
H	-0.40783800	-1.90926100	-2.72910200
H	0.98344800	-2.96541200	-2.83692800
H	-0.46995900	-3.52678800	-2.00712700
C	-1.68952600	-3.06267700	0.39899300
H	-1.21224000	-4.02938800	0.16257200
H	-2.49595500	-3.26397300	1.11357500
H	-2.14846200	-2.69140800	-0.51312300
C	-0.17166500	-2.64441700	2.17365000
H	0.40747800	-1.90911900	2.72912500
H	-0.98412300	-2.96484000	2.83704000
H	0.46912500	-3.52674100	2.00732000
C	-3.97387600	-0.68704800	0.08583300
H	-4.38547600	-1.49917700	0.69503300
H	-4.80320500	0.00692400	-0.13401000
H	-3.64973900	-1.12248800	-0.85825100
C	-3.33019200	0.46468900	2.06905400
H	-4.03693800	1.30901300	1.98606700
H	-3.85370000	-0.33718700	2.60145700
H	-2.50622900	0.77805500	2.70669400
C	-3.11714600	1.16259400	-2.25345700
H	-4.16734700	0.84295800	-2.16516800
H	-3.09383600	1.98838900	-2.97662200
H	-2.55757800	0.33985100	-2.69394900
C	-3.34016100	2.68638800	-0.43393500
H	-3.47036900	3.47510100	-1.18440100
H	-4.34817400	2.35997700	-0.12846300
H	-2.85929900	3.14142600	0.43147100
C	3.11722300	1.16228800	2.25346600
H	4.16740200	0.84256800	2.16521600
H	3.09394700	1.98807800	2.97663500
H	2.55757300	0.33958600	2.69392800
C	3.34041200	2.68610300	0.43398100
H	3.47064500	3.47478300	1.18447600
H	4.34841300	2.35964000	0.12852700
H	2.85960000	3.14119600	-0.43142400
C	3.97405600	-0.68726100	-0.08581600

H	4.38565000	-1.49941800	-0.69498200
H	4.80339400	0.00670800	0.13400100
H	3.64991200	-1.12266000	0.85828500
C	3.33040000	0.46439600	-2.06908300
H	4.03717200	1.30870100	-1.98612200
H	3.85388200	-0.33751400	-2.60146200
H	2.50644700	0.77776800	-2.70673000

$6H^+$

E= -1195.13321918, ZPE= 0.692996

C	-0.05526300	-2.40084600	-0.04370400
H	-0.65555600	-3.03686700	0.60463500
H	0.52423100	-3.04726400	-0.70506100
C	0.87512100	-1.54346500	0.83195700
H	1.44264800	-2.20247200	1.48950900
C	-0.95650300	-1.48665000	-0.88736100
H	-1.54393900	-2.11222500	-1.55820300
C	-1.90554900	-0.64850600	0.03522000
C	0.01311900	-0.61150800	1.70769000
H	0.63470600	-0.00634800	2.36705700
H	-0.59082600	-1.24258100	2.35491000
C	-0.90924600	0.29541000	0.85216200
H	-1.50146800	0.92043400	1.51621300
C	0.01934600	1.24040000	-0.01720400
C	1.82434100	-0.74090000	-0.09681300
C	-0.06521600	-0.57792400	-1.75501300
H	0.50165600	-1.20286500	-2.44602600
H	-0.67636900	0.09421300	-2.35028800
C	0.90495700	0.26527600	-0.88663200
H	1.53661100	0.86725200	-1.53568000
N	2.82043400	0.14093100	0.85335300
N	0.96073900	2.03245500	0.94842700
N	2.58558000	-1.57247800	-0.96782800
N	-0.71395100	2.13577200	-0.88753000
N	-2.86683900	0.13571200	-0.77286500
N	-2.53917600	-1.58800100	1.01284600
C	1.63566600	3.14705700	0.25271400
H	0.96145000	3.98606300	0.05817400
H	2.45244400	3.51355100	0.88037300
H	2.05579200	2.82649000	-0.69852600
C	0.37849400	2.58145000	2.19236600
H	-0.08973300	1.81224400	2.80075600
H	1.19011200	3.01575700	2.78223900
H	-0.35187000	3.37473200	2.00579700
C	-1.70921900	3.03688500	-0.33254200
H	-1.31953600	4.05798400	-0.19269900
H	-2.56370600	3.10568700	-1.01270100
H	-2.08315100	2.68995300	0.62530000

C	-0.26461000	2.61986500	-2.18490900
H	0.44306800	1.95516500	-2.67315300
H	-1.13288600	2.69867600	-2.85002600
H	0.19461600	3.61941300	-2.13809600
C	-3.97563000	0.72897900	-0.03113900
H	-4.41660700	1.53287000	-0.62692700
H	-4.77982100	0.01408200	0.19673700
H	-3.64371400	1.16594500	0.90965700
C	-3.36883100	-0.40869000	-2.03510700
H	-4.03018300	-1.28153000	-1.92461100
H	-3.95211800	0.37439600	-2.52726400
H	-2.56659600	-0.67638400	-2.72052800
C	-3.11377500	-1.12571100	2.27570100
H	-4.16288900	-0.80928800	2.19995100
H	-3.07881100	-1.95154800	2.99605000
H	-2.55309500	-0.30046300	2.71156200
C	-3.36996300	-2.65288300	0.45803500
H	-3.49276500	-3.43415200	1.21525000
H	-4.37777100	-2.32012800	0.16875400
H	-2.90748000	-3.11796600	-0.41165900
C	3.10421000	-1.17169100	-2.27349800
H	4.19397300	-1.03618300	-2.26105600
H	2.88467200	-1.95409400	-3.00868400
H	2.65817900	-0.25073200	-2.63782100
C	3.21361200	-2.80907500	-0.51106700
H	3.10013000	-3.58157300	-1.27910600
H	4.29254500	-2.68769100	-0.33485900
H	2.76099400	-3.18987100	0.40044600
C	3.97046900	0.69876700	0.09194700
H	4.47020600	1.44791500	0.70687400
H	4.67568000	-0.09518600	-0.14677500
H	3.63047000	1.16620000	-0.82702000
C	3.34271100	-0.53380600	2.07498800
H	3.92557000	-1.41247500	1.80230700
H	3.99092100	0.16702300	2.60314400
H	2.53201000	-0.82212000	2.73616500
H	2.16125400	0.96061700	1.12334600

6aH$^+$

E= -1195.45879441, ZPE= 0.708747

C	-0.00008800	-2.42454100	-0.00004900
H	0.57796100	-3.07007000	-0.66067900
H	-0.57818000	-3.07005500	0.66056100
C	-0.92552100	-1.53651500	-0.85038500
H	-1.51519300	-2.17680600	-1.50461000
C	0.92539900	-1.53659800	0.85031900
H	1.51502200	-2.17694200	1.50453600
C	1.84759300	-0.72467100	-0.10448300

C	-0.05501100	-0.62077600	-1.73524900
H	-0.66323500	0.00657500	-2.38428100
H	0.53091900	-1.25485400	-2.39847300
C	0.89112400	0.26915200	-0.88717100
H	1.49284000	0.88215200	-1.55339700
C	0.00004300	1.23000000	-0.00001700
C	-1.84765100	-0.72457000	0.10446500
C	0.05495000	-0.62081100	1.73520000
H	-0.53103300	-1.25486000	2.39840700
H	0.66321800	0.00648100	2.38424900
C	-0.89111200	0.26920400	0.88713400
H	-1.49278200	0.88223900	1.55336800
N	-2.86126100	0.17391400	-0.83438800
N	-0.89128700	2.06056900	-0.89335700
N	-2.58906200	-1.54899700	0.98655800
N	0.89146000	2.06049200	0.89330700
N	2.86115300	0.17378400	0.83445300
N	2.58904500	-1.54908800	-0.98655200
C	-1.64588100	3.13097300	-0.20574900
H	-1.04493200	4.02494500	-0.01807200
H	-2.48020200	3.43536200	-0.84250600
H	-2.05412800	2.78924300	0.74256900
C	-0.38391700	2.60530900	-2.17427000
H	0.15722000	1.86411800	-2.75607300
H	-1.24727400	2.91267500	-2.76946000
H	0.25232100	3.48537400	-2.05020100
C	1.64590900	3.13101700	0.20572500
H	1.04489400	4.02498800	0.01825100
H	2.48031100	3.43536100	0.84239700
H	2.05402800	2.78942600	-0.74269800
C	0.38426100	2.60504000	2.17436900
H	-0.15675900	1.86374900	2.75615500
H	1.24769600	2.91235800	2.76947000
H	-0.25203000	3.48509700	2.05051600
C	4.00350700	0.73223000	0.05124200
H	4.50817800	1.48624500	0.65501700
H	4.70641100	-0.06373000	-0.18304700
H	3.65319700	1.18823500	-0.86939300
C	3.40778000	-0.49758600	2.05517700
H	3.96720000	-1.38695700	1.77280500
H	4.08240300	0.19864100	2.55417700
H	2.61222700	-0.76359000	2.74380100
C	3.10704300	-1.13331900	-2.29499500
H	4.19408500	-0.99458500	-2.28091500
H	2.89132200	-1.91351500	-3.03193600
H	2.65932300	-0.21088800	-2.65504400
C	3.25751800	-2.77272400	-0.53084600
H	3.17552300	-3.53728200	-1.30867800
H	4.32829400	-2.61544000	-0.34639800
H	2.81123400	-3.17919600	0.37283600
C	-3.10697100	-1.13325700	2.29504600

H	-4.19401100	-0.99450100	2.28103800
H	-2.89121900	-1.91348000	3.03195000
H	-2.65921000	-0.21084600	2.65509700
C	-3.25757600	-2.77261400	0.53086300
H	-3.17554500	-3.53719100	1.30867300
H	-4.32836100	-2.61531300	0.34648100
H	-2.81134900	-3.17907000	-0.37285300
C	-4.00374700	0.73206700	-0.05116000
H	-4.50847400	1.48612300	-0.65483500
H	-4.70656200	-0.06403000	0.18293400
H	-3.65356600	1.18795200	0.86958300
C	-3.40771900	-0.49732000	-2.05526400
H	-3.96703900	-1.38681600	-1.77308100
H	-4.08240300	0.19890200	-2.55418600
H	-2.61208600	-0.76309900	-2.74388200
H	-2.22513100	0.96714500	-1.11522200
H	2.22492900	0.96687000	1.11547800

Optimized geometry at M06-2X/6-31+G(d) level of theory, gas phase electronic energies and Cartesian coordinates for 2 and its complexes with lithium and sodium ions (All energies are given in Hartee).

2

E= -722.54107451

C	0.00004400	-2.12308300	0.00017200
H	-0.58948700	-2.75965400	0.66552000
H	0.58960400	-2.75974200	-0.66506900
C	0.92540000	-1.22858600	0.83899400
H	1.58327700	-1.85643500	1.46089300
C	-0.92534500	-1.22876000	-0.83881100
H	-1.58317900	-1.85673300	-1.46063000
C	-1.80706800	-0.37409300	0.09691300
C	0.07896700	-0.31934100	1.75176500
H	0.72358000	0.31316300	2.36834500
H	-0.51040100	-0.94745900	2.42432400
C	-0.86519200	0.56081100	0.90217500
H	-1.46511200	1.20747500	1.56167100
C	-0.00001900	1.49373900	-0.00004100
C	1.80706200	-0.37406600	-0.09692600
C	-0.07895600	-0.31960200	-1.75170600
H	0.51046900	-0.94779800	-2.42414400
H	-0.72358200	0.31275700	-2.36841800
C	0.86513500	0.56073800	-0.90222800
H	1.46501600	1.20735000	-1.56181000
N	2.74515900	0.40614500	0.72882100
H	3.37165500	-0.23566100	1.21514300
H	3.33258400	0.98086500	0.12348100
N	0.73656000	2.40660100	0.87622600
H	1.51006800	1.92083000	1.32466100

H	1.14636500	3.12563200	0.27948900
N	2.49466500	-1.25655600	-1.05064000
H	3.07611500	-0.69892600	-1.67620700
H	3.12069000	-1.88657700	-0.54905300
N	-0.73655400	2.40668700	-0.87626100
H	-1.51022000	1.92103600	-1.32455300
H	-1.14617000	3.12580200	-0.27949600
N	-2.74501700	0.40604600	-0.72906800
H	-3.37151800	-0.23579500	-1.21533800
H	-3.33244900	0.98093600	-0.12389800
N	-2.49485100	-1.25641900	1.05065300
H	-3.07635200	-0.69867200	1.67607100
H	-3.12085200	-1.88646200	0.54906300

7. (Li^+)

E= -729.94285139

C	-0.15123000	-2.14824800	0.14457500
H	-0.73697600	-2.69598000	0.88703000
H	0.36974600	-2.87174500	-0.48594400
C	0.86309900	-1.24468900	0.86783800
H	1.50896300	-1.85765700	1.51432300
C	-1.06170800	-1.27025200	-0.72723400
H	-1.76691500	-1.90882300	-1.27849700
C	-1.87410500	-0.30671600	0.16676500
C	0.08174300	-0.23665400	1.73300900
H	0.74567500	0.37864500	2.36061000
H	-0.53153700	-0.79450900	2.44363700
C	-0.84370200	0.64232300	0.85952900
H	-1.39584800	1.35265700	1.49880700
C	0.00537300	1.44690100	-0.16745700
C	1.73900900	-0.52859500	-0.18262800
C	-0.21175600	-0.47913000	-1.74089000
H	0.32339000	-1.18335200	-2.37928000
H	-0.84428600	0.12846800	-2.39104000
C	0.81644200	0.41582300	-1.00350800
H	1.41325500	0.97431100	-1.74078200
N	2.82815300	0.23319800	0.52775300
H	3.45590700	-0.46874600	0.92767600
H	3.39409600	0.68964800	-0.19333600
N	0.88626400	2.38634400	0.59112800
H	1.33048000	2.96757600	-0.12717300
N	2.30613500	-1.50749400	-1.08903800
H	2.88285800	-1.08014100	-1.81135000
H	2.86185000	-2.20900800	-0.60354900
N	-0.71370500	2.30549000	-1.10229200
H	-1.48439800	1.79160300	-1.52792600
H	-1.16089100	3.06851900	-0.59238800
N	-2.79147700	0.45603400	-0.68813500
H	-3.43404600	-0.18792300	-1.14972200

H	-3.36939300	1.07723800	-0.12102500
N	-2.54689900	-1.07062900	1.21832500
H	-3.18730900	-0.47088500	1.73755800
H	-3.11147800	-1.81444300	0.80831800
H	0.26350100	3.03837100	1.07737000
Li	2.17168900	1.57033700	1.74750100

7. (Na^+)

E=-884.66417907

C	0.80761600	2.03576300	0.62201400
H	1.35623900	2.22851900	1.54727700
H	0.60043600	2.99202100	0.13774500
C	-0.50571400	1.30653200	0.95580000
H	-1.10385400	1.91762300	1.64893100
C	1.63655300	1.15120800	-0.32189100
H	2.55978300	1.67955400	-0.60111300
C	2.02444700	-0.16207700	0.39400000
C	-0.15322000	-0.03261200	1.63071900
H	-1.05088200	-0.56881000	1.95749100
H	0.41899200	0.17647300	2.53700200
C	0.69395000	-0.92274400	0.69222400
H	0.93820700	-1.87328200	1.19801200
C	-0.11774500	-1.23819500	-0.59882000
C	-1.31001900	1.09326500	-0.34450900
C	0.83215700	0.84376300	-1.60099600
H	0.60657300	1.78142400	-2.10976100
H	1.41925900	0.23505700	-2.29107000
C	-0.49516700	0.12492000	-1.24603900
H	-1.05526800	-0.08574800	-2.17034300
N	-2.67063600	0.55011700	-0.01506500
H	-3.19596900	1.34176300	0.36462000
H	-3.13193300	0.36170700	-0.90997900
N	-1.31004300	-2.05348500	-0.22259000
H	-1.73679000	-2.30490400	-1.12019700
N	-1.42971800	2.36377900	-1.04428200
H	-1.96789400	2.27570800	-1.90453100
H	-1.86934800	3.07704500	-0.46491800
N	0.55269400	-2.03252900	-1.62748300
H	1.48713500	-1.66518700	-1.80324100
H	0.70698800	-2.98040300	-1.28169200
N	2.88608200	-0.94067600	-0.50564300
H	3.73111100	-0.40568300	-0.70673800
H	3.19402400	-1.79776900	-0.04524600
N	2.65312000	0.14955800	1.67899500
H	3.01082300	-0.70181100	2.11141100
H	3.45573800	0.76267100	1.53704200
H	-0.93564100	-2.94582500	0.11441000
Na	-2.97139800	-1.35967600	1.21021400

8. $(Li^+)_2$

E= -737.23066914

C	0.00014900	-2.18412800	0.00015200
H	-0.51923800	-2.82465900	0.71461300
H	0.51968600	-2.82462900	-0.71424100
C	1.00130300	-1.28889900	0.75167100
H	1.69478400	-1.91905500	1.32560700
C	-1.00117800	-1.28917300	-0.75148300
H	-1.69457900	-1.91954600	-1.32529200
C	-1.80837300	-0.46112800	0.27362200
C	0.21987600	-0.38400200	1.72687000
H	0.87722900	0.22506600	2.36000000
H	-0.32737500	-1.01985200	2.42373900
C	-0.79774800	0.50846700	0.97014400
H	-1.34408100	1.13828400	1.69251900
C	-0.00007200	1.42262800	-0.00014700
C	1.80838700	-0.46105900	-0.27361300
C	-0.21978000	-0.38448400	-1.72688300
H	0.32761900	-1.02049300	-2.42348600
H	-0.87714900	0.22426200	-2.36029200
C	0.79769900	0.50832400	-0.97028500
H	1.34399800	1.13805700	-1.69275100
N	2.89875900	0.28464200	0.44019000
H	3.56593600	-0.42687100	0.75370900
H	3.42814200	0.80700800	-0.26494900
N	0.88440300	2.30241700	0.81779000
H	1.36403300	2.95084100	0.18620300
N	2.34992400	-1.33453500	-1.29112200
H	2.95876000	-0.85102800	-1.94912600
H	2.86528500	-2.12151500	-0.90015600
N	-0.88449000	2.30231800	-0.81800300
H	-1.36409600	2.95093400	-0.18664700
H	-0.28904400	2.90030300	-1.39802200
N	-2.89878800	0.28434100	-0.44018000
H	-3.56605800	-0.42716500	-0.75347700
H	-3.42804500	0.80710400	0.26474100
N	-2.34995200	-1.33436200	1.29138400
H	-2.95907400	-0.85068500	1.94902000
H	-2.86519700	-2.12147700	0.90050300
H	0.28875300	2.90072500	1.39730100
Li	2.34751300	1.47206200	1.85960000
Li	-2.34780000	1.47172700	-1.85967100

8. $(Na^+)_2$

E= -1046.68916680

C	-0.00029000	-2.36970800	-0.00007900

H	0.25080700	-3.01021900	-0.84728500
H	-0.25155400	-3.01020100	0.84709700
C	-1.19365400	-1.47324000	-0.37579500
H	-2.04006800	-2.10177800	-0.68694400
C	1.19328200	-1.47355100	0.37573800
H	2.03957900	-2.10231000	0.68676200
C	1.61745600	-0.64176400	-0.85544600
C	-0.77889900	-0.56953300	-1.55354100
H	-1.60759500	0.05255500	-1.89791300
H	-0.49960700	-1.20087500	-2.39721200
C	0.43165100	0.32286300	-1.17714500
H	0.70441000	0.95266500	-2.04125600
C	0.00013800	1.23846000	0.00025500
C	-1.61772400	-0.64152200	0.85545000
C	0.77864100	-0.57005900	1.55370800
H	0.49901900	-1.20166200	2.39708000
H	1.60738100	0.05168800	1.89861100
C	-0.43168700	0.32272200	1.17743500
H	-0.70434500	0.95240400	2.04165900
N	-2.88854400	0.09231000	0.55504300
H	-3.61828400	-0.62639500	0.56245700
H	-3.11229100	0.65593400	1.38083900
N	-1.10600700	2.11711900	-0.47561800
H	-1.41274400	2.68368600	0.32022800
N	-1.78284100	-1.52194700	1.99822100
H	-2.16044600	-1.03844300	2.81150700
H	-2.39207100	-2.31229000	1.79252500
N	1.10668500	2.11650000	0.47636700
H	1.41373800	2.68304500	-0.31938200
H	0.69722200	2.79219600	1.12716100
N	2.88848500	0.09166800	-0.55519700
H	3.61804800	-0.62721700	-0.56250000
H	3.11237600	0.65514300	-1.38105500
N	1.78215000	-1.52209000	-1.99839100
H	2.15992800	-1.03857700	-2.81159600
H	2.39115500	-2.31264800	-1.79283600
H	-0.69621900	2.79272500	-1.12630500
Na	3.23487000	1.44649200	1.29913900
Na	-3.23409100	1.44693200	-1.29987700

Li^+

E= -7.28104871

Li	0.00000000	0.00000000	0.00000000

Na^+

E= -162.04450829

Na	0.00000000	0.00000000	0.00000000

M06-2X/6-31+G(d) level of theory optimized, gas phase electronic energies (E) and Cartesian coordinates for hydrogen, carbon dioxide and carbon monoxide trapped litiated adamantane (9-11) (All energies are given in Hartee).

9. $(Li^+)_2$ - (H_2)

E=-738.40086308

C	-0.19992000	-2.18557000	0.25506100
H	-0.68094500	-2.68257600	1.09943300
H	0.19466300	-2.95497400	-0.41060300
C	0.93347700	-1.28233900	0.77142600
H	1.64349400	-1.88495500	1.35480300
C	-1.21483500	-1.32056100	-0.51304000
H	-2.00503800	-1.96448100	-0.92346000
C	-1.85236300	-0.29937700	0.45490500
C	0.31864200	-0.20415600	1.68799000
H	1.07384900	0.42683300	2.17297600
H	-0.19626800	-0.70317300	2.50970200
C	-0.71000700	0.66393600	0.91679200
H	-1.13348900	1.42318000	1.59561300
C	0.04092900	1.37877300	-0.23989200
C	1.67612500	-0.65980300	-0.43262000
C	-0.48559600	-0.61727400	-1.67629000
H	-0.05563200	-1.37979200	-2.32630300
H	-1.16659500	-0.05043500	-2.32358300
C	0.66123300	0.28661200	-1.15366700
H	1.16552800	0.77204900	-2.00610500
N	2.88284500	0.08039500	0.06388500
H	3.53210000	-0.63663400	0.40104500
H	3.36632200	0.47006600	-0.75124000
N	1.07035000	2.27479600	0.35928000
H	1.53476900	2.78299100	-0.39908700
N	2.04791300	-1.70027800	-1.36710400
H	2.62157300	-1.35770200	-2.13592700
H	2.54417400	-2.46914100	-0.91942100
N	-0.86155300	2.22142400	-1.07591500
H	-1.23287000	2.97422800	-0.48873700
H	-0.28850200	2.70120200	-1.77626300
N	-2.95373600	0.43085800	-0.25893900
H	-3.69168600	-0.26177400	-0.41767500
H	-3.38022100	1.07851100	0.41085700
N	-2.35053800	-0.98081300	1.62911200
H	-2.85396400	-0.36349300	2.26403300
H	-2.95890900	-1.76493800	1.39949100
H	0.58788800	2.99917900	0.89879100
Li	2.56966300	1.46496100	1.37314300

H	3.35132200	1.97188800	3.29683500
H	3.85257200	1.46608200	3.08917200
Li	-2.46207000	1.38895300	-1.86999900

9.$(Li^+)_2$-$(H_2)_2$

E=-739.57081325

C	-0.07133200	-2.22346300	0.24768900
H	0.27322400	-2.96227700	-0.47765600
H	-0.46027400	-2.75697800	1.11680100
C	-1.16971700	-1.35420500	-0.39073800
H	-1.98584500	-1.99942900	-0.74473500
C	1.09034100	-1.31485200	0.68675300
H	1.86154000	-1.92161100	1.18138100
C	1.70824400	-0.63868400	-0.55711000
C	-0.56319000	-0.60361200	-1.59382300
H	-1.30987300	-0.03031600	-2.15648000
H	-0.18348700	-1.33886100	-2.30406500
C	0.61220100	0.30629000	-1.15146600
H	1.02571200	0.82644500	-2.03199300
C	0.05615300	1.35845900	-0.15373900
C	-1.72790100	-0.37864200	0.66862000
C	0.54932600	-0.27592600	1.68973900
H	0.12499600	-0.80756300	2.54232400
H	1.33826000	0.35539200	2.11782800
C	-0.56377000	0.59396400	1.04916100
H	-0.93320700	1.32357800	1.78928000
N	-2.90428300	0.35079100	0.08915500
H	-3.64565000	-0.34884000	-0.01174800
H	-3.26971400	0.97822800	0.81210300
N	-0.94343000	2.19644800	-0.87516400
H	-1.28063200	2.91872800	-0.23195800
N	-2.09579800	-1.10960800	1.86161800
H	-2.55971600	-0.52757100	2.55689100
H	-2.69747000	-1.90724500	1.66289600
N	1.11668300	2.26359000	0.37021600
H	1.49721700	2.80145100	-0.41394900
H	0.67130500	2.96255100	0.97169000
N	2.93930700	0.11376700	-0.14403200
H	3.62867700	-0.59810000	0.11615500
H	3.34314500	0.53505400	-0.98627300
N	2.01472600	-1.64019400	-1.55526600
H	2.50860000	-1.26070400	-2.36122300
H	2.56544700	-2.41060800	-1.17974800
H	-0.45274200	2.71407900	-1.61007600
Li	-2.59460100	1.34315000	-1.54744700
H	-3.66502300	1.18929300	-3.39141900
H	-4.08893500	0.76178000	-2.95820800
Li	2.71524500	1.46395300	1.22319800

H	3.12965000	2.68478700	2.92549300
H	3.79030200	2.35788300	2.84322000

9.$(Li^+)_2$-$(H_2)_3$

E=-740.73896144

C	0.24787300	-2.26405700	0.11110500
H	0.63872000	-2.91148400	-0.67612800
H	-0.04221200	-2.89344100	0.95430100
C	-0.96456100	-1.48278100	-0.42480700
H	-1.72059300	-2.18950700	-0.79447100
C	1.32007500	-1.26120000	0.57158400
H	2.17409100	-1.80795200	0.99511700
C	1.80552400	-0.43761400	-0.64200100
C	-0.49849100	-0.59145300	-1.59367400
H	-1.32911500	-0.06646200	-2.07803800
H	-0.07463200	-1.22999100	-2.36959100
C	0.58802200	0.41263300	-1.13142700
H	0.90354900	1.03276000	-1.98742800
C	-0.03759100	1.32869700	-0.04418100
C	-1.57979000	-0.64578000	0.71962200
C	0.71267500	-0.35712100	1.66312400
H	0.38621900	-0.98660000	2.49174300
H	1.44798800	0.32744500	2.10443400
C	-0.51425100	0.42385400	1.12490500
H	-0.92831200	1.05794700	1.92709300
N	-2.85340800	-0.01584100	0.23808200
H	-3.51859000	-0.78563300	0.11830600
H	-3.24873200	0.51769400	1.01853900
N	-1.15469500	2.09095800	-0.66980700
H	-1.54693900	2.72463900	0.03287700
N	-1.81390800	-1.49113400	1.87054000
H	-2.30475500	-1.01084000	2.62283000
H	-2.33816900	-2.33284700	1.63713900
N	0.93744400	2.31296700	0.50351600
H	1.22125700	2.94079900	-0.25424700
H	0.44273800	2.91609000	1.16694900
N	2.96146700	0.42296600	-0.22040400
H	3.73830200	-0.21962500	-0.03884000
H	3.27570800	0.94501500	-1.04425700
N	2.17996700	-1.32800300	-1.71876900
H	2.58811000	-0.83948500	-2.51401200
H	2.83434800	-2.04923300	-1.41992800
H	-0.75750100	2.70906700	-1.38297000
Li	-2.75175600	1.12335900	-1.33581200
H	-3.57673500	0.57427200	-3.27677000
H	-3.99940300	0.14843800	-2.84118500
Li	2.64681900	1.65103100	1.24554500
H	2.98102000	2.66159800	3.10298200

H	3.64193200	2.76272500	2.78216700
H	-4.31506600	2.74013000	-1.33073100
H	-4.53339600	2.24684300	-0.82268900

9.$(Li^+)_2$-$(H_2)_4$

E=-741.90726387

C	-0.04474500	-2.31499200	0.14716900
H	0.26169100	-3.01458200	-0.63237300
H	-0.38026600	-2.89454300	1.00909600
C	-1.18122200	-1.42504500	-0.38599100
H	-2.01367500	-2.05818500	-0.72358200
C	1.13539300	-1.42003500	0.56404600
H	1.93654300	-2.04391800	0.98435700
C	1.67761700	-0.67918300	-0.67824600
C	-0.65046800	-0.61112200	-1.58329000
H	-1.43273600	-0.01120500	-2.06234800
H	-0.31314400	-1.30550900	-2.35365700
C	0.54555400	0.28274400	-1.16492700
H	0.90635500	0.84743500	-2.04135800
C	0.04016500	1.28271700	-0.08933300
C	-1.68255200	-0.50470500	0.74885400
C	0.65013600	-0.43116300	1.64269600
H	0.28263200	-1.00232800	2.49611900
H	1.46397400	0.18646000	2.03984800
C	-0.50356800	0.45646600	1.10856800
H	-0.83373800	1.14662600	1.90342300
N	-2.89403400	0.24358600	0.27671400
H	-3.63617300	-0.45594700	0.18064500
H	-3.21926500	0.82571500	1.05473100
N	-1.00323300	2.14421600	-0.71301900
H	-1.30611000	2.83578500	-0.02086900
N	-1.97799700	-1.29455300	1.92451700
H	-2.39675800	-0.74848700	2.67545800
H	-2.59260000	-2.08162000	1.72326900
N	1.12252400	2.17373000	0.41481700
H	1.44754000	2.75255800	-0.36514400
H	0.70712700	2.83769000	1.07452800
N	2.92502000	0.06427500	-0.30083400
H	3.63046600	-0.65245900	-0.10570100
H	3.28032300	0.52096000	-1.14658700
N	1.93170800	-1.62875800	-1.74032600
H	2.37281100	-1.20591300	-2.55519000
H	2.50999700	-2.41017900	-1.43596500
H	-0.55872400	2.69576900	-1.45257300
Li	-2.70970900	1.34191600	-1.31810500
H	-3.70222100	0.99408500	-3.19701700
H	-4.12399400	0.56906200	-2.75954600
Li	2.80128400	1.38874600	1.11448500
H	-4.08624300	3.14715200	-1.31269000

H	-4.18852100	2.82191800	-0.65495300
H	3.66953700	1.66919900	3.08532400
H	3.01102200	1.99939200	3.16988100
H	4.51501100	2.87973400	0.53069800
H	3.86864600	3.23178000	0.61268800

9.$(Li^{+})_2$-$(H_2)_5$

E=-743.07518786

C	-0.14804900	-2.31152000	0.25498400
H	0.08361900	-3.06356200	-0.50167100
H	-0.43655900	-2.83065600	1.17076500
C	-1.29719300	-1.42108300	-0.24941400
H	-2.16687800	-2.04776400	-0.49184300
C	1.07989100	-1.42747900	0.53565200
H	1.89501300	-2.04823900	0.93396400
C	1.55088100	-0.77047300	-0.78110300
C	-0.83273500	-0.69219400	-1.52566000
H	-1.63337700	-0.09971900	-1.98360900
H	-0.56672800	-1.43799500	-2.27597200
C	0.40966400	0.18998700	-1.24480100
H	0.72126200	0.69315400	-2.17588700
C	0.01314800	1.26396200	-0.19475900
C	-1.69631200	-0.42065100	0.85909100
C	0.69103100	-0.36968100	1.58860700
H	0.36446500	-0.88429000	2.49312700
H	1.54284400	0.24518400	1.90321800
C	-0.47013400	0.52305400	1.08205500
H	-0.72471900	1.26685200	1.85624200
N	-2.91628200	0.33547100	0.42237400
H	-3.67942300	-0.34767600	0.40714000
H	-3.17886500	0.96664900	1.18551200
N	-1.04712900	2.12380500	-0.79004600
H	-1.28816800	2.85295900	-0.11231300
N	-1.93378500	-1.13441900	2.09528200
H	-2.29246100	-0.53623900	2.83744700
H	-2.57802800	-1.91467900	1.97778400
N	1.15663200	2.13763400	0.18414000
H	1.46096000	2.64889900	-0.64931000
H	0.80786600	2.85968800	0.82079600
N	2.83113700	-0.03469000	-0.52928200
H	3.54353900	-0.75280600	-0.36921800
H	3.12268800	0.39728600	-1.41145300
N	1.71100900	-1.78418300	-1.80192700
H	2.11467800	-1.41760300	-2.66227500
H	2.28729900	-2.56407400	-1.48991000
H	-0.63929400	2.63071100	-1.58083200
Li	-2.80267900	1.33381100	-1.24584600
Li	2.83750400	1.32224600	0.88664400

H	4.11801300	0.05877000	2.24746600
H	4.62577800	0.56248700	2.05439300
H	2.77295000	2.39861300	2.97902900
H	2.98266700	2.91674700	2.49352000
H	4.14663700	2.97125100	0.20479500
H	4.66674000	2.44346600	0.20192300
H	-4.08562300	3.19537200	-1.06004800
H	-3.98360800	3.10993000	-1.78900900
H	-4.00311400	0.33892800	-2.82314600
H	-4.51687300	0.53131900	-2.32473100

9. $(Li^+)_2$-$(H_2)_6$

E=-744.24302807

C	0.01962500	-2.34728000	0.05318800
H	-0.19316900	-2.96746700	0.92581600
H	0.24156000	-3.00775000	-0.78694600
C	1.22167400	-1.43498600	0.35595600
H	2.08508200	-2.05061400	0.64499800
C	-1.19484000	-1.46886000	-0.29583200
H	-2.04938600	-2.11069400	-0.55267500
C	-1.57161800	-0.60315500	0.92759700
C	0.84921800	-0.50863800	1.53091900
H	1.69037400	0.11073800	1.86350900
H	0.59612000	-1.12646800	2.39338000
C	-0.37625000	0.37220900	1.18017100
H	-0.61870700	1.02338000	2.03717800
C	-0.00431500	1.25753200	-0.04051600
C	1.58687700	-0.62897700	-0.91101200
C	-0.83575500	-0.59864300	-1.51697600
H	-0.57627800	-1.25590400	-2.34779400
H	-1.68603000	-0.00728200	-1.87829600
C	0.37856400	0.31529600	-1.21413800
H	0.61279400	0.92391400	-2.10394200
N	2.84745100	0.14061800	-0.65347200
H	3.59600400	-0.55650100	-0.60148300
H	3.07106900	0.66646600	-1.50375400
N	1.12017200	2.14646300	0.35839100
H	1.35927600	2.74321000	-0.43868600
N	1.73355500	-1.52913900	-2.03500800
H	2.07229900	-1.06185200	-2.87428200
H	2.35828200	-2.30799000	-1.83284100
N	-1.13894000	2.11232800	-0.48436100
H	-1.37923100	2.75052700	0.27958100
H	-0.80373100	2.72078800	-1.23647400
N	-2.84084300	0.13486600	0.63080400
H	-3.58137300	-0.57258800	0.61259300
H	-3.07276900	0.70078000	1.45272300
N	-1.70661000	-1.44639300	2.09681800

H	-2.05298400	-0.94080700	2.91045500
H	-2.32183200	-2.24196800	1.93430600
H	0.77700700	2.79319100	1.07392400
Li	2.86123500	1.33538500	0.89763900
Li	-2.87699000	1.26132100	-0.96981500
H	-4.27921500	-0.15795900	-2.08879700
H	-4.78371600	0.34728200	-1.89168600
H	-2.90183700	1.87561200	-3.19394700
H	-3.00321400	2.53418100	-2.87100500
H	-4.12030600	3.03916100	-0.57041300
H	-4.61822900	2.52975100	-0.36631200
H	4.45465200	2.76328300	0.25222200
H	4.36137000	2.89912100	0.97491500
H	4.14332400	0.20042700	2.34601300
H	4.65890000	0.23368500	1.81531200
H	2.68176700	2.01191100	3.17639500
H	2.78681200	2.67012400	2.85419700

9. $(Li^{+})_2$-$(H_2)_7$

E= -745.40880411

C	0.16210000	-2.35223100	0.05467600
H	-0.06313300	-2.97419500	0.92291700
H	0.42848400	-3.00999600	-0.77455100
C	1.32985800	-1.40798700	0.39175000
H	2.19885500	-2.00017500	0.71152700
C	-1.06282700	-1.50770900	-0.33837500
H	-1.89116200	-2.17317000	-0.61988400
C	-1.50257800	-0.64765600	0.86798100
C	0.89462500	-0.48755500	1.54949500
H	1.70768700	0.15492400	1.90728000
H	0.62941600	-1.10944900	2.40534000
C	-0.34145400	0.35892900	1.15465200
H	-0.62829000	1.00719800	2.00008700
C	0.04695900	1.24878200	-0.05727400
C	1.71438200	-0.59821300	-0.86713200
C	-0.68760400	-0.63281800	-1.55129100
H	-0.38611600	-1.28585600	-2.37120900
H	-1.54066900	-0.06370200	-1.94033600
C	0.49290500	0.31303000	-1.21345500
H	0.74036300	0.92457100	-2.09759500
N	2.94564600	0.20478900	-0.57440800
H	3.71015200	-0.47197300	-0.49448700
H	3.18234900	0.73200600	-1.42023000
N	1.13399500	2.16904500	0.37488100
H	1.38347300	2.76890200	-0.41673800
N	1.91969000	-1.49902600	-1.98168000
H	2.26623700	-1.02499200	-2.81402400
H	2.56401000	-2.25571900	-1.75799800
N	-1.09441400	2.07204700	-0.54124400

H	-1.37600300	2.70583800	0.21218200
H	-0.75108500	2.68672400	-1.28454100
N	-2.78052400	0.05420400	0.52703000
H	-3.50080100	-0.67280100	0.48444400
H	-3.05932400	0.61324300	1.33924000
N	-1.65312100	-1.48967000	2.03658000
H	-2.03238500	-0.98755600	2.83768900
H	-2.24951800	-2.29652600	1.85976400
H	0.74947600	2.80928600	1.07497700
Li	2.87863700	1.40653700	0.97300000
Li	-2.79974800	1.18155200	-1.07267800
H	-4.16978600	-0.23196500	-2.22546600
H	-4.67514100	0.27339400	-2.03015700
H	-2.76453400	1.78328600	-3.31363600
H	-2.86576100	2.44236700	-2.99183700
H	-4.02880500	2.97378100	-0.73535300
H	-4.52822400	2.46709300	-0.52751300
H	4.47414500	2.83712900	0.35279000
H	4.37985000	2.97184200	1.07556900
H	4.14646900	0.29166200	2.46385700
H	4.66281800	0.32207500	1.93375600
H	2.63100000	2.08915600	3.22144400
H	2.73576000	2.74729100	2.89894600
H	-5.78617200	0.39779000	0.46012200
H	-6.10741100	0.49509000	1.11837500

9. $(Li^{+})_2$-$(H_2)_8$

E= -746.57438923

C	-0.00813300	-2.36938400	0.02982500
H	-0.28188000	-2.99761000	0.87937300
H	0.26078100	-3.02228700	-0.80247800
C	1.18131700	-1.47405000	0.41979700
H	2.01826700	-2.10293400	0.75477100
C	-1.19011000	-1.47527400	-0.38467400
H	-2.03243400	-2.10628300	-0.70175600
C	-1.63432500	-0.62120000	0.82446100
C	0.74566000	-0.55679900	1.57987700
H	1.57069600	0.05132600	1.96983000
H	0.43515100	-1.18152200	2.41830100
C	-0.44846600	0.33866100	1.16317600
H	-0.73836100	0.98273500	2.01067000
C	0.00685300	1.23333200	-0.02135300
C	1.63263900	-0.65771400	-0.81235300
C	-0.74693100	-0.59480900	-1.57031500
H	-0.44260700	-1.24501800	-2.39149600
H	-1.56632900	0.01094700	-1.97626600
C	0.45512900	0.30161500	-1.17932100
H	0.75088300	0.91886000	-2.04451800
N	2.88131500	0.09515900	-0.46812300
H	3.61504100	-0.61170500	-0.36537600

H	3.17208100	0.61842100	-1.29971700
N	1.11109100	2.10886600	0.45665400
H	1.40782800	2.70672700	-0.32007200
N	1.84031200	-1.54631800	-1.93639700
H	2.22530200	-1.06995900	-2.75034200
H	2.45356500	-2.32713800	-1.70832400
N	-1.09025400	2.10375400	-0.52585300
H	-1.37298100	2.73486800	0.22943900
H	-0.70259200	2.71792400	-1.24740000
N	-2.87662000	0.13109700	0.46146500
H	-3.62003700	-0.56919500	0.38523800
H	-3.15853400	0.68524700	1.27589300
N	-1.84758700	-1.47704400	1.97315600
H	-2.22874500	-0.97436600	2.77303800
H	-2.46909600	-2.25746000	1.76670300
H	0.72600100	2.75567700	1.15028400
Li	2.81952600	1.28876900	1.08667000
Li	-2.81048600	1.28358700	-1.12185400
H	-4.18596000	-0.07636000	-2.32323900
H	-4.68938000	0.43043700	-2.12659200
H	-2.69696700	1.90902100	-3.34303500
H	-2.79752700	2.56796500	-3.02066100
H	-4.01613800	3.09815900	-0.78956700
H	-4.51614100	2.59256300	-0.58042500
H	4.39291000	2.71399700	0.46276300
H	4.11917200	3.04412900	1.06718000
H	4.15491500	0.21464700	2.51446700
H	4.66744300	0.25951300	1.98152600
H	2.66863100	1.93916700	3.34295300
H	2.58891800	2.59595100	3.01085100
H	-5.88158300	0.56446400	0.34467600
H	-6.20271600	0.66108600	1.00308800
H	5.96734700	0.36915000	-0.68316700
H	6.28836200	1.02691600	-0.78208700

H_2

E=-1.16356551

H	0.00000000	0.00000000	0.36826300
H	0.00000000	0.00000000	-0.36826300

10.$(Li^+)_2$-(CO_2)

E=-925.77153461

C	-1.66616200	1.21983400	-1.65916500
H	-2.03297400	2.24795400	-1.64876900
H	-1.75472600	0.83921000	-2.67815300
C	-2.50719200	0.37051300	-0.68994300
H	-3.56736600	0.43705500	-0.97171300
C	-0.19245300	1.16382100	-1.22022000

H	0.42221300	1.73397700	-1.93068000
C	-0.04972600	1.79641400	0.18155800
C	-2.32855700	0.93509600	0.73404300
H	-2.97200100	0.43853300	1.47170400
H	-2.65459500	1.97581100	0.73777300
C	-0.84204800	0.88407400	1.17379100
H	-0.74568000	1.29500400	2.19293300
C	-0.38726900	-0.60177300	1.17840500
C	-2.05736000	-1.10474900	-0.77886100
C	0.26753300	-0.30852200	-1.22752000
H	0.14331400	-0.70517400	-2.23569000
H	1.33426900	-0.41883800	-1.00450200
C	-0.58603700	-1.16453500	-0.25560100
H	-0.23700900	-2.21059300	-0.28429100
N	-2.98695500	-1.94940500	0.04492200
H	-3.88731200	-1.93313300	-0.44353400
H	-2.68571900	-2.92420400	-0.04923300
N	-1.19833600	-1.32946200	2.19832100
H	-0.86657700	-2.29778400	2.23589500
N	-2.05066800	-1.52965700	-2.16193100
H	-1.84583100	-2.52121600	-2.27250800
H	-2.93031500	-1.33231700	-2.63630300
N	1.04589500	-0.75921300	1.53947500
H	1.17570900	-0.43804500	2.50296600
H	1.26511300	-1.75892000	1.56495800
N	1.40374000	1.88273500	0.53506200
H	1.80474500	2.58587600	-0.09241800
H	1.47428900	2.32146200	1.45816400
N	-0.67493500	3.10241800	0.19396400
H	-0.52416900	3.60337800	1.06808100
H	-0.35144100	3.69520600	-0.56879200
H	-0.96718900	-0.94330000	3.11828300
Li	-3.13947700	-1.48240600	1.91850900
Li	2.44789100	0.23279500	0.52604300
C	5.27492800	-0.68287000	-0.36401500
O	6.33819200	-0.95834200	-0.69198400
O	4.18091700	-0.40501300	-0.02693300

10.$(Li^+)_2$0-$(CO_2)_2$

E=-1114.31076091

C	0.00159400	-2.75349900	-0.00372500
H	0.16809800	-3.39465200	0.86377400
H	-0.16400400	-3.39230300	-0.87313000
C	1.23322200	-1.85671800	-0.21656900
H	2.12800000	-2.48449200	-0.33158900
C	-1.23134600	-1.85912600	0.21174600
H	-2.12520800	-2.48855200	0.32482800
C	-1.04215800	-1.02666100	1.49936400

C	1.40951700	-0.95567000	1.02217600
H	2.31855400	-0.34578400	0.97113400
H	1.54116100	-1.59293000	1.89762000
C	0.16182600	-0.06324700	1.24483200
H	0.31424500	0.56522500	2.13885000
C	-0.00100600	0.85385100	0.00170600
C	1.04278700	-1.02065500	-1.50168100
C	-1.40893400	-0.95462500	-1.02427200
H	-1.53961500	-1.58941200	-1.90165600
H	-2.31889700	-0.34626500	-0.97139700
C	-0.16257000	-0.05970600	-1.24421800
H	-0.31589000	0.57128400	-2.13630600
N	2.30797200	-0.27147000	-1.78926100
H	3.00280600	-0.97827000	-2.04725400
H	2.16888500	0.25333900	-2.65800400
N	1.19890100	1.73027900	-0.08580200
H	1.07258100	2.36926800	-0.87583800
N	0.68282900	-1.89262400	-2.60098400
H	0.63808700	-1.40337600	-3.49327500
H	1.32739800	-2.67497300	-2.70236500
N	-1.20212100	1.72834000	0.09180200
H	-1.07678800	2.36514500	0.88375800
H	-1.21550600	2.33649100	-0.73164700
N	-2.30841000	-0.28011400	1.78913100
H	-3.00215900	-0.98865000	2.04527000
H	-2.16997900	0.24245900	2.65933000
N	-0.68104300	-1.90137500	2.59608800
H	-0.63694400	-1.41469600	3.48981600
H	-1.32453600	-2.68490400	2.69518300
H	1.21132300	2.33603300	0.73943400
Li	2.98923400	0.93826200	-0.41079800
Li	-2.99140600	0.93279000	0.41434900
C	-5.88449600	1.67361700	-0.42382800
O	-6.97226700	1.92685600	-0.68256800
O	-4.76629000	1.41461300	-0.16056600
C	5.88448900	1.67210500	0.42656900
O	6.97198500	1.92616300	0.68567400
O	4.76662800	1.41206900	0.16288500

10.$(Li^+)_2$-$(CO_2)_3$

E=-1302.84272651

C	0.84983100	-2.55434300	1.43737300
H	1.04430500	-2.60410900	2.51028000
H	0.81219900	-3.57432300	1.05083000
C	1.97420700	-1.75813300	0.75296000
H	2.94329500	-2.22750400	0.97365500

C	-0.49198100	-1.85575900	1.16076100
H	-1.30746500	-2.43788000	1.61290600
C	-0.47690300	-0.44804000	1.79594700
C	1.97176900	-0.32042900	1.31147300
H	2.80287900	0.28109100	0.92610300
H	2.12950300	-0.36821600	2.38957700
C	0.61479400	0.37818800	1.04188100
H	0.63949100	1.40083100	1.45581600
C	0.40895600	0.45890300	-0.49610200
C	1.75070000	-1.77145400	-0.77553700
C	-0.71765200	-1.77691700	-0.36214100
H	-0.73735600	-2.79020500	-0.76535900
H	-1.68596300	-1.33134300	-0.60556000
C	0.42715500	-0.99093900	-1.05141700
H	0.24911000	-0.96072700	-2.14008800
N	2.93174800	-1.13668000	-1.44579800
H	3.71591200	-1.77980300	-1.30368600
H	2.77237100	-1.17569000	-2.45691300
N	1.50256900	1.29917800	-1.06126300
H	1.33951300	1.40086600	-2.06690100
N	1.55797400	-3.13386000	-1.22889400
H	1.48571500	-3.20362000	-2.24257000
H	2.30594400	-3.75399700	-0.92260500
N	-0.88769100	1.08071100	-0.86453500
H	-0.88094500	2.05589900	-0.55285900
H	-0.94109700	1.13173200	-1.88539100
N	-1.83350300	0.16489600	1.66729900
H	-2.45545400	-0.39561200	2.25647000
H	-1.80884300	1.07403700	2.13881200
N	-0.07040200	-0.54692300	3.18532000
H	-0.14086700	0.34282000	3.67647800
H	-0.62349400	-1.23171900	3.69840700
H	1.40053000	2.24577300	-0.68516300
Li	3.38771900	0.68595200	-0.93011200
Li	-2.64619500	0.52239100	-0.08619400
C	-5.07669400	-1.08747600	-1.28173200
O	-5.97592400	-1.66337000	-1.70406600
O	-4.15534700	-0.49746700	-0.85077500
C	6.03802100	2.21829700	-0.42839300
O	7.05499600	2.72473600	-0.27306400
O	4.99207400	1.70104300	-0.58543900
C	-4.40269000	3.14626700	0.13148100
O	-5.22421400	3.94699400	0.18971800
O	-3.55481100	2.33261800	0.07393100

10.$(Li^+)_2$-$(CO_2)_4$

E=-1491.37444975

C	0.00031500	-3.18622200	-0.00011000

H	0.07814600	-3.82655300	0.88062600
H	-0.07736800	-3.82662200	-0.88081000
C	1.24691400	-2.29002900	-0.08968400
H	2.14895600	-2.91767900	-0.11614300
C	-1.24648600	-2.29030000	0.08939400
H	-2.14839000	-2.91814500	0.11588600
C	-1.18516500	-1.45567100	1.38730700
C	1.30497500	-1.38306400	1.15542200
H	2.20582700	-0.76486000	1.16426700
H	1.35711200	-2.01395000	2.04368200
C	0.03838000	-0.49536900	1.25331400
H	0.09912100	0.13524800	2.15698100
C	-0.00007600	0.42025800	-0.00023900
C	1.18539700	-1.45551200	-1.38765800
C	-1.30474700	-1.38343100	-1.15576900
H	-1.35674700	-2.01438900	-2.04398400
H	-2.20573600	-0.76543800	-1.16466200
C	-0.03834900	-0.49546400	-1.25373100
H	-0.09922900	0.13507500	-2.15744400
N	2.47011000	-0.70854000	-1.55273300
H	3.18807600	-1.41516400	-1.73531800
H	2.41524400	-0.18722500	-2.43285300
N	1.20460900	1.29159000	0.02972700
H	1.15618200	1.93517600	-0.76502500
N	0.93393200	-2.33151400	-2.51696000
H	0.98174700	-1.84029600	-3.40810300
H	1.59169700	-3.10877000	-2.55293900
N	-1.20495000	1.29135200	-0.03025800
H	-1.15657200	1.93505500	0.76440300
H	-1.14273500	1.89158000	-0.85695100
N	-2.47004300	-0.70897100	1.55227700
H	-3.18784800	-1.41573500	1.73495100
H	-2.41531700	-0.18749800	2.43231000
N	-0.93352500	-2.33151800	2.51668800
H	-0.98152200	-1.84024500	3.40778900
H	-1.59107700	-3.10895300	2.55269200
H	1.14227300	1.89191300	0.85634000
Li	3.07220200	0.59898100	-0.21302700
Li	-3.07231300	0.59836700	0.21245000
C	-5.37207300	0.10671800	-1.91294700
O	-6.21411000	-0.09289000	-2.66822900
O	-4.50898900	0.31279100	-1.14187500
C	5.37153900	0.10576300	1.91274000
O	6.21231300	-0.09539800	2.66901800
O	4.50978100	0.31346200	1.14062500
C	-4.77961000	2.83202100	1.62969100
O	-5.57868800	3.55814300	2.02196100
O	-3.95498200	2.09294600	1.23320100
C	4.77970400	2.83324200	-1.62831100
O	5.57935400	3.55901700	-2.02006000
O	3.95447500	2.09455300	-1.23235000

10.$(Li^+)_2$-$(CO_2)_5$

E=-1679.90053374

C	-0.38563500	-3.07988000	0.79719400
H	-0.47719500	-3.94412200	0.13645100
H	-0.26379000	-3.44370200	1.81934400
C	-1.64988400	-2.21256400	0.67576200
H	-2.53434100	-2.81882300	0.91812400
C	0.83533700	-2.22910000	0.40881200
H	1.75204700	-2.82507900	0.52739800
C	0.71380900	-1.79713700	-1.06898700
C	-1.77155300	-1.70406500	-0.77394700
H	-2.68656900	-1.12513300	-0.92494400
H	-1.83873900	-2.56455400	-1.44123300
C	-0.53259200	-0.86449800	-1.17039400
H	-0.63789400	-0.52199800	-2.21435300
C	-0.47196500	0.37397900	-0.23809000
C	-1.56789000	-1.03742300	1.67511600
C	0.90949100	-1.00534200	1.34277200
H	0.99692500	-1.35834600	2.37106900
H	1.80069300	-0.40104800	1.15314400
C	-0.37150200	-0.14007100	1.22468500
H	-0.29434700	0.72596500	1.90450600
N	-2.86444800	-0.29345000	1.66369600
H	-3.56107500	-0.93031700	2.06013600
H	-2.79893900	0.45603700	2.35885200
N	-1.69674000	1.18765700	-0.46975600
H	-1.62922500	2.03429300	0.10214600
N	-1.26233100	-1.54694500	2.99954300
H	-1.29145200	-0.81814500	3.71084900
H	-1.90569400	-2.28464400	3.28253300
N	0.71382600	1.21747000	-0.51132500
H	0.63700000	1.59520600	-1.45896300
H	0.68970900	2.03243100	0.10688200
N	1.96881000	-1.09840000	-1.47521000
H	2.69550800	-1.81750700	-1.51616500
H	1.86355100	-0.80238700	-2.44988700
N	0.45590500	-2.96304900	-1.89564600
H	0.46687100	-2.73970800	-2.88961600
H	1.13817800	-3.70264700	-1.73546800
H	-1.66934100	1.52633500	-1.43532000
Li	-3.53051000	0.57451800	0.02904800
Li	2.60994600	0.50751600	-0.46627700
C	5.44926600	-1.03016900	0.50177600
O	6.37296600	-1.67361200	0.73745400
O	4.50341400	-0.37579100	0.25944800
C	-5.93813000	-0.57153000	-1.66707100
O	-6.80924700	-1.03547900	-2.25473400
O	-5.04640100	-0.09620800	-1.06655000

C	4.31552300	2.24710800	-2.49656900
O	5.08410500	2.85067900	-3.10252800
O	3.52573800	1.63150100	-1.88223200
C	-5.23013200	3.12158300	0.79084000
O	-6.03649200	3.92343600	0.95480300
O	-4.39900600	2.30606000	0.62615800
C	3.99243200	2.01764700	1.85008600
O	4.90155800	2.11176100	2.55072400
O	3.06901600	1.91110200	1.13185400

10.$(Li^+)_2$-$(CO_2)_6$

E=-1868.42704703

C	-0.00027500	-3.15868700	0.00613900
H	0.13426100	-3.79679800	0.88194400
H	-0.13471500	-3.80013200	-0.86724300
C	1.23804200	-2.26248100	-0.16484100
H	2.13707300	-2.89013700	-0.25091500
C	-1.23869300	-2.26198700	0.17369200
H	-2.13766900	-2.88938800	0.26218700
C	-1.09753000	-1.41780100	1.45932300
C	1.37343400	-1.36041900	1.07691800
H	2.27931100	-0.74893700	1.04419000
H	1.47092700	-1.99587600	1.95851800
C	0.12115500	-0.46611100	1.24826400
H	0.24149100	0.16709000	2.14439300
C	-0.00045000	0.44748100	-0.00077600
C	1.09682700	-1.42325300	-1.45369600
C	-1.37415700	-1.36463200	-1.07146700
H	-1.47172400	-2.00340000	-1.95066200
H	-2.27996300	-0.75297400	-1.04093400
C	-0.12197000	-0.47090600	-1.24630800
H	-0.24237900	0.15880700	-2.14487500
N	2.36359500	-0.66738400	-1.68151300
H	3.06568400	-1.36148000	-1.94988100
H	2.24543200	-0.10002100	-2.52580600
N	1.20519900	1.30722500	-0.06290900
H	1.11375200	1.93739100	-0.86371200
N	0.78609400	-2.29931700	-2.57026100
H	0.79359000	-1.80414900	-3.46053200
H	1.44336000	-3.07473300	-2.64071600
N	-1.20621200	1.30726400	0.05810000
H	-1.11471400	1.94063400	0.85635500
H	-1.21193000	1.91489400	-0.76507200
N	-2.36443000	-0.66125300	1.68428900
H	-3.06643700	-1.35448100	1.95509200
H	-2.24634300	-0.09094500	2.52660600
N	-0.78664900	-2.28955900	2.57919600
H	-0.79396700	-1.79097700	3.46755900

H	-1.44390300	-3.06469500	2.65272300
H	1.21062100	1.91816200	0.75781400
Li	3.07681400	0.56995400	-0.27775800
Li	-3.07800800	0.57098700	0.27565700
C	-5.90017400	-1.24886800	-0.05856100
O	-6.81192800	-1.95009200	-0.04257100
O	-4.96703000	-0.53464500	-0.07204600
C	4.56774600	1.30827600	2.32816300
O	5.48198900	1.17740400	3.01613500
O	3.63812300	1.43426400	1.62124900
C	-4.76465400	2.80877500	1.78130600
O	-5.52444100	3.56406600	2.19914400
O	-3.98378500	2.03952700	1.35915500
C	4.76672200	2.79698100	-1.79088400
O	5.53290600	3.54545000	-2.20932900
O	3.97922400	2.03479600	-1.36817800
C	-4.56742200	1.29691800	-2.33409900
O	-5.48158400	1.16196600	-3.02140200
O	-3.63788500	1.42693200	-1.62782000
C	5.90013100	-1.24824600	0.06263600
O	6.81102500	-1.95065400	0.04987000
O	4.96791800	-0.53273200	0.07280500

10.$(Li^{+})_2$-$(CO_2)_7$

E=-2056.95114883

C	-0.53868800	-3.52889800	0.00284400
H	-0.75454200	-4.15388400	-0.86619200
H	-0.45891800	-4.17769100	0.87752800
C	-1.67379100	-2.50738500	0.18786500
H	-2.63202500	-3.03697300	0.29306800
C	0.78428800	-2.76820200	-0.19008000
H	1.61071400	-3.48726700	-0.28779200
C	0.71123000	-1.91993900	-1.47922600
C	-1.73413300	-1.60301000	-1.05829200
H	-2.57109300	-0.90069100	-1.01642200
H	-1.91131800	-2.22992100	-1.93354000
C	-0.39794600	-0.84562900	-1.25506000
H	-0.46557600	-0.20851200	-2.15382400
C	-0.15926700	0.05882100	-0.01550600
C	-1.42448500	-1.67911900	1.46800300
C	1.03032400	-1.88418400	1.04840300
H	1.06877000	-2.52626100	1.92950500
H	1.99572300	-1.37352400	1.00549200
C	-0.11668400	-0.86119600	1.23438800
H	0.08438600	-0.24304700	2.12650800
N	-2.60034700	-0.79334400	1.71075700
H	-3.36633100	-1.40660600	2.00025600
H	-2.40591000	-0.23354900	2.54590800
N	-1.26812600	1.04156700	0.05846200

H	-1.08984500	1.66792000	0.84744400
N	-1.18936500	-2.57601800	2.58673900
H	-1.12393400	-2.07620300	3.47208400
H	-1.92679800	-3.27323900	2.67762300
N	1.12774300	0.78433100	-0.09831500
H	1.09856900	1.42311600	-0.89676400
H	1.21765900	1.39893800	0.71469100
N	2.04481500	-1.30049300	-1.72740900
H	2.66777100	-2.06066200	-2.01101900
H	1.97363400	-0.71562500	-2.56486700
N	0.29273300	-2.75884100	-2.58971000
H	0.33777200	-2.26403400	-3.47916600
H	0.86994800	-3.59463300	-2.67164100
H	-1.22299500	1.63995700	-0.77034000
Li	-3.20453900	0.49539600	0.31297800
Li	2.90120100	-0.16482100	-0.32545700
C	5.50506100	-2.30068600	-0.06458400
O	6.36109400	-3.06237200	-0.16853900
O	4.62723800	-1.52650800	0.03841500
C	4.57732600	2.14252500	-1.54765600
O	5.13385100	3.14170100	-1.68721300
O	4.01535800	1.12241700	-1.41390400
C	2.74045400	4.63164000	-0.08139800
O	2.94253200	5.75656600	0.06982200
O	2.52957200	3.48620700	-0.23109400
C	4.49071800	0.29163700	2.25123000
O	5.36219400	-0.04060200	2.92717600
O	3.60382200	0.62505800	1.55703300
C	-6.18131100	-1.05083700	-0.03263900
O	-7.15096600	-1.66971200	-0.02264000
O	-5.18896700	-0.42144100	-0.04031800
C	-4.66919400	2.87757600	1.81604200
O	-5.35724300	3.69968200	2.23266800
O	-3.96172700	2.04000900	1.39487700
C	-4.63864600	1.39018900	-2.29519100
O	-3.69517200	1.41852800	-1.59638000
O	-5.56775500	1.35551800	-2.97485700

10.$(Li^+)_2$-$(CO_2)_8$

E=-2245.47671795

C	0.40297400	-3.32125700	-0.38097400
H	0.65112400	-4.02875200	0.41284000
H	0.41513500	-3.85728500	-1.33212500
C	1.43506900	-2.18162000	-0.38722800
H	2.44352500	-2.59966900	-0.51949800
C	-0.99366500	-2.72001200	-0.15066400
H	-1.74846800	-3.51944900	-0.17915600
C	-1.03939700	-2.04565600	1.23757100
C	1.37386200	-1.43421900	0.95850800

H	2.12600300	-0.64368600	1.01669000
H	1.60122500	-2.13873300	1.76053600
C	-0.03942500	-0.85002100	1.19760800
H	-0.06342700	-0.33210100	2.17197300
C	-0.33170600	0.18072500	0.07440600
C	1.14296900	-1.22720900	-1.56565400
C	-1.29370400	-1.70723000	-1.27386600
H	-1.25518400	-2.22889400	-2.23116800
H	-2.30347900	-1.29522900	-1.19244000
C	-0.24409200	-0.56768900	-1.28435700
H	-0.47701600	0.14076100	-2.09788100
N	2.24109100	-0.22057400	-1.65582300
H	3.08787800	-0.73915100	-1.90300800
H	2.06149800	0.36743400	-2.47489500
N	0.67014900	1.27078300	0.17765300
H	0.43619800	1.99037900	-0.51160600
N	1.02323200	-1.99521600	-2.79353000
H	0.91429600	-1.39729400	-3.61134200
H	1.83628600	-2.58913800	-2.94986800
N	-1.68678500	0.76255400	0.19571800
H	-1.74067900	1.29676000	1.06646600
H	-1.81629200	1.46278900	-0.53863700
N	-2.43415800	-1.59788000	1.51242900
H	-2.98356700	-2.44680100	1.66773000
H	-2.44406500	-1.12972200	2.42316100
N	-0.56587400	-2.97945800	2.24662400
H	-0.68228300	-2.61150000	3.18960100
H	-1.05999700	-3.86948600	2.19964500
H	0.54979800	1.72904800	1.08492400
Li	2.62304400	1.05055500	-0.19457400
Li	-3.38031700	-0.34907000	0.26663900
C	-5.79694100	-2.59188600	-0.34314000
O	-6.59179300	-3.42285600	-0.38005500
O	-4.98255900	-1.74591700	-0.30395200
C	4.65228500	1.25529900	1.91258400
O	5.74302100	1.10404400	2.25082800
O	3.54237400	1.41304300	1.56404200
C	-5.17196000	1.63204900	1.83352900
O	-5.81632700	2.54638700	2.10833000
O	-4.51976600	0.69587200	1.56266800
C	-3.54745300	4.47628700	0.70962100
O	-3.81204000	5.59842100	0.71330700
O	-3.27259500	3.33487100	0.70153000
C	-5.00037500	0.42167700	-2.22262500
O	-5.84156600	0.15657400	-2.96353500
O	-4.14420600	0.68626300	-1.46328200
C	5.29491600	-2.23704700	1.12512400
O	5.81447500	-3.15845400	1.58245800
O	4.75357000	-1.30418100	0.65908700
C	6.06901300	0.51925500	-0.98222300
O	7.04832900	-0.08239700	-1.06255800

O	5.06444700	1.12225100	-0.89904800
C	3.76423500	3.57199900	-1.40015600
O	2.85823700	2.89536100	-1.07821800
O	4.64765700	4.23735900	-1.71635500

CO_2

E=-188.51605286

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16289500
O	0.00000000	0.00000000	-1.16289500

11.$(Li^+)_2$-(CO)

E=-850.52437047

C	1.29537100	1.51979400	1.42117200
H	1.52376900	2.57479100	1.25920100
H	1.51611700	1.28209200	2.46330000
C	2.15587600	0.66306100	0.47603900
H	3.21796900	0.88992600	0.64323800
C	-0.18990400	1.23549400	1.13666800
H	-0.81263900	1.81281400	1.83406000
C	-0.52698500	1.66674200	-0.30751000
C	1.78855700	1.01866900	-0.97821700
H	2.42932300	0.51499100	-1.71313600
H	1.97386600	2.08235400	-1.13216700
C	0.29013000	0.73555100	-1.26218800
H	0.05773600	1.00045200	-2.30737800
C	0.03168400	-0.78271500	-1.05139600
C	1.91149400	-0.83349800	0.77370100
C	-0.45134000	-0.26880300	1.35773400
H	-0.19493100	-0.51697500	2.38822600
H	-1.51040100	-0.53458100	1.25823500
C	0.42089300	-1.13336200	0.41026500
H	0.21450400	-2.20138300	0.59263700
N	2.87093900	-1.65470600	-0.04026700
H	3.79909000	-1.47198800	0.35294700
H	2.70800800	-2.63988500	0.18927500
N	0.84064800	-1.53265000	-2.05538100
H	0.64210700	-2.53132100	-1.94444000
N	2.07735400	-1.08285900	2.18876100
H	2.01271600	-2.07059200	2.42918300
H	2.96127700	-0.72643700	2.54847200
N	-1.39604400	-1.15083300	-1.25234000
H	-1.64336400	-0.96564600	-2.22872200

H	-1.48339200	-2.16596400	-1.15023800
N	-2.00489200	1.53958300	-0.52413000
H	-2.43674000	2.26550800	0.05547400
H	-2.20724900	1.84986400	-1.47943100
N	-0.07722900	3.02484700	-0.52828200
H	-0.36501400	3.39552100	-1.43243900
H	-0.40284000	3.66539600	0.19389500
H	0.48177800	-1.30108800	-2.98626000
Li	2.80008500	-1.40350400	-1.96232100
Li	-2.81082800	-0.20391400	-0.22699300
C	-5.48770500	-1.39265500	0.98245400
O	-4.50666400	-0.99486700	0.55789400

11.$(Li^+)_2$-$(CO)_2$

E=-963.81617562

C	-0.00164000	-2.52182300	0.00887600
H	0.11302200	-3.15881900	0.88777100
H	-0.11719900	-3.16514200	-0.86527800
C	1.24178600	-1.62807100	-0.13770400
H	2.14021900	-2.25803000	-0.19740300
C	-1.24372800	-1.62519500	0.14892100
H	-2.14315000	-2.25329000	0.21328300
C	-1.12690300	-0.78698400	1.44158800
C	1.34787200	-0.72160900	1.10522400
H	2.26051000	-0.11447300	1.10647100
H	1.42666200	-1.35471000	1.98980900
C	0.09111200	0.17470500	1.25124600
H	0.19252300	0.80750800	2.14922300
C	0.00109700	1.08467100	-0.00448800
C	1.12640100	-0.79918300	-1.43654100
C	-1.34842100	-0.72765600	-1.10065900
H	-1.42832400	-1.36712100	-1.98054500
H	-2.26009000	-0.11908400	-1.10626400
C	-0.09030300	0.16557500	-1.25341500
H	-0.19081000	0.79181500	-2.15608000
N	2.40835200	-0.05279000	-1.65595500
H	3.11346200	-0.76207100	-1.87714000
H	2.31735600	0.47097500	-2.53187700
N	1.20509100	1.96105900	-0.02771000
H	1.12916200	2.58915200	-0.83298600
N	0.82855700	-1.67585200	-2.54917900
H	0.83296200	-1.19280400	-3.44595200
H	1.47406600	-2.46160800	-2.61017400
N	-1.20163400	1.96295800	0.01232800
H	-1.12458400	2.59713800	0.81271200
H	-1.16077700	2.57396700	-0.80811700
N	-2.40783500	-0.03730900	1.65578300
H	-3.11394500	-0.74407700	1.88178800

H	-2.31616300	0.49238100	2.52806000
N	-0.82985200	-1.65593700	2.56048400
H	-0.83347300	-1.16639900	3.45372800
H	-1.47630300	-2.44044600	2.62726300
H	1.16485100	2.57840300	0.78800100
Li	2.99961100	1.14955600	-0.24381900
Li	-2.99707600	1.15588100	0.23506400
C	-5.85214900	1.65528100	-1.05024600
O	-4.82540400	1.47423800	-0.58833600
C	5.85078400	1.66382900	1.04305000
O	4.82518300	1.47879800	0.58016000

11.$(Li^+)_2$-$(CO)_3$

E=-1077.10440274

C	0.73544300	-2.39981800	1.08593300
H	0.87689700	-2.57866800	2.15338600
H	0.78140200	-3.36140200	0.57157700
C	1.84195200	-1.45980000	0.57603300
H	2.82539600	-1.89933000	0.79407600
C	-0.63113800	-1.74586300	0.82136300
H	-1.43129300	-2.42642000	1.14491600
C	-0.73753400	-0.43379900	1.63072700
C	1.71889100	-0.11055300	1.31292900
H	2.53201300	0.58172900	1.06439100
H	1.82188300	-0.29073800	2.38360000
C	0.33776400	0.54308300	1.05319700
H	0.27785600	1.50303200	1.59371500
C	0.20847600	0.81099200	-0.47128100
C	1.70045100	-1.28752300	-0.95310500
C	-0.77729400	-1.48456800	-0.69090100
H	-0.70735900	-2.43718100	-1.21742400
H	-1.75977000	-1.07547400	-0.94445600
C	0.34699200	-0.55068900	-1.20646100
H	0.22285200	-0.38935800	-2.29083700
N	2.87205700	-0.50636400	-1.46784800
H	3.68721600	-1.11773600	-1.36410100
H	2.76728900	-0.42054600	-2.48334200
N	1.27236600	1.78016200	-0.86114400
H	1.15875700	1.99650400	-1.85558200
N	1.61563200	-2.58797900	-1.58422600
H	1.60744100	-2.53213100	-2.60129300
H	2.37810200	-3.20452400	-1.30787200
N	-1.10621100	1.40339100	-0.83479900
H	-1.17872500	2.32287700	-0.38994000
H	-1.10079100	1.60051700	-1.83951700
N	-2.12464400	0.11265900	1.49657100
H	-2.73757300	-0.54999700	1.98060400
H	-2.18268700	0.95662200	2.07444600

N	-0.40083500	-0.68748000	3.01711900
H	-0.55107500	0.12491900	3.61309200
H	-0.93018800	-1.46562200	3.40736200
H	1.08621300	2.66544700	-0.38155700
Li	3.17321900	1.24800400	-0.69135200
Li	-2.82585100	0.56349700	-0.27401900
C	-5.16802900	-1.09171200	-1.71034200
O	-4.31909200	-0.52063100	-1.20869100
C	5.83155900	2.68095100	0.25299200
O	4.85778600	2.18178100	-0.06851100
C	-4.88996800	3.02338500	0.10804600
O	-4.09993100	2.21357000	-0.02575000

11.$(Li^+)_2$-$(CO)_4$

E=-1190.39224724

C	0.00001300	-2.89317300	-0.00013500
H	0.01669000	-3.53438000	0.88307900
H	-0.01664900	-3.53425900	-0.88343900
C	1.25093100	-1.99758200	-0.00351500
H	2.15155200	-2.62648300	0.03324600
C	-1.25091900	-1.99759900	0.00336000
H	-2.15153200	-2.62650700	-0.03347500
C	-1.27908600	-1.16373500	1.30333700
C	1.21946200	-1.09268900	1.24455000
H	2.12108700	-0.47899500	1.33118900
H	1.20579700	-1.72539100	2.13264300
C	-0.04953100	-0.20168000	1.25369100
H	-0.05056700	0.42789900	2.15974000
C	-0.00000400	0.71379900	0.00007200
C	1.27907700	-1.16358400	-1.30340200
C	-1.21946100	-1.09256600	-1.24460300
H	-1.20578300	-1.72517200	-2.13276700
H	-2.12109100	-0.47887000	-1.33117800
C	0.04952300	-0.20154300	-1.25364500
H	0.05055200	0.42813400	-2.15962600
N	2.57450000	-0.41706100	-1.37923300
H	3.30195700	-1.12540600	-1.51249900
H	2.58198400	0.10174100	-2.26255600
N	1.19889300	1.58869000	0.11818100
H	1.20373000	2.23570700	-0.67537400
N	1.10563400	-2.03707300	-2.44680400
H	1.20656300	-1.54646600	-3.33382300
H	1.76351800	-2.81497900	-2.44167500
N	-1.19890700	1.58868700	-0.11796100
H	-1.20376400	2.23562100	0.67566200
H	-1.07616200	2.18652500	-0.94006200
N	-2.57451400	-0.41723000	1.37922200
H	-3.30196700	-1.12559400	1.51240600

H	-2.58201600	0.10148200	2.26259800
N	-1.10569400	-2.03733400	2.44666400
H	-1.20665200	-1.54680700	3.33372400
H	-1.76359300	-2.81522800	2.44144200
H	1.07615300	2.18644100	0.94034500
Li	3.04418300	0.83730200	0.04192800
Li	-3.04418600	0.83726700	-0.04181800
C	-5.34256900	0.43622500	-2.23259100
O	-4.51401200	0.58432700	-1.46453400
C	5.34269400	0.43596400	2.23251200
O	4.51412400	0.58419700	1.46449400
C	-4.84908200	3.19013100	1.30772200
O	-4.13736200	2.41089200	0.87929800
C	4.84902900	3.19023700	-1.30755500
O	4.13729400	2.41099700	-0.87915800

11.$(Li^{+})_2$-$(CO)_5$

E=-1303.67786129

C	-0.34768900	-2.83758800	0.73674800
H	-0.42537900	-3.70236700	0.07516200
H	-0.29356700	-3.20063900	1.76498500
C	-1.57956500	-1.93665000	0.54249100
H	-2.49212200	-2.51929500	0.73237200
C	0.91705400	-2.02201600	0.41619600
H	1.80813600	-2.64248100	0.58895800
C	0.88994600	-1.59299900	-1.06807700
C	-1.60123700	-1.43030500	-0.91303400
H	-2.49435100	-0.83647100	-1.12832500
H	-1.64945600	-2.29170300	-1.58048400
C	-0.32038500	-0.62301000	-1.23921400
H	-0.35833800	-0.27953100	-2.28718300
C	-0.27786700	0.61347200	-0.30302000
C	-1.52421500	-0.76272800	1.54471900
C	0.96654400	-0.80233600	1.35708400
H	0.97745600	-1.16132300	2.38697500
H	1.88811500	-0.22349400	1.24269100
C	-0.27894000	0.10071600	1.16361900
H	-0.21719400	0.96540700	1.84663700
N	-2.79862000	0.01916300	1.45449200
H	-3.53533900	-0.59826900	1.80802300
H	-2.75452400	0.76416400	2.15622100
N	-1.46092100	1.46514500	-0.61029900
H	-1.40695000	2.30741600	-0.03042300
N	-1.31285300	-1.27461900	2.88393500
H	-1.35816400	-0.54562200	3.59404200
H	-1.98759000	-1.99668600	3.13158500
N	0.94743100	1.42778800	-0.50282400
H	0.94932200	1.78217100	-1.46311300

H	0.88000400	2.26217000	0.08578800
N	2.18457500	-0.92899400	-1.40987200
H	2.89477700	-1.66636000	-1.40076700
H	2.14226400	-0.64848700	-2.39397800
N	0.64522000	-2.75317200	-1.90318300
H	0.71669200	-2.53994600	-2.89675800
H	1.28933400	-3.51593600	-1.69980500
H	-1.36106300	1.80663900	-1.57034400
Li	-3.31049000	0.83756500	-0.24678300
Li	2.78264300	0.61382500	-0.32142700
C	5.56719900	-0.82342700	0.78146500
O	4.60611500	-0.34833300	0.40076600
C	-5.79246500	-0.21113100	-1.99130100
O	-4.89755600	0.14612700	-1.38329400
C	4.63507000	2.44450600	-2.26337300
O	3.93287800	1.82818800	-1.61295800
C	-5.01506500	3.52485900	0.40456900
O	-4.35689300	2.62077800	0.18824200
C	3.73523900	2.71848800	2.15856000
O	3.35244300	2.03826300	1.33124800

11.$(Li^+)_2$-$(CO)_6$

E=-1416.96375087

C	0.00005400	-2.94995900	0.00007700
H	0.09612600	-3.59012300	0.87920200
H	-0.09598800	-3.59021300	-0.87899600
C	1.24551000	-2.05401100	-0.11649700
H	2.14657700	-2.68213500	-0.16366000
C	-1.24546000	-2.05406400	0.11661800
H	-2.14648200	-2.68224800	0.16382600
C	-1.15696400	-1.21568000	1.41111300
C	1.32607200	-1.15473100	1.13271900
H	2.23484900	-0.54567300	1.14934600
H	1.38491000	-1.79185800	2.01618900
C	0.06763600	-0.26038200	1.25262300
H	0.14856300	0.37087300	2.15432300
C	-0.00003500	0.65422500	-0.00003600
C	1.15695300	-1.21578800	-1.41102100
C	-1.32611300	-1.15487600	-1.13263200
H	-1.38499100	-1.79204000	-2.01606500
H	-2.23490300	-0.54584800	-1.14921400
C	-0.06769500	-0.26050800	-1.25263200
H	-0.14863600	0.37066400	-2.15438700
N	2.43122800	-0.45717000	-1.58896300
H	3.14859100	-1.15177400	-1.81492900
H	2.34986700	0.09403000	-2.44830000
N	1.20757900	1.52066300	-0.00442500
H	1.15933400	2.13645100	-0.82072200

N	0.89093700	-2.09019200	-2.53766200
H	0.93037300	-1.59810200	-3.42878700
H	1.54626600	-2.86906200	-2.58241500
N	-1.20766300	1.52066000	0.00429500
H	-1.15942600	2.13651700	0.82053900
H	-1.15108000	2.14942400	-0.80110600
N	-2.43126800	-0.45710200	1.58895500
H	-3.14861500	-1.15173900	1.81486100
H	-2.34998600	0.09408900	2.44830700
N	-0.89092200	-2.08987400	2.53790000
H	-0.93038900	-1.59764800	3.42895100
H	-1.54623700	-2.86874800	2.58276400
H	1.15093400	2.14950100	0.80091400
Li	3.06473600	0.72930500	-0.13425400
Li	-3.06476900	0.72933000	0.13419100
C	-5.78106200	-1.12953200	-0.53770600
O	-4.86226500	-0.50466900	-0.29439400
C	4.17162400	2.15176500	2.68840000
O	3.74788200	1.70891800	1.73032600
C	-4.99765100	2.81165100	1.68391400
O	-4.26123800	2.10464900	1.18003100
C	4.99761900	2.81170900	-1.68386600
O	4.26127800	2.10450600	-1.18015900
C	-4.17142300	2.15154600	-2.68862300
O	-3.74779500	1.70882300	-1.73044100
C	5.78100300	-1.12961200	0.53767100
O	4.86223800	-0.50468400	0.29440100

11.$(Li^+)_2$-$(CO)_7$

E= -1530.24559457

C	0.59402700	-3.22942200	-0.17134300
H	0.78512300	-3.89706900	0.67114100
H	0.58229100	-3.82831700	-1.08395200
C	1.70174000	-2.16295600	-0.23618200
H	2.68131800	-2.65573800	-0.31754300
C	-0.76351100	-2.52380700	-0.00762100
H	-1.56807900	-3.27310500	0.00338100
C	-0.78776500	-1.75140200	1.32984200
C	1.66218100	-1.33502200	1.06344800
H	2.47977400	-0.61004700	1.12230900
H	1.81089600	-2.00916200	1.90834200
C	0.29306800	-0.63001100	1.22902400
H	0.29090100	-0.04421900	2.16437200
C	0.09327600	0.33427500	0.02930000
C	1.48956400	-1.27369000	-1.48189900
C	-0.97576000	-1.57740800	-1.20507700
H	-0.95031800	-2.16719500	-2.12212900
H	-1.96189700	-1.10295800	-1.18794800
C	0.14525700	-0.50995900	-1.27221400
H	-0.02970200	0.15357400	-2.13673900

N	2.64450800	-0.33490300	-1.61487900
H	3.44907200	-0.90789800	-1.88349200
H	2.47857700	0.24932000	-2.43954800
N	1.17228200	1.35766300	0.07720300
H	1.03467600	2.00462000	-0.70398900
N	1.34324200	-2.11156000	-2.65681600
H	1.29780000	-1.56884100	-3.51775400
H	2.10634700	-2.78029300	-2.74905400
N	-1.21733400	1.02603400	0.07584100
H	-1.25399100	1.60734600	0.91751600
H	-1.25838200	1.69629800	-0.69583300
N	-2.15487100	-1.18626300	1.54089000
H	-2.76832700	-1.98564400	1.72159100
H	-2.14918000	-0.68088000	2.43170200
N	-0.40258000	-2.63931100	2.41069800
H	-0.49811300	-2.20085700	3.32534900
H	-0.95352300	-3.49638000	2.41718800
H	1.02999900	1.92744700	0.91530600
Li	3.11203400	0.83144700	-0.08838400
Li	-2.94957800	0.00477200	0.16326500
C	-5.55091400	-1.96530800	-0.49030500
O	-4.65537000	-1.30392900	-0.25696300
C	4.02262000	2.16547300	2.86413300
O	3.64719100	1.74232700	1.87758700
C	-4.88922200	1.92978000	1.92633500
O	-4.18439700	1.25933600	1.33631100
C	-3.01250000	4.81854400	-0.19868400
O	-2.71762700	3.72218800	-0.14421900
C	-4.23379300	1.56534700	-2.49675700
O	-3.75007000	1.02371800	-1.62205600
C	6.10399600	-0.57417600	0.39762000
O	5.08361300	-0.09813900	0.23627400
C	4.65441600	3.32766000	-1.48459800
O	4.06423000	2.48352700	-1.00012700

11.$(Li^{+})_2$-$(CO)_8$

E= -1643.52638658

C	-0.56743500	-2.96475100	0.72700600
H	-0.87383100	-3.71090600	-0.00885800
H	-0.54058200	-3.44458900	1.70736500
C	-1.57391000	-1.80082900	0.71936800
H	-2.58466000	-2.18515800	0.91931000
C	0.83010200	-2.41479900	0.39126400
H	1.56519400	-3.23168100	0.42887800
C	0.81916100	-1.82200800	-1.03515500
C	-1.55805000	-1.14215100	-0.67309000
H	-2.31344300	-0.35683200	-0.77067800
H	-1.82925800	-1.89373300	-1.41538500
C	-0.14936400	-0.59864200	-1.01270500

H	-0.16510500	-0.13599700	-2.01491900
C	0.22200100	0.48355600	0.03615000
C	-1.19838500	-0.78783300	1.82436300
C	1.20573100	-1.35134500	1.44222900
H	1.19245600	-1.81962400	2.42762900
H	2.22453000	-0.97387700	1.31109000
C	0.18793100	-0.18498500	1.43703400
H	0.47976600	0.56074000	2.19679100
N	-2.25660200	0.26325600	1.90408500
H	-3.09016400	-0.19848400	2.27797700
H	-1.99040400	0.91924800	2.64409000
N	-0.76224700	1.59073900	-0.07885800
H	-0.51506000	2.31322400	0.60275200
N	-1.03956000	-1.48480200	3.08706900
H	-0.88505500	-0.84623800	3.86572800
H	-1.85055200	-2.05932200	3.31128400
N	1.58476600	1.03071600	-0.17860700
H	1.61413000	1.49376700	-1.09093600
H	1.74141400	1.78609200	0.49326700
N	2.20742200	-1.41985100	-1.40786200
H	2.73430200	-2.28856600	-1.53309900
H	2.17533300	-1.01817100	-2.34943300
N	0.27699100	-2.79834200	-1.96269000
H	0.35186300	-2.49288700	-2.93169300
H	0.74408400	-3.70049100	-1.88403700
H	-0.63195800	2.03682800	-0.99058200
Li	-2.72994500	1.28576700	0.27710100
Li	3.20369000	-0.16894800	-0.23597100
C	5.43819600	-2.42973700	0.77290500
O	4.68112900	-1.66447700	0.40559200
C	-3.79044900	2.04025700	-2.77868800
O	-3.35266000	1.86440100	-1.74397000
C	5.38416500	0.98516100	-2.35256800
O	4.60199800	0.58205600	-1.63148700
C	3.86105200	4.48321800	-0.83077800
O	3.41190300	3.45198900	-0.66830000
C	4.87865600	1.62576500	2.04972100
O	4.26965000	1.00755400	1.31533400
C	-5.24025900	-2.54209300	-2.04342600
O	-4.68753800	-1.72119300	-1.48681100
C	-5.95566300	0.45120300	0.43654800
O	-4.86101200	0.75741200	0.40834300
C	-3.68121600	4.23208200	1.32376000
O	-3.27887200	3.22872900	0.96811100

CO

E=-113.27699443

C	0.00000000	0.00000000	-0.64624400

O 0.00000000 0.00000000 0.48468300

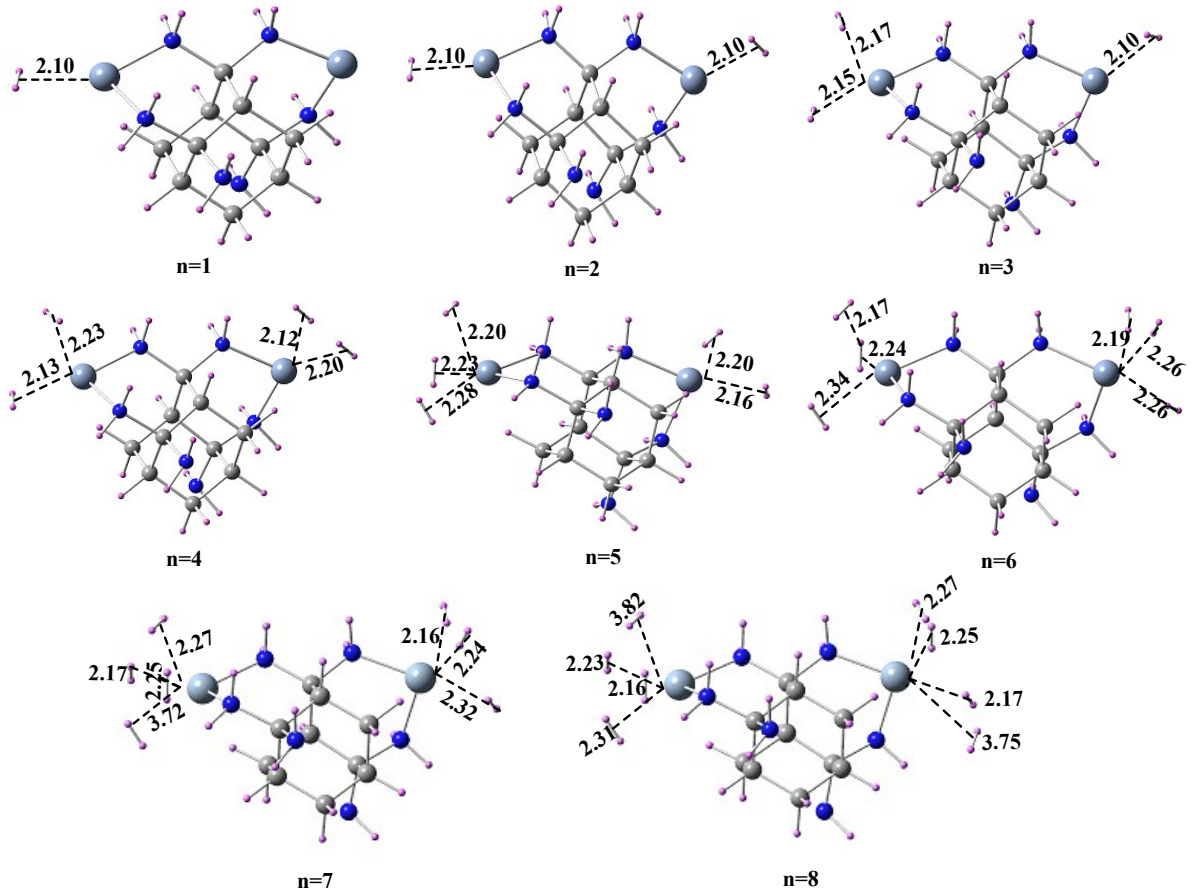

Figure S1: Optimized geometries of sequential adsorption of H_2 molecules (**n=1-8**) with lithiated adamantane **8** at M06-2X/6-31+G(d) level of theory. Distances are given in Å. (Colour of atoms: grey-C, pink-H, blue-N and sky blue-lithium)

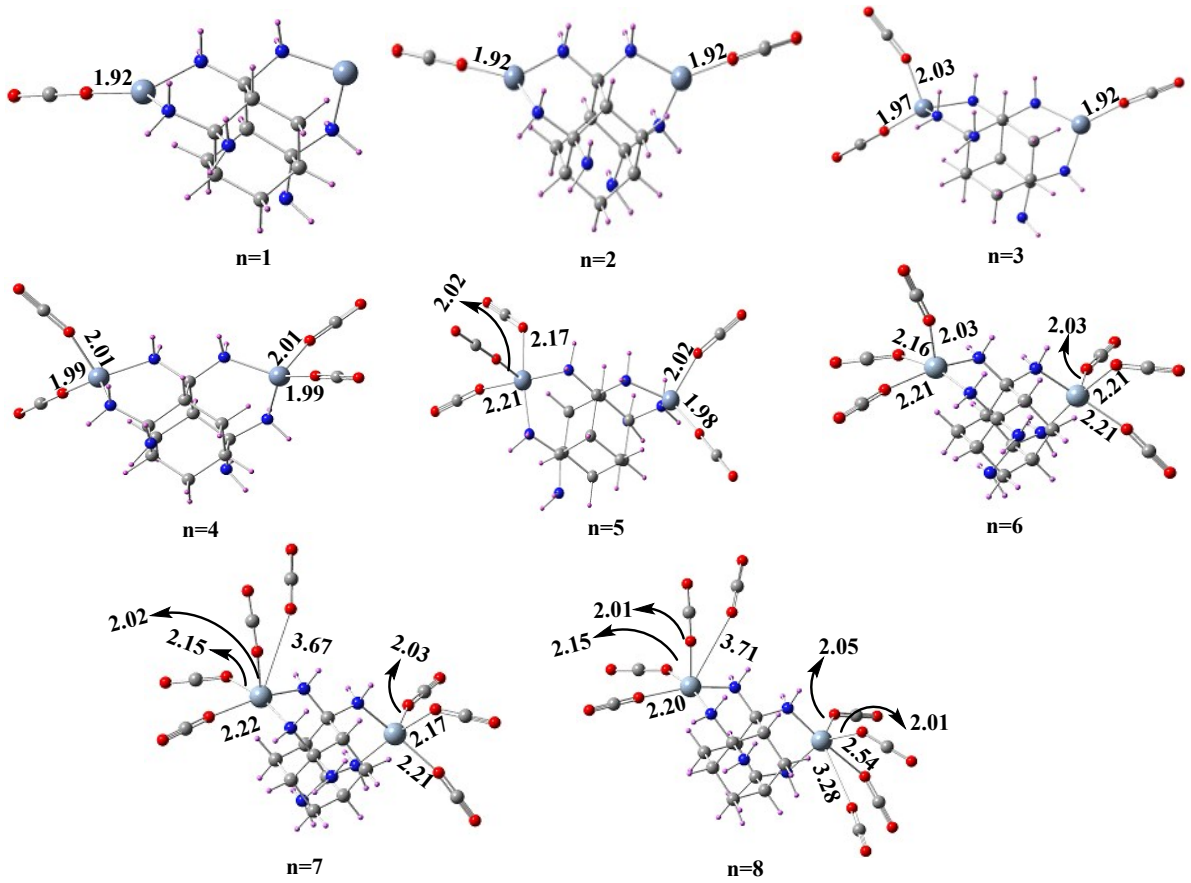

Figure S2: Optimized geometries of sequential adsorption of CO_2 molecules (**n=1-8**) with lithiated adamantane **8** at M06-2X/6-31+G(d) level of theory. Distances are given in Å. (Colour of atoms: grey-C, pink-H, blue-N and sky blue-lithium, red-oxygen)

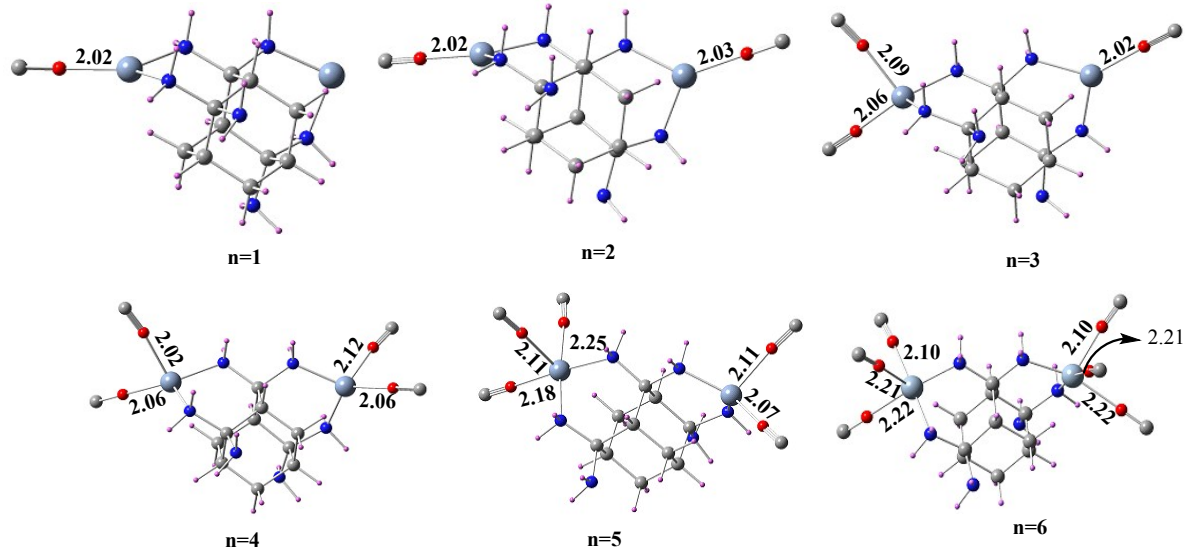

Figure S3: Optimized geometries of sequential adsorption of CO molecules (**n=1-6**) with lithiated adamantane **8** at M06-2X/6-31+G(d) level of theory. Distances are given in Å. (Colour of atoms: grey-C, pink-H, blue-N and sky blue-lithium, red-oxygen)