

The rational design of Li-doped nitrogen adsorbents for natural gas purification

*Jialuo He,^{‡a,b} Seyed Hesam Mousavi,^{‡c} Guoliang Li,^{*a} Zhikao Li,^b Abdol Hadi Mokarizadeh,^d Jin Shang,^e Eric F. May,^b Gang (Kevin) Li^{*b,c}*

^aMOE Key Laboratory of Theoretical Chemistry of Environment, School of Chemistry, South China Normal University, Guangzhou 510006, P. R. China

^bCentre for Energy, Department of Chemical Engineering, The University of Western Australia, 35 Stirling Highway, Crawley, Western Australia 6009, Australia

^cDepartment of Chemical Engineering, The University of Melbourne, Parkville, Victoria 3010, Australia

^dDepartment of Polymer Science, University of Akron, Akron, OH 44325, USA

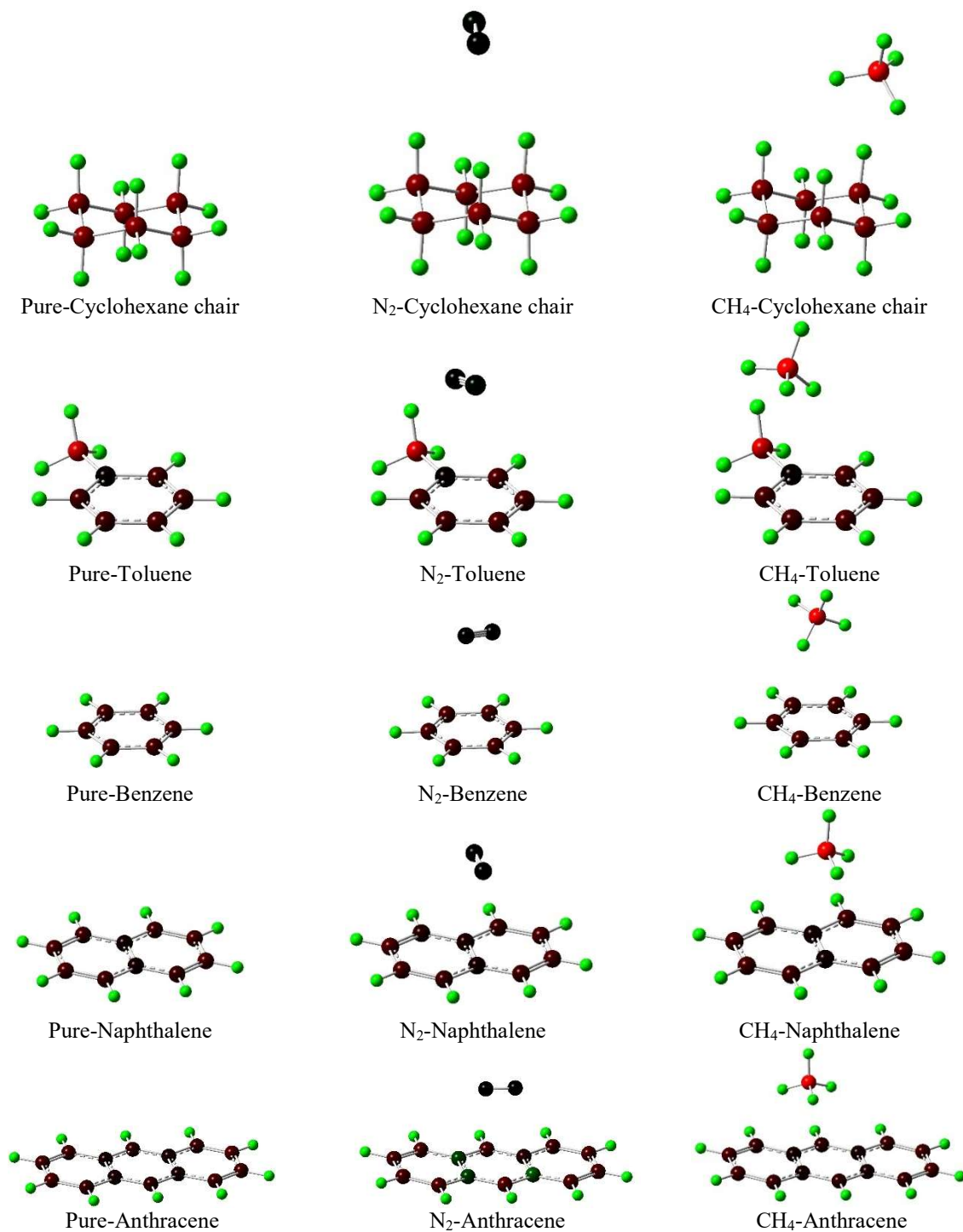
^eSchool of Energy and Environment, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong SAR, P. R. China

[‡]These authors contributed equally to this work

e-mails: glli@scnu.edu.cn and li.g@unimelb.edu.au

Supporting Information

Fig. S1. Optimized structures and graphical NBO charge distributions of N_2 and CH_4 complexes with pure organic molecular systems.



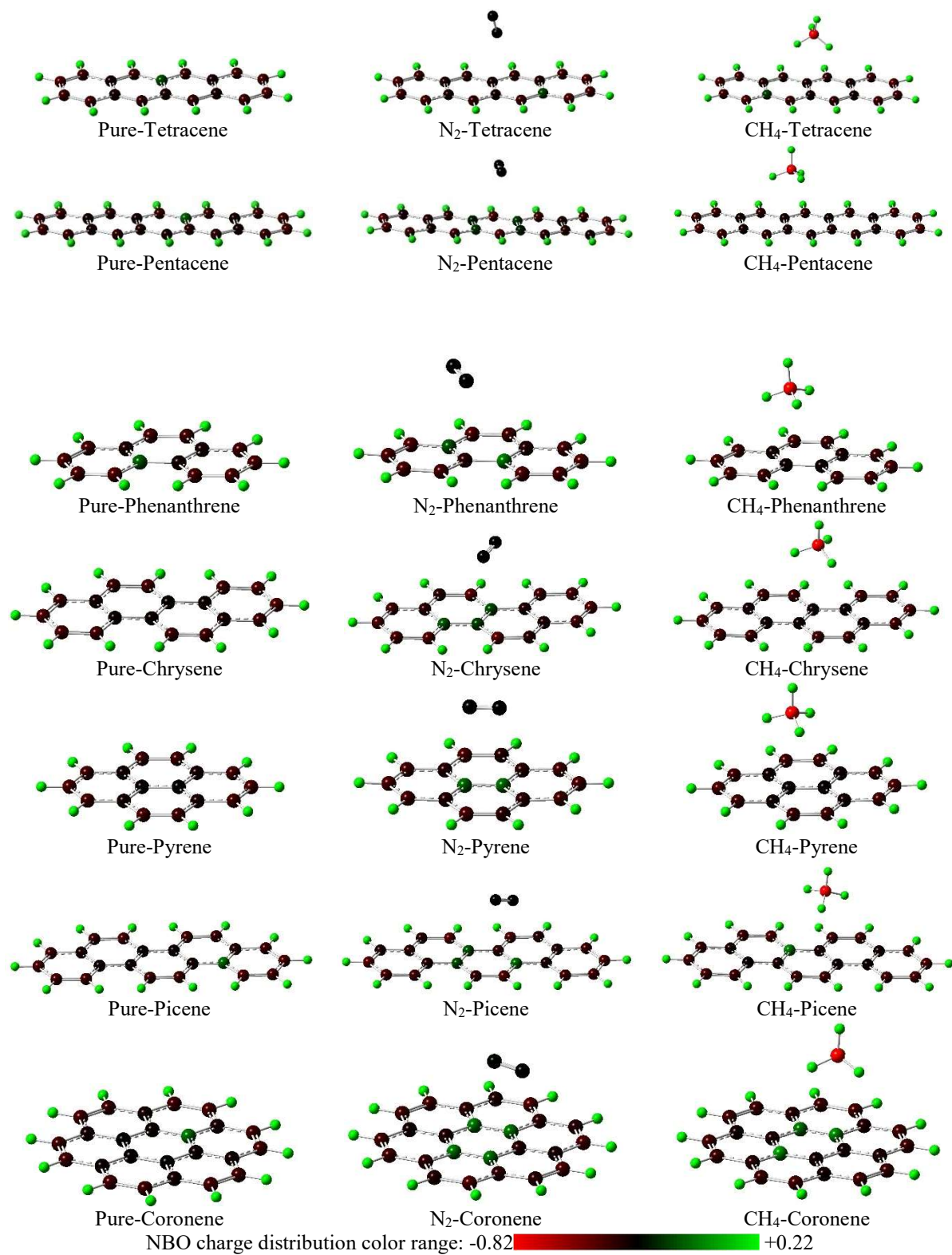


Table S1. Cartesian coordinates for optimized geometries of N₂/CH₄ adsorbed on the Li-free/Li-doped organic molecular systems at the M06/6-311++G(d,p) level.

N₂-Cyclohexane chair

C	-1.29478600	-0.61528600	-1.25623000
C	-0.56728900	0.72286900	-1.25763300
C	-0.88211100	1.52275200	0.00001300
C	-0.56729400	0.72286000	1.25765400
C	-1.29479000	-0.61529400	1.25623800
C	-0.97368500	-1.41480700	0.00000200
H	-0.33114400	2.47087700	0.00001700
H	0.51763700	0.54212600	-1.30846900
H	-0.82581300	1.29987200	-2.15350500
H	-2.38011200	-0.43382800	-1.29912500
H	-1.04078900	-1.19136400	-2.15397800
H	0.51763300	0.54211600	1.30849400
H	-0.82582100	1.29985700	2.15352900
H	-1.04079700	-1.19137900	2.15398300
H	-2.38011700	-0.43383700	1.29913100
H	0.09688000	-1.67277000	0.00000300
H	-1.52065600	-2.36514300	-0.00000200
H	-1.95178300	1.78437400	0.00001200
N	3.37156400	0.33096500	-0.00003700
N	3.00623800	-0.70088900	-0.00001300

N₂-Toluene

C	-1.12932900	-0.29914900	0.00031200
C	-0.47799300	-0.59321700	1.19636100
C	0.79277100	-1.15066900	1.19904300
C	1.43477800	-1.42822200	-0.00038900
C	0.79232500	-1.15014500	-1.19954600
C	-0.47835900	-0.59273100	-1.19615700
H	-0.97655200	-0.37742300	2.13890700
H	1.28374800	-1.37171200	2.14225900
H	2.42874400	-1.86474100	-0.00065900
H	1.28299100	-1.37077900	-2.14302100
H	-0.97729500	-0.37649700	-2.13842200
C	-2.47885000	0.34919300	0.00025200
H	-3.05437700	0.07979100	0.89069200

CH₄-Cyclohexane chair

C	0.07566700	1.14629500	0.77698700
C	0.21042700	-0.20004200	1.47710700
C	0.24377400	-1.34607500	0.47374800
C	1.34492000	-1.14337700	-0.55881500
C	1.19714100	0.19972900	-1.26160200
C	1.17702100	1.34378600	-0.25628900
H	0.37375200	-2.30423500	0.99099300
H	1.14249800	-0.20864300	2.06356000
H	-0.60760100	-0.34207200	2.19429300
H	-0.90166600	1.19375400	0.27258800
H	0.08625100	1.96169600	1.51014100
H	2.32320200	-1.17867500	-0.05435000
H	1.34225700	-1.96209400	-1.28826700
H	2.00299300	0.34266600	-1.99136100
H	0.25508600	0.20568600	-1.83260400
H	2.15022500	1.38711000	0.25730300
H	1.05388400	2.30496700	-0.76948500
H	-0.72682700	-1.40066900	-0.04318200
C	-3.39893900	-0.00023800	-0.52170700
H	-3.53865300	1.07695500	-0.41720600
H	-3.06951200	-0.41801100	0.43169000
H	-4.34234700	-0.46282300	-0.81538300
H	-2.64361000	-0.19608900	-1.28530100

CH₄-Toluene

C	-0.39309000	-0.96172100	0.10718500
C	0.05632200	-0.28474400	1.23838900
C	1.22143400	0.46827100	1.20368400
C	1.96071400	0.55522300	0.03194500
C	1.52881800	-0.12243700	-1.10032300
C	0.36366900	-0.87541400	-1.05945000
H	-0.52149900	-0.34595900	2.15819700
H	1.55422900	0.98943700	2.09659200
H	2.87270900	1.14342900	0.00284900
H	2.10422700	-0.06694500	-2.01974800
H	0.02963300	-1.40482600	-1.94929500
C	-1.68064600	-1.72588100	0.12962600
H	-1.91013200	-2.09904200	1.13194600

H	-2.38292700	1.44190100	-0.00922700
H	-3.06117500	0.06525400	-0.88126300
N	1.59558300	2.29167500	0.00082400
N	0.50795800	2.41744400	-0.00061300

N₂-Benzene

C	1.02057800	-1.10323800	-0.75258100
C	0.84786400	0.12021500	-1.38678100
C	0.67875600	1.27459700	-0.63355300
C	0.68619600	1.20608700	0.75372100
C	0.86304700	-0.01664000	1.38789900
C	1.02877800	-1.17166700	0.63471700
H	1.15062300	-2.00654700	-1.34106000
H	0.84303200	0.17377000	-2.47137600
H	0.53990300	2.23092700	-1.12884400
H	0.55290500	2.10896100	1.34215600
H	0.87007000	-0.06988900	2.47249800
H	1.16492800	-2.12835200	1.13004400
N	-2.57415700	-0.70191400	-0.00310200
N	-2.55052500	0.39262800	-0.00031800

N₂-Naphthalene

C	-2.41881100	-0.54467600	0.70527600
C	-1.23728100	-0.56904800	1.39522300
C	-0.00002000	-0.58457600	0.71118500
C	-0.00001800	-0.58484800	-0.71100600
C	-1.23727900	-0.56958200	-1.39505000
C	-2.41881000	-0.54494700	-0.70511500
H	1.23125200	-0.56598200	2.48249300
H	-3.36256400	-0.52544400	1.24161100
H	-1.23129200	-0.56593500	2.48249100
C	1.23724200	-0.56909400	1.39522400
C	1.23724400	-0.56962600	-1.39504900
H	-1.23129000	-0.56688700	-2.48232000
H	-3.36256300	-0.52592100	-1.24145700
C	2.41877500	-0.54503300	-0.70511200
C	2.41877300	-0.54476400	0.70527900

H	-2.51716100	-1.08662400	-0.17994900
H	-1.65439700	-2.57919000	-0.55458500
C	-1.83086100	2.31324500	-0.40035900
H	-1.11753300	2.95896300	0.11421700
H	-2.39942200	2.89926500	-1.12430900
H	-1.28589000	1.51671800	-0.91146100
H	-2.51291900	1.87551900	0.33136600

CH₄-Benzene

C	-0.86578700	-1.05802100	-0.81429300
C	-0.59402000	-1.30916200	0.52440300
C	-0.41738900	-0.25200000	1.40728200
C	-0.51311700	1.05628300	0.95157400
C	-0.78462900	1.30761900	-0.38713600
C	-0.96057000	0.25049700	-1.27029600
H	-1.00506400	-1.88511000	-1.50415900
H	-0.51933900	-2.33212800	0.88106400
H	-0.20468200	-0.44810000	2.45398800
H	-0.37543700	1.88325800	1.64193800
H	-0.85962900	2.33061600	-0.74367800
H	-1.17326900	0.44656600	-2.31698800
C	2.89613100	0.00326100	-0.28866500
H	3.74145300	0.05133400	-0.97705600
H	2.43261600	0.98761500	-0.20499800
H	2.15556800	-0.70652600	-0.66170400
H	3.24406800	-0.31839700	0.69438000

CH₄-Naphthalene

C	-2.42091200	-0.66247000	-0.50325300
C	-1.23904100	-0.92877400	-1.13972700
C	-0.00151500	-0.67850800	-0.50332800
C	-0.00145700	-0.14752300	0.81579800
C	-1.23893100	0.11457800	1.44754200
C	-2.42085600	-0.13471200	0.80459100
H	1.23013800	-1.33967300	-2.14662400
H	-3.36483700	-0.85757500	-1.00301500
H	-1.23328200	-1.33515400	-2.14826200
C	1.23599600	-0.93248000	-1.13840200
C	1.23612500	0.11050700	1.44901200
H	-1.23298900	0.52191800	2.45574700
H	-3.36468700	0.07254700	1.29955600
C	2.41804900	-0.14123600	0.80699100
C	2.41804600	-0.66881100	-0.50095600

H	1.23125600	-0.56692900	-2.48231900
H	3.36252900	-0.52603900	-1.24145400
H	3.36252700	-0.52556800	1.24161500
N	0.00008100	2.72337700	0.54702500
N	0.00009800	2.72317600	-0.54785300

N₂-Anthracene

C	3.66509100	-0.49169100	-0.58644500
C	2.49146900	-1.09883100	-0.91309900
C	1.24421000	-0.45670400	-0.67311500
C	1.24571000	0.84865300	-0.07775100
C	2.49508200	1.44995000	0.24368800
C	3.66688200	0.80174000	-0.00029900
C	0.02791700	-1.06086900	-0.98098200
C	0.03081700	1.48068300	0.17659000
C	-1.18590800	0.86747700	-0.11252000
C	-1.18719700	-0.43733800	-0.70916100
C	-2.43658600	-1.06287200	-0.97974400
H	-2.43237400	-2.05261700	-1.42964800
C	-3.60950500	-0.44276500	-0.67546100
C	-3.60830200	0.84976700	-0.08743900
C	-2.43439400	1.48466500	0.18044300
H	0.02627700	-2.05371800	-1.42782200
H	4.60935600	-0.99407800	-0.77236700
H	2.48489600	-2.08888500	-1.36226900
H	2.49167800	2.44004100	0.69282700
H	4.61262800	1.27090400	0.25286500
H	0.03207800	2.47110400	0.62866100
H	-4.55560900	-0.93388800	-0.88109100
H	-4.55359600	1.32944200	0.14705100
H	-2.42882300	2.47415200	0.63090700
N	-0.74156800	-1.29768200	2.46536300
N	0.35325000	-1.30998300	2.49073200

N₂-Tetracene

C	0.01821100	0.84433800	-0.08854900
C	0.01755300	-0.47139200	-0.67834300

H	1.23030100	0.51754600	2.45734400
H	3.36192800	0.06350100	1.30288700
H	3.36188100	-0.86602600	-1.00002800
C	0.00993700	2.76484600	-1.04544800
H	0.04926100	3.04101800	0.00974000
H	0.09423300	3.66139000	-1.66209500
H	0.83338400	2.08396800	-1.27014600
H	-0.93797800	2.26403800	-1.25203000

CH₄-Anthracene

C	-3.49488800	0.73504500	-0.53410800
C	-2.32208100	1.42078200	-0.44396900
C	-1.07625700	0.73495500	-0.38808500
C	-1.07768800	-0.69856500	-0.43420400
C	-2.32504800	-1.37673400	-0.53247000
C	-3.49638200	-0.68449300	-0.57850900
C	0.13727000	1.40968800	-0.28075000
C	0.13453600	-1.38128300	-0.37077500
C	1.34823400	-0.70700800	-0.25966300
C	1.34960000	0.72700600	-0.21325100
C	2.59617200	1.40450900	-0.09860900
H	2.59227600	2.49116800	-0.06431800
C	3.76596600	0.71140400	-0.03344200
C	3.76458700	-0.70797900	-0.07944000
C	2.59338200	-1.39302800	-0.18922600
H	0.13824400	2.49778600	-0.24461700
H	-4.43834000	1.27081100	-0.57353300
H	-2.31578100	2.50747800	-0.40929300
H	-2.32119200	-2.46351700	-0.56591000
H	-4.44103400	-1.21468800	-0.65041000
H	0.13317900	-2.46951600	-0.40443600
H	4.70962300	1.24107100	0.05389800
H	4.70714700	-1.24410200	-0.02655700
H	2.58720100	-2.47962600	-0.22502700
C	-1.27367300	-0.13001900	2.97389100
H	-2.04228000	0.38334700	2.39226800
H	-1.34361600	-1.20423600	2.79397800
H	-0.28893500	0.22483900	2.66334400
H	-1.41887100	0.07351500	4.03626700

CH₄-Tetracene

C	0.00158300	-0.71740300	-0.28385100
C	0.00157800	0.72423400	-0.27272900

C	-2.41673300	0.83592900	-0.06795900
C	-2.41723900	-0.47827700	-0.66098000
C	2.45215300	0.82164500	-0.04087600
C	2.45164100	-0.49473700	-0.62940100
C	1.24591000	1.45408800	0.20744200
C	1.24494900	-1.09900700	-0.93768100
C	-1.20928000	1.45959500	0.19721400
C	-1.21042500	-1.09035500	-0.95440000
C	-3.67115800	1.45038000	0.22659000
C	-3.67196800	-1.10614900	-0.92427100
C	3.70684600	1.42903500	0.26685700
C	3.70544800	-1.13163800	-0.87481600
C	-4.84148600	0.81575500	-0.04191900
C	-4.84188500	-0.48415600	-0.62612300
C	4.87620300	0.78569900	0.01576100
C	4.87550700	-0.51633600	-0.56387300
H	1.24816500	2.44827300	0.65086900
H	1.24487300	-2.09280200	-1.38210700
H	-1.20946600	2.45098500	0.64695800
H	-1.21145700	-2.08446200	-1.39816000
H	-3.66639000	2.44263700	0.67086500
H	-3.66777900	-2.09765200	-1.37025300
H	3.70314400	2.42285300	0.70766800
H	3.70026000	-2.12450800	-1.31772200
H	-5.78794600	1.29610100	0.18641400
H	-5.78851000	-0.97465000	-0.83099100
H	5.82290800	1.26028700	0.25489600
H	5.82151300	-1.01345600	-0.75519700
N	-0.00200900	-1.14424200	2.48770200
N	-0.29724800	-1.72434600	3.36782800

N₂-Pentacene

C	3.65601200	-0.72254200	-0.27941100
C	4.91329200	-1.40301800	-0.26621100
C	6.08154300	-0.71365400	-0.25397000
C	6.08155200	0.71402800	-0.25388100
C	4.91330800	1.40340700	-0.26603200
C	3.65602000	0.72294700	-0.27930300
C	1.21927900	-0.72311500	-0.30352400

C	2.43681500	-0.71766100	-0.26740300
C	2.43679500	0.72410000	-0.25699900
C	-2.43372600	-0.71758200	-0.27016700
C	-2.43376300	0.72417100	-0.25957000
C	-1.22670300	-1.39557800	-0.28424900
C	-1.22665900	1.40247500	-0.26349400
C	1.22981300	-1.39567600	-0.28237400
C	1.22975300	1.40242400	-0.26207600
C	3.69147700	-1.39874100	-0.26111900
C	3.69153300	1.40496200	-0.24121500
C	-3.68837300	-1.39871000	-0.26477800
C	-3.68851800	1.40502600	-0.24484700
C	4.86160100	-0.70955400	-0.24587100
C	4.86160800	0.71551800	-0.23582100
C	-4.85850900	-0.70954900	-0.25042800
C	-4.85855000	0.71552500	-0.24044900
H	-1.22715800	-2.48418900	-0.29124000
H	-1.22697900	2.49103700	-0.25466000
H	1.23022000	-2.48428100	-0.28919800
H	1.23009300	2.49096800	-0.25316600
H	3.68678800	-2.48587800	-0.26884100
H	3.68694300	2.49210500	-0.23384900
H	-3.68364000	-2.48584400	-0.27241900
H	-3.68399000	2.49216900	-0.23755000
H	5.80812500	-1.24120700	-0.24123900
H	5.80815000	1.24703400	-0.22385700
H	-5.80503100	-1.24120700	-0.24640200
H	-5.80511400	1.24702000	-0.22931900
C	-0.01853500	-0.03835100	3.11746200
H	-0.85051000	0.43188400	2.58903900
H	-0.07768000	-1.12099100	2.99303100
H	0.92406400	0.32249600	2.70081500
H	-0.06959100	0.21109500	4.17872700

CH₄-Pentacene

C	3.73079200	-0.69211200	-0.21299400
C	4.98659700	-1.37500900	-0.24276700
C	6.15594900	-0.69309800	-0.15475200
C	6.15864100	0.72911500	-0.02965300
C	4.99199800	1.42046200	0.00336500
C	3.73350600	0.74778200	-0.08613700
C	1.29432100	-0.68292600	-0.27060500

C	2.45368400	-1.40059500	-0.29146200
C	2.45369900	1.40101500	-0.29114300
C	1.21928500	0.72355200	-0.30318700
C	-1.21907100	-0.72317400	-0.30380100
C	0.00011700	-1.40090400	-0.30484300
C	0.00010400	1.40129500	-0.30378800
C	-1.21905200	0.72349900	-0.30298900
C	-3.65580500	-0.72257300	-0.28000400
C	-4.91309800	-1.40303600	-0.26733800
C	-6.08133800	-0.71365900	-0.25472400
C	-6.08132200	0.71402300	-0.25369800
C	-4.91306600	1.40338900	-0.26533500
C	-3.65579000	0.72291600	-0.27899500
C	-2.45348800	-1.40063800	-0.29232500
C	-2.45345800	1.40097100	-0.29049100
H	4.90887700	-2.49013800	-0.26612500
H	7.02850600	-1.24440800	-0.24407200
H	7.02852000	1.24477000	-0.24391600
H	4.90890600	2.49052700	-0.26579900
H	2.45425700	-2.48904300	-0.29033000
H	2.45428200	2.48946300	-0.28972200
H	0.00015400	-2.48926300	-0.29933400
H	0.00006800	2.48964800	-0.29758000
H	-4.90870200	-2.49015600	-0.26795300
H	-7.02831000	-1.24440300	-0.24523300
H	-7.02828200	1.24477400	-0.24344200
H	-4.90864400	2.49050900	-0.26440000
H	-2.45407600	-2.48908700	-0.29179900
H	-2.45402800	2.48941800	-0.28853600
N	-0.00029200	-0.54957200	2.92240700
N	-0.00198800	0.54565600	2.92287400

N₂-Phenanthrene

C	3.68107300	-0.27461900	-0.04882300
C	2.95851900	0.89025400	-0.12197800
C	1.55997600	0.86822400	-0.27547400
C	0.88353600	-0.37303900	-0.35982600
C	1.65077200	-1.54965400	-0.27864700
C	3.01687200	-1.50502700	-0.12752600

C	2.52755400	-1.36249400	-0.30142700
C	2.53294400	1.42798800	-0.05500600
C	1.29704100	0.75836400	-0.14290700
C	-1.14281100	-0.67377900	-0.31869400
C	0.07435200	-1.35307800	-0.35751700
C	0.07953300	1.43830900	-0.11063100
C	-1.14027900	0.76718700	-0.19253700
C	-3.57972100	-0.66824600	-0.33425200
C	-4.83835600	-1.34354400	-0.39835700
C	-6.00553400	-0.65433200	-0.34456600
C	-6.00310400	0.76809100	-0.22228700
C	-4.83363800	1.45243900	-0.15755000
C	-3.57725700	0.77193800	-0.20972100
C	-2.37828400	-1.34598300	-0.38723500
C	-2.37372200	1.44489300	-0.14428500
H	4.98010700	-2.45795300	-0.33810800
H	7.10166700	-1.22562400	-0.17883600
H	7.10641500	1.25405900	0.03921200
H	4.98981800	2.50341900	0.09872800
H	2.52612300	-2.44676100	-0.39729700
H	2.53591300	2.51231300	0.04018400
H	0.07202700	-2.43758100	-0.45111600
H	0.08151400	2.52253300	-0.01475100
H	-4.83580600	-2.42666800	-0.49184400
H	-6.95343200	-1.18119200	-0.39437200
H	-6.94921400	1.29891800	-0.18138800
H	-4.82746600	2.53555700	-0.06424200
H	-2.38053200	-2.43062900	-0.47968500
H	-2.37284900	2.52923300	-0.04907000
C	-1.12187100	-0.58394200	3.08943900
H	-2.12429500	-0.52740400	2.66031000
H	-0.48320300	0.16487600	2.61623700
H	-1.17187300	-0.39811100	4.16366500
H	-0.70682200	-1.57714000	2.90883700

CH₄-Phenanthrene

C	3.59692400	-0.25930500	-0.20151700
C	2.88668800	0.90906200	-0.07957600
C	1.48117500	0.91477300	-0.14731900
C	0.78412100	-0.30156700	-0.34834600
C	1.53960100	-1.48252300	-0.46825500
C	2.91276700	-1.46553800	-0.39683900

C	0.81840500	2.08774500	-0.34614100
C	-0.55832100	-0.38099000	-0.50490500
C	-1.25145600	0.85199300	-0.56643000
C	-0.52550200	2.08019300	-0.48923600
C	-2.65475900	0.85809300	-0.66699800
H	-3.16734800	1.81607100	-0.70767000
C	-3.36717500	-0.31502100	-0.70149400
C	-2.68662600	-1.53772500	-0.64385700
C	-1.31475600	-1.56640300	-0.55179000
H	1.36456000	3.02536800	-0.28030500
H	4.75959700	-0.24475300	0.07020200
H	3.45805600	1.85406900	-0.06119400
H	1.16413400	-2.51749500	-0.33570900
H	3.58243000	-2.42986400	-0.06846500
H	-1.08418500	3.01136100	-0.53884300
H	-4.45019300	-0.29736400	-0.77229500
H	-3.24403600	-2.46898400	-0.67073600
H	-0.81605300	-2.52853800	-0.50197300
N	-0.77352300	-0.46441200	2.64873200
N	-1.34509300	0.46098200	2.77494500

N₂-Chrysene

C	3.78833500	-1.13022300	-0.32269600
C	4.65457600	-0.06910000	-0.27814900
C	4.14498900	1.23761100	-0.26200700
C	2.78991700	1.45888000	-0.28986400
C	1.87092500	0.38966500	-0.33745700
C	2.39444000	-0.92683900	-0.35275900
C	1.49819500	-2.02797100	-0.39956800
C	0.43917300	0.57947100	-0.35698100
C	-0.41660500	-0.53626000	-0.40251600
C	0.15574500	-1.84025400	-0.42869000
C	-3.76648500	1.16742500	-0.27564500
C	-4.63267500	0.10594200	-0.31257300
C	-4.12290000	-1.19877900	-0.38509600
C	-2.76760800	-1.41770200	-0.41880400
C	-0.13339100	1.88231000	-0.29829100
C	-1.47602200	2.06809600	-0.27024700
C	-2.37229900	0.96663000	-0.30908800

C	0.75227900	2.13611600	-0.00880200
C	-0.66364100	-0.28358200	-0.40548800
C	-1.34360500	0.94917500	-0.25555600
C	-0.59830800	2.15232700	-0.05961300
C	-2.75007500	0.97683400	-0.28731400
H	-3.25258500	1.93359300	-0.16765700
C	-3.47733700	-0.17466100	-0.46142100
C	-2.80960700	-1.39624900	-0.61538000
C	-1.43564800	-1.44517700	-0.58977700
H	1.31333700	3.05493100	0.14229400
H	4.68095000	-0.25083900	-0.14605500
H	3.40182100	1.85416100	0.07424700
H	1.03789100	-2.43262600	-0.61904500
H	3.46848800	-2.39334600	-0.49218400
H	-1.14699500	3.08433200	0.05036800
H	-4.56212300	-0.14076700	-0.48158100
H	-3.37872100	-2.31018900	-0.75509600
H	-0.94664000	-2.40649000	-0.70766600
C	-0.58723300	-0.73694900	2.90639300
H	-0.19950800	-1.68290500	2.52287100
H	-0.71427900	-0.80505700	3.98825500
H	0.11828200	0.06214500	2.66955300
H	-1.54852500	-0.52335400	2.43455500

CH₄-Chrysene

C	3.81723600	-1.08914400	-0.29675500
C	4.68357000	-0.03531500	-0.16476200
C	4.17405600	1.26585800	-0.04298900
C	2.81898800	1.48864300	-0.05551200
C	1.89965300	0.42684600	-0.18970700
C	2.42333600	-0.88425600	-0.31184500
C	1.52718000	-1.97801300	-0.44895200
C	0.46794900	0.61889200	-0.20373700
C	-0.38765500	-0.49026800	-0.33570900
C	0.18497300	-1.78819600	-0.46178900
C	-3.73871500	1.20848800	-0.17586300
C	-4.60450900	0.15183400	-0.28657700
C	-4.09368800	-1.14794200	-0.41790400
C	-2.73794800	-1.36615800	-0.43885300
C	-0.10526300	1.91606000	-0.07235700
C	-1.44826200	2.10315600	-0.06718200
C	-2.34418400	1.00781100	-0.19211400

C	-1.84850800	-0.34786600	-0.38311500
H	4.16289700	-2.15080500	-0.33597400
H	5.72701300	-0.23509100	-0.25546800
H	4.82630400	2.08218500	-0.22642400
H	2.43330700	2.48262800	-0.27623700
H	1.91293000	-3.03278200	-0.41249100
H	-0.49094600	-2.70936400	-0.46237600
H	-4.14143000	2.18640700	-0.21955100
H	-5.70529500	0.27015100	-0.28599400
H	-4.80417600	-2.04361500	-0.41431000
H	-2.41076400	-2.43993300	-0.47507600
H	0.51346100	2.75117000	-0.26305600
H	-1.89102900	3.07142200	-0.21648500
N	-0.44966700	-0.58243500	2.95252600
N	0.25951200	0.23977800	2.81100400

N₂-Pyrene

C	3.50290500	0.00512700	-0.33397900
C	2.81707700	-1.19961100	-0.35070000
C	1.42158400	-1.22534200	-0.38472200
C	0.70931100	0.00118900	-0.40761100
C	1.41801100	1.22981800	-0.38425400
C	2.81359800	1.20794100	-0.34976600
C	0.67988400	-2.44969800	-0.37367200
C	-0.71002000	-0.00091200	-0.40687900
C	-1.41871600	-1.22952600	-0.38348700
C	-0.67339700	-2.45174100	-0.37299100
C	-2.81429900	-1.20776900	-0.34895800
H	-3.35571600	-2.15016700	-0.32915700
C	-3.50366300	-0.00499900	-0.33269600
C	-2.81784700	1.19976800	-0.34899000
C	-1.42238500	1.22554800	-0.38339100
C	-0.68066000	2.44992300	-0.37264500
C	0.67261300	2.45197000	-0.37299700
H	1.22381100	3.38892200	-0.35790000
H	-1.23461100	3.38523300	-0.35706100
H	1.23388900	-3.38498600	-0.35875400
H	4.58814900	0.00667900	-0.30355500
H	3.36122700	-2.14043400	-0.33129400

C	-1.81935200	-0.30100100	-0.32943600
H	4.19201100	-2.10523600	-0.39266400
H	5.75594600	-0.20288200	-0.15399700
H	4.85523300	2.10474100	0.06200400
H	2.46221200	2.50798300	0.04053000
H	1.94198200	-2.97840200	-0.54353200
H	-0.46177400	-2.65175400	-0.56612900
H	-4.11442200	2.22339800	-0.07128200
H	-5.67738100	0.31582900	-0.27170600
H	-4.77444600	-1.98935700	-0.50377300
H	-2.38046600	-2.38475100	-0.54133600
H	0.54109100	2.78023800	0.02828100
H	-1.86351400	3.10260400	0.03542000
C	-0.47782000	-0.73650600	2.98392700
H	0.53295000	-0.84513500	2.58566300
H	-0.44422700	-0.73249000	4.07483000
H	-0.90886500	0.20068200	2.62613400
H	-1.09360100	-1.57020700	2.64025400

CH₄-Pyrene

C	-3.43513300	0.00502700	-0.42919300
C	-2.74693500	1.20861800	-0.40175700
C	-1.35169900	1.23132500	-0.35108300
C	-0.64257400	0.00299600	-0.32805300
C	-1.35322900	-1.22425600	-0.35888400
C	-2.74838400	-1.19948000	-0.40836400
C	-0.60856000	2.45399600	-0.30867700
C	0.77536500	0.00200600	-0.26193300
C	1.48561400	1.22929500	-0.21696800
C	0.74324500	2.45314100	-0.24473700
C	2.87979900	1.20418700	-0.14240700
H	3.42271800	2.14538400	-0.10903700
C	3.56596000	-0.00022700	-0.11002000
C	2.87825600	-1.20352700	-0.14971700
C	1.48407700	-1.22631600	-0.22408800
C	0.74032800	-2.44911400	-0.25997700
C	-0.61151500	-2.44814900	-0.32467700
H	-1.16421200	-3.38403100	-0.34983800
H	1.29153600	-3.38581700	-0.23263700
H	-1.16018700	3.39063800	-0.32703900
H	-4.52019400	0.00573700	-0.46708900
H	-3.28921700	2.15064700	-0.41772200

H	3.35511300	2.15028500	-0.32980200
H	-1.22460500	-3.38867000	-0.35759700
H	-4.58890900	-0.00657800	-0.30227500
H	-3.36198900	2.14058300	-0.32902400
N	-0.54332900	0.03963500	2.77314800
N	0.54899500	-0.04120600	2.77011700

N₂-Picene

C	-3.70052900	-1.63009200	-0.23788700
C	-2.93377100	-0.44709900	-0.24347000
C	-5.07338100	-1.59287100	-0.19920100
C	-3.62679600	0.78665200	-0.20695300
C	-1.48822700	-0.44261600	-0.28382100
C	-5.03430200	0.80196200	-0.16785300
C	-2.88284600	1.99835600	-0.21051900
C	-5.75187000	-0.36646600	-0.16421400
C	-0.78255700	0.77789000	-0.28283900
C	-1.52878600	1.99444400	-0.24587000
C	0.65623700	0.77758800	-0.30770000
C	-0.74412300	-1.64545000	-0.33090500
C	0.61629800	-1.64534100	-0.36893400
C	1.36107000	-0.44261600	-0.35064000
C	2.80697300	-0.44772800	-0.35239500
C	1.40330300	1.99322300	-0.26753500
C	3.50104900	0.78480900	-0.30120200
C	2.75770200	1.99615800	-0.26030900
C	4.90901700	0.79938700	-0.29402700
C	3.57302400	-1.63032000	-0.39654500
C	4.94651500	-1.59378000	-0.38940100
C	5.62602300	-0.36863100	-0.33705700
H	-3.20958800	-2.59662500	-0.26298600
H	-5.63596900	-2.52140400	-0.19548100
H	-5.54145100	1.76327400	-0.14056000
H	-3.42745000	2.93888500	-0.18469700
H	-6.83668600	-0.34542600	-0.13382700
H	-1.01050100	2.94553200	-0.24955100
H	-1.26032700	-2.59864300	-0.33884400
H	1.13137800	-2.59857900	-0.40412300
H	0.88572700	2.94414400	-0.23410200

H	-3.29187600	-2.14069200	-0.42895500
H	1.29542300	3.38906900	-0.21132800
H	4.65007500	-0.00105800	-0.05152300
H	3.41993800	-2.14559400	-0.12160300
C	-0.69825800	-0.02608800	2.98465500
H	-0.44823500	-1.02381000	2.61812800
H	-0.74765300	-0.03859800	4.07496300
H	0.06887600	0.68069100	2.66151300
H	-1.66513000	0.27683000	2.57744600

CH₄-Picene

C	-3.68973800	-1.68390200	-0.01166900
C	-2.91899100	-0.50979400	-0.13262900
C	-5.06265400	-1.63896900	0.01822100
C	-3.60802100	0.72324500	-0.22450400
C	-1.47320000	-0.51352500	-0.16392800
C	-5.01552500	0.74675600	-0.19096600
C	-2.85974000	1.92591700	-0.34898500
C	-5.73713200	-0.41317000	-0.07141300
C	-0.76358400	0.69699100	-0.29753000
C	-1.50566900	1.91331600	-0.38647200
C	0.67486600	0.69026400	-0.32145300
C	-0.73212400	-1.71428800	-0.05723600
C	0.62889200	-1.72009400	-0.07451100
C	1.37687000	-0.52595600	-0.20302000
C	2.82278000	-0.53372500	-0.20131400
C	1.42433100	1.89811000	-0.45148900
C	3.51985000	0.69232000	-0.32470100
C	2.77888700	1.89941600	-0.45188300
C	4.92797200	0.70427000	-0.32142100
C	3.58650300	-1.71225900	-0.07785800
C	4.95999900	-1.67831100	-0.07614700
C	5.64235400	-0.45977300	-0.19905000
H	-3.20200700	-2.64984800	0.05886800
H	-5.62834900	-2.56093200	0.11171700
H	-5.51953400	1.70745700	-0.26258400
H	-3.40096800	2.86642600	-0.41555900
H	-6.82194600	-0.38583700	-0.04656700
H	-0.98422200	2.85795200	-0.48273300
H	-1.25053400	-2.66078500	0.04548200
H	1.14166000	-2.67105200	0.01458800
H	0.90845700	2.84561500	-0.54956600

H	3.30324500	2.93573800	-0.22260300
H	5.41710400	1.75974400	-0.25387500
H	3.08134100	-2.59593100	-0.43885200
H	5.50873600	-2.52189500	-0.42471500
H	6.71126500	-0.34812200	-0.33118000
N	0.19915400	-0.38687700	3.08957200
N	1.11842200	0.11467000	2.76914800

N₂-Coronene

C	-2.95332500	-2.37924900	-0.10603500
C	-1.53917200	-2.42906000	-0.18837200
C	-0.81714400	-1.21727400	-0.24009100
C	-1.50767100	0.02288300	-0.19997300
C	-2.91621100	0.04374100	-0.11378000
C	-3.61683700	-1.18772600	-0.07099900
C	0.60020600	-1.23787600	-0.32265500
C	-0.78047100	1.24212600	-0.23787600
C	0.63686700	1.22117100	-0.32158500
C	1.32715600	-0.01879200	-0.36683600
C	1.36073600	2.43282300	-0.33398600
C	0.64697500	3.65640800	-0.28146600
C	-0.71544500	3.67650600	-0.21205800
C	-1.46637500	2.47456300	-0.18563400
C	-2.88140100	2.46654900	-0.10310700
C	-3.58005800	1.29512100	-0.06943700
H	-4.66522500	1.30406900	-0.00462100
H	-3.40393200	3.41907900	-0.06501400
H	-3.50352800	-3.31613400	-0.06908900
H	-4.70178800	-1.16494300	-0.00629000
H	1.21000800	4.58625000	-0.29554300
H	-1.24981000	4.62240000	-0.17179200
C	-0.82397400	-3.65251100	-0.21627600
C	0.53846500	-3.67235800	-0.28538600
C	1.28791000	-2.47023300	-0.33630700
H	-1.38549700	-4.58255800	-0.17722000
H	1.07433400	-4.61813100	-0.30065000
C	2.70415600	-2.46200300	-0.39660600
C	3.40241600	-1.29055300	-0.43911200
C	2.73706300	-0.03966700	-0.42337600

H	3.32603600	2.83371700	-0.55008200
H	5.43818400	1.65947800	-0.41834900
H	3.09264000	-2.67274100	0.01932900
H	5.52010600	-2.60326800	0.02122900
H	6.72764700	-0.44116200	-0.19702900
C	0.67937100	0.91550300	3.00785800
H	0.70877300	1.00972700	4.09483600
H	0.40033400	-0.10437000	2.73572000
H	-0.05716400	1.61103100	2.60007900
H	1.66311500	1.14455400	2.59323300

CH₄-Coronene

C	0.87002200	-3.64482300	-0.14609600
C	1.56951400	-2.41239500	-0.11302700
C	0.83215800	-1.20971100	-0.16183500
C	-0.58489600	-1.24854200	-0.24491000
C	-1.25646700	-2.48941700	-0.26921500
C	-0.49175000	-3.68195700	-0.22018200
C	1.50715800	0.03899100	-0.12379200
C	-1.32669400	-0.03858500	-0.28864000
C	-0.65202500	1.20982000	-0.24980700
C	0.76479100	1.24894300	-0.16530400
C	-1.39023600	2.41260000	-0.27734500
C	-2.80440200	2.34515600	-0.34576000
C	-3.45278300	1.14514800	-0.38407600
C	-2.73570700	-0.07704400	-0.35711500
C	-3.38512900	-1.33649900	-0.38181800
C	-2.67223700	-2.49927100	-0.33924300
H	-3.18398400	-3.45826800	-0.35819700
H	-4.47084500	-1.35894300	-0.43374000
H	1.44317100	-4.56783600	-0.10879600
H	-1.01509100	-4.63462100	-0.24207500
H	-3.36725800	3.27506600	-0.36596000
H	-4.53814500	1.10889100	-0.43437800
C	2.98284700	-2.34501000	-0.03038800
C	3.63147800	-1.14519000	0.00500100
C	2.91557200	0.07744800	-0.03872300
H	3.54474900	-3.27499100	0.00555700
H	4.71609800	-1.10900000	0.06937400
C	3.56371500	1.33726900	0.00143700
C	2.85054800	2.49975900	-0.03733600
C	1.43553100	2.48997900	-0.12028300

H	3.22824300	-3.41441000	-0.40567300
H	4.48869600	-1.29947300	-0.48072100
C	2.77598200	2.38270500	-0.39513200
H	3.32775600	3.31936700	-0.40351500
C	3.43912000	1.19114400	-0.43872200
H	4.52515700	1.16829500	-0.48071500
N	0.46684500	-0.05370900	3.04613400
N	1.51912400	0.00878900	2.74953500

Li-Cyclohexane chair

C	-0.12487900	1.21818000	0.77715400
C	-0.71110500	1.29190800	-0.62680900
C	-0.31830800	0.07261700	-1.45092600
C	-0.72662000	-1.21778800	-0.75233800
C	-0.13993900	-1.29115700	0.65148400
C	-0.53290400	-0.07224800	1.47590600
H	-0.76382100	0.12562500	-2.45149300
H	-1.80903500	1.34039600	-0.55637600
H	-0.39200400	2.21350700	-1.12814500
H	0.97373300	1.25894700	0.71003400
H	-0.43197200	2.08922400	1.36825900
H	-1.82505100	-1.25857800	-0.68507400
H	-0.41963600	-2.08886700	-1.34344600
H	-0.45826600	-2.21298700	1.15290100
H	0.95777700	-1.33839900	0.58051200
H	-1.62451000	-0.07278700	1.62107000
H	-0.08692300	-0.12518100	2.47626700
H	0.77336000	0.07278100	-1.59546000
Li	6.80962400	-0.00425300	-0.19862700

Li-Benzene

C	1.22309400	0.68672400	-0.15608800
C	1.22299400	-0.68684400	-0.15629200
C	-0.00013300	-1.42670400	0.00134700
C	-1.22312600	-0.68662500	-0.15627500
C	-1.22298400	0.68694100	-0.15607100
C	0.00012600	1.42678600	0.00184800
H	2.16409700	1.22342800	-0.24443700
H	2.16394300	-1.22369400	-0.24433600
H	-0.00022200	-2.50812600	-0.05522700

H	4.64872500	1.35996900	0.06589700
H	3.36143800	3.45877900	-0.00375800
C	-0.69163900	3.64509400	-0.23036200
H	-1.26578500	4.56794600	-0.25411700
C	0.67015200	3.68243100	-0.15596500
H	1.19278300	4.63505200	-0.12031400
C	-1.39640400	-0.00269600	3.02339100
H	-2.11168800	-0.71759000	2.61128200
H	-1.48482400	0.01785400	4.11115900
H	-0.38390200	-0.30240500	2.74560300
H	-1.60414000	0.99109300	2.62084400

Li-Toluene

C	-0.95584300	0.02914100	-0.05433500
C	-0.24824200	-1.22124000	0.06084500
C	1.16921200	-1.20534800	-0.18169600
C	1.86407400	-0.01865300	-0.21987600
C	1.18978700	1.22927200	-0.03012800
C	-0.24945000	1.20841500	-0.08499700
H	-0.80190100	-2.15362800	0.02317900
H	1.70206600	-2.14549700	-0.29630900
H	2.94128200	-0.02976100	-0.36417000
H	1.72768600	2.16577400	-0.11120700
H	-0.79407600	2.14956700	-0.12832300
C	-2.44909700	0.00275500	-0.09652500
H	-2.80193300	-0.50178500	-1.00458000
H	-2.85962000	-0.56265600	0.75134700
H	-2.87650900	1.00943500	-0.07852000
Li	0.61345500	-0.02583300	1.61628400

Li-Naphthalene

C	2.39422700	-0.69424800	-0.20381500
C	1.18261900	-1.40619400	-0.02893400
C	-0.07926500	-0.71918700	-0.05464500
C	-0.07935200	0.71937600	-0.05442100
C	1.18244200	1.40638400	-0.02803400
C	2.39409200	0.69459100	-0.20350100
H	-1.30758500	-2.47837100	-0.04972900
H	3.32797400	-1.23857500	-0.31085300
H	1.18138300	-2.49224600	-0.03404000

H	-2.16415800	-1.22332600	-0.24431300
H	-2.16390200	1.22379600	-0.24441300
H	0.00021400	2.50813800	-0.05621000
Li	0.00006700	-0.00062900	1.60604200

Li-Anthracene 1

C	-3.74939000	0.70119000	0.02616800
C	-2.55806700	1.39148100	-0.00055100
C	-1.32234900	0.71485500	-0.02940900
C	-1.32234100	-0.71486900	-0.02939100
C	-2.55804800	-1.39150600	-0.00053300
C	-3.74937900	-0.70122900	0.02617100
C	-0.08583200	1.39851700	-0.05487300
C	-0.08578700	-1.39846800	-0.05481900
C	1.13283100	-0.72834400	-0.08356300
C	1.13283800	0.72849300	-0.08353000
C	2.39416400	1.40124400	-0.07277200
H	2.39513300	2.48817700	-0.06736400
C	3.60750900	0.69967100	-0.14556200
C	3.60756500	-0.69971700	-0.14555400
C	2.39413200	-1.40121500	-0.07278400
H	-0.08831700	2.48738600	-0.06152100
H	-4.69079900	1.24214700	0.04518900
H	-2.55352900	2.47931700	-0.00301900
H	-2.55349400	-2.47934200	-0.00300000
H	-4.69078100	-1.24219800	0.04517500
H	-0.08817700	-2.48733500	-0.06128200
H	4.54511800	1.24507600	-0.19058700
H	4.54512000	-1.24510800	-0.19147400
H	2.39490900	-2.48814900	-0.06778400
Li	2.58591300	-0.00019900	1.62722400

Li-Tetracene 1

C	0.10820000	-0.72345400	-0.04715900
C	0.10820400	0.72346100	-0.04719600
C	-2.35010000	-0.73079100	-0.09303800
C	-2.35008400	0.73086900	-0.09287800

C	-1.31066300	-1.39070500	-0.03982200
C	-1.31083900	1.39070400	-0.04003500
H	1.18125200	2.49243000	-0.03397700
H	3.32769100	1.23923000	-0.31021800
C	-2.51512900	0.69390400	-0.01324600
C	-2.51506100	-0.69405400	-0.01307100
H	-1.30787900	2.47837300	-0.04996400
H	-3.45404700	1.23922700	0.00156200
H	-3.45391200	-1.23947700	0.00197000
Li	1.48223100	-0.00133900	1.62080000

Li-Anthracene 2

C	-3.67945700	0.69956000	-0.11350700
C	-2.48606300	1.39248600	-0.07077800
C	-1.24645800	0.71990300	-0.03312900
C	-1.24645300	-0.71985900	-0.03344100
C	-2.48606900	-1.39243200	-0.07119500
C	-3.67946000	-0.69949100	-0.11370500
C	0.00005000	1.40092400	0.06260800
C	0.00003700	-1.40095200	0.06211600
C	1.24654800	-0.71982100	-0.03317600
C	1.24656300	0.71989000	-0.03319800
C	2.48611000	1.39249600	-0.07120500
H	2.48180200	2.48019900	-0.07912000
C	3.67951800	0.69955100	-0.11378900
C	3.67953200	-0.69948500	-0.11338500
C	2.48613100	-1.39242900	-0.07056900
H	0.00003900	2.48901400	0.06978100
H	-4.61912000	1.24211300	-0.15170600
H	-2.48177500	2.48019400	-0.07843600
H	-2.48178400	-2.48013900	-0.07915300
H	-4.61913000	-1.24202400	-0.15201300
H	0.00002900	-2.48904200	0.06850200
H	4.61917900	1.24208400	-0.15230600
H	4.61920600	-1.24202900	-0.15145700
H	2.48186300	-2.48013900	-0.07800500
Li	-0.00115700	-0.00076000	1.75401000

Li-Tetracene 2

C	-3.74277500	-1.39422300	-0.04138500
C	4.87386700	-0.70316200	-0.12083200
C	2.44195500	0.72064300	-0.04950800
C	2.44196100	-0.72065200	-0.04944600

C	2.55199400	-0.71606700	-0.00459800
C	2.55199500	0.71606600	-0.00465000
C	1.32560900	-1.39513300	-0.02551700
C	1.32560500	1.39513300	-0.02561700
C	-1.13392400	-1.40258100	-0.06399200
C	-1.13392700	1.40261600	-0.06399000
C	-3.61033100	-1.39941300	-0.08169000
C	-3.61033400	1.39951700	-0.08107200
C	3.79526100	-1.39494300	0.01621300
C	3.79525900	1.39494000	0.01611900
C	-4.82015200	-0.70312700	-0.10841500
C	-4.82017500	0.70327400	-0.10813500
C	4.97755500	-0.70628700	0.03629700
C	4.97755500	0.70628400	0.03625200
H	1.32757400	-2.48417200	-0.02759000
H	1.32757900	2.48417200	-0.02775000
H	-1.13328600	-2.49135800	-0.06893100
H	-1.13322100	2.49139200	-0.06869700
H	-3.61103300	-2.48677100	-0.07633500
H	-3.61100700	2.48687000	-0.07640600
H	3.79015400	-2.48269700	0.01481100
H	3.79015600	2.48269400	0.01464700
H	-5.75886200	-1.24767800	-0.12749900
H	-5.75885900	1.24785100	-0.12756500
H	5.92118300	-1.24348400	0.05131500
H	5.92118300	1.24348200	0.05124000
Li	-3.73361000	-0.00082900	1.64238200

Li-Pentacene 1

C	-3.56851700	-0.73154300	-0.09269900
C	-4.82819800	-1.39917100	-0.07805700
C	-6.03476800	-0.70542800	-0.08192500
C	-6.03473800	0.70558200	-0.08150400
C	-4.82817500	1.39930000	-0.07738900
C	-3.56848700	0.73170200	-0.09259200
C	-1.11029800	-0.72761100	-0.05720400
C	-2.35296100	-1.40408500	-0.06804100
C	-2.35293700	1.40420400	-0.06808600
C	-1.11028200	0.72770000	-0.05722400
C	1.33815100	-0.72210000	-0.02510200
C	0.10153800	-1.39893100	-0.04116300
C	0.10156400	1.39899000	-0.04113200

C	1.20202300	-1.39984500	0.03537500
C	-1.27320200	-1.39764600	-0.02150300
C	3.68701600	1.39455800	-0.07984400
C	4.87386200	0.70318100	-0.12085800
C	-4.92748500	0.70492900	-0.05028400
C	-2.50102800	0.71622500	-0.03274400
C	-0.04948800	-0.72860000	-0.02172000
C	-3.74277400	1.39422800	-0.04128500
C	-1.27320100	1.39764200	-0.02144200
C	-0.04948500	0.72858600	-0.02173100
C	1.20201600	1.39984200	0.03524800
C	-2.50102900	-0.71622500	-0.03279000
C	-4.92748500	-0.70492100	-0.05033700
C	3.68702800	-1.39455100	-0.07977600
H	3.68258600	2.48223700	-0.08749000
H	5.81475700	-1.24343800	-0.15752100
H	-3.73808600	-2.48194100	-0.04402800
H	-3.73808100	2.48194600	-0.04385100
H	3.68261100	-2.48222900	-0.08739200
H	-1.27522400	-2.48655500	-0.02729400
H	-5.87042700	1.24325300	-0.05959900
H	1.20497100	2.48824700	0.04803200
H	-1.27521800	2.48655100	-0.02718100
H	1.20498200	-2.48825000	0.04824500
H	-5.87042800	-1.24324400	-0.05969100
H	5.81474900	1.24346300	-0.15755100
Li	1.27737700	-0.00003400	1.74816000

Li-Pentacene 2

C	-3.64785100	-0.72137700	-0.05848100
C	-4.89634700	-1.39622300	-0.07527800
C	-6.07943400	-0.70535000	-0.10378600
C	-6.07940700	0.70554800	-0.10357200
C	-4.89628900	1.39634300	-0.07495500
C	-3.64781300	0.72141700	-0.05845500
C	-1.15947900	-0.73203600	-0.03655400
C	-2.41138700	-1.39968700	0.00643900
C	-2.41135800	1.39969800	0.00613600
C	-1.15951500	0.73204200	-0.03661200
C	1.29608400	-0.72304600	-0.02343700
C	0.05963400	-1.40170800	-0.02275400
C	0.05963800	1.40168400	-0.02293300

C	1.33816600	0.72213100	-0.02504100
C	3.77776300	-0.71840800	0.00785600
C	5.02712700	-1.39785400	0.02438500
C	6.20372400	-0.70961200	0.04030800
C	6.20373600	0.70954300	0.04045900
C	5.02715100	1.39780900	0.02466300
C	3.77777700	0.71838900	0.00797400
C	2.56076800	-1.39625500	-0.00877200
C	2.56079300	1.39626000	-0.00859000
H	-4.82881700	-2.48671200	-0.07525000
H	-6.97396600	-1.24918700	-0.08909800
H	-6.97392900	1.24935900	-0.08833800
H	-4.82878600	2.48683900	-0.07430400
H	-2.35322600	-2.49290200	-0.07258300
H	-2.35318000	2.49301900	-0.07244400
H	0.10294500	-2.48778400	-0.04334400
H	0.10299500	2.48784200	-0.04328100
H	5.02214600	-2.48549500	0.02347100
H	7.14873000	-1.24439200	0.05232600
H	7.14875200	1.24430500	0.05260700
H	5.02218900	2.48545000	0.02397500
H	2.56194500	-2.48525700	-0.00996100
H	2.56199100	2.48526200	-0.00963400
Li	-4.91105700	-0.00134200	1.65970300

Li-Pentacene 3

C	-3.69507600	-0.71754600	-0.04319300
C	-4.94061400	-1.39628800	-0.06377300
C	-6.12084900	-0.70719600	-0.08327800
C	-6.12083600	0.70735400	-0.08316200
C	-4.94057800	1.39639600	-0.06357000
C	-3.69506200	0.71759800	-0.04313400
C	-1.24613200	-0.72841000	-0.01272200
C	-2.47365800	-1.39789300	-0.02043700
C	-2.47362700	1.39788200	-0.02046500
C	-1.24610900	0.72831700	-0.01296000
C	1.24633900	-0.72837500	-0.01242100
C	0.00008700	-1.40032000	0.05504600
C	0.00006200	1.40025800	0.05413400
C	1.24626200	0.72827800	-0.01263100
C	3.69520500	-0.71755100	-0.04319400
C	4.94072500	-1.39627200	-0.06395400

C	1.29607900	0.72302000	-0.02350600
C	3.73754200	-0.71779700	-0.01908500
C	4.98525500	-1.39719100	-0.01740500
C	6.16333400	-0.70863000	-0.01552300
C	6.16332600	0.70869900	-0.01550100
C	4.98523500	1.39723900	-0.01736700
C	3.73753600	0.71782300	-0.01907800
C	2.51802600	-1.39608600	-0.02111700
C	2.51800900	1.39608900	-0.02116300
H	-4.89190700	-2.48382900	-0.08373700
H	-7.02161400	-1.24377300	-0.13109300
H	-7.02156900	1.24401700	-0.13060800
H	-4.89178500	2.48395000	-0.08317400
H	-2.41531500	-2.48826100	0.02170700
H	-2.41534700	2.48826900	0.02164700
H	0.06064700	-2.49044000	-0.02733000
H	0.06069100	2.49041800	-0.02783500
H	4.98039400	-2.48480000	-0.01873000
H	7.10805900	-1.24393700	-0.01500700
H	7.10804200	1.24402100	-0.01495300
H	4.98035900	2.48484900	-0.01866100
H	2.51958100	-2.48503500	-0.02365000
H	2.51955000	2.48503700	-0.02372100
Li	-2.48822700	-0.00110000	1.73302200

Li-Phenanthrene 1

C	3.61643400	-0.34152800	0.01849400
C	2.92841900	0.84163000	0.01650700
C	1.51666500	0.87123100	-0.01246000
C	0.79229900	-0.35982200	-0.03690200
C	1.53780200	-1.56275200	-0.04005200
C	2.90782800	-1.55904900	-0.01252900
C	0.81136700	2.09310200	-0.02468700
C	-0.64372900	-0.34550100	-0.04815800
C	-1.31486300	0.90998400	-0.05740600
C	-0.55751900	2.10614800	-0.05559000
C	-2.75339000	0.94165900	-0.01922100
H	-3.25148400	1.90600400	-0.03629000
C	-3.49495700	-0.25146000	-0.20733900
C	-2.84871600	-1.47325300	-0.19846400
C	-1.43863000	-1.53931400	-0.00607900
H	1.37383600	3.02320800	-0.01607500

C	6.12096700	-0.70715800	-0.08356800	H	4.70194400	-0.34540600	0.03927400
C	6.12093200	0.70736600	-0.08340100	H	3.46119100	1.78986700	0.03336400
C	4.94064400	1.39639400	-0.06366900	H	1.01952300	-2.51544700	-0.07399300
C	3.69516900	0.71757700	-0.04311400	H	3.45091400	-2.49938100	-0.02045000
C	2.47375700	-1.39791400	-0.02034100	H	-1.09675900	3.05051800	-0.07451200
C	2.47369300	1.39786700	-0.02030300	H	-4.57373000	-0.20404600	-0.32581200
H	-4.93593100	-2.48387600	-0.06667000	H	-3.41461900	-2.39301800	-0.31304800
H	-7.06468900	-1.24356300	-0.10126400	H	-0.96043000	-2.51080700	-0.00213400
H	-7.06466000	1.24374800	-0.10105200	Li	-2.35481400	-0.42931300	1.63099300
H	-4.93584800	2.48398500	-0.06631400				
H	-2.47540600	-2.48678100	-0.02610900				
H	-2.47530900	2.48677100	-0.02626400				
H	0.00011800	-2.48871500	0.07226100				
H	0.00002200	2.48865400	0.07125800				
H	4.93606200	-2.48386000	-0.06690200				
H	7.06480900	-1.24351800	-0.10167000				
H	7.06474000	1.24378800	-0.10136400				
H	4.93591000	2.48398200	-0.06639200				
H	2.47549500	-2.48679800	-0.02594300				
H	2.47540700	2.48675500	-0.02611000				
Li	-0.00284000	-0.00092100	1.77906200				

Li-Phenanthrene 2

C	3.55988400	-0.34808700	-0.05287600
C	2.85697400	0.83255000	-0.06948000
C	1.43550700	0.85168400	-0.06641900
C	0.74351700	-0.40868500	-0.04823500
C	1.49809700	-1.58342700	-0.03449800
C	2.88648400	-1.57242800	-0.03334200
C	0.70783700	2.06686600	-0.05596100
C	-0.73622100	-0.40889600	-0.03049200
C	-1.43155400	0.85081000	-0.11312900
C	-0.70899200	2.06373500	-0.10870800
C	-2.85610100	0.82420500	-0.14259500
H	-3.38263100	1.77185000	-0.22972500
C	-3.55371100	-0.35514000	-0.07393500
C	-2.87760000	-1.57628500	0.03651700
C	-1.49050700	-1.58248900	0.05561600
H	1.25613400	3.00367800	-0.09036600
H	4.64622200	-0.32727600	-0.06253500
H	3.38119300	1.78499300	-0.09692400
H	0.99019300	-2.54293000	-0.03841600

Li-Phenanthrene 3

C	3.54886300	-0.27544000	0.04460000
C	2.81580700	0.91829300	0.04211400
C	1.43053100	0.91682600	-0.05201300
C	0.71207200	-0.32189100	-0.16544600
C	1.48573400	-1.53584300	-0.14810200
C	2.87566600	-1.48198300	-0.05678300
C	0.67529700	2.13722500	-0.02673700
C	-0.71206200	-0.32190800	-0.16540100
C	-1.43048800	0.91682900	-0.05190100
C	-0.67525400	2.13721200	-0.02662600
C	-2.81578100	0.91832100	0.04219800
H	-3.32877400	1.87459500	0.11440200
C	-3.54885300	-0.27539600	0.04452400
C	-2.87570100	-1.48195400	-0.05688200
C	-1.48572700	-1.53584100	-0.14805000
H	1.22556300	3.07458300	0.01415600
H	4.63118600	-0.25437800	0.11428900
H	3.32882300	1.87455500	0.11430400
H	1.01661600	-2.48931700	-0.37501100

H	3.43879000	-2.50605700	-0.02920400
H	-1.25739600	2.99940500	-0.17107800
H	-4.63979100	-0.33912600	-0.10515700
H	-3.42859600	-2.50855400	0.09786600
H	-0.98021700	-2.53825300	0.12723900
Li	-0.07519400	1.09193000	1.67450800

Li-Chrysene 1

C	3.86348200	-1.15621400	0.01527100
C	4.74514200	-0.10243600	0.05023100
C	4.24827800	1.20579900	0.05680300
C	2.89174000	1.43683800	0.02750400
C	1.96288000	0.37903900	-0.00973900
C	2.47446400	-0.94199700	-0.01447200
C	1.56618900	-2.04235800	-0.05624900
C	0.52851200	0.58875500	-0.04231200
C	-0.34676400	-0.53890000	-0.06018600
C	0.22647900	-1.84466100	-0.07772600
C	-3.71516400	1.16885200	-0.02970200
C	-4.59761900	0.07232900	-0.16118500
C	-4.09660800	-1.21813400	-0.13894000
C	-2.70210600	-1.44358400	0.01089900
C	-0.03471000	1.87193000	-0.06468700
C	-1.39902200	2.05714300	-0.09183000
C	-2.29390700	0.97128100	-0.07532200
C	-1.76713600	-0.35847800	-0.05561300
H	4.22862900	-2.18065100	0.00872600
H	5.81575400	-0.28067200	0.07231500
H	4.93558700	2.04615400	0.08484800
H	2.54158800	2.46352200	0.03501800
H	1.97559600	-3.04928600	-0.07773600
H	-0.42440500	-2.71114400	-0.12215300
H	-4.09588500	2.18552900	-0.04848200
H	-5.66632800	0.24434200	-0.24962900
H	-4.76824400	-2.06832000	-0.21097100
H	-2.34786500	-2.46640400	0.03805700
H	0.60506700	2.74742000	-0.06926200
H	-1.81046900	3.06331700	-0.12047400
Li	-3.43793700	-0.20834400	1.65442300

Li-Pyrene 1

C	3.47129000	0.00000100	-0.15198800
C	2.79670100	1.21669500	-0.08824100

H	3.43942500	-2.41096800	-0.08569100
H	-1.22552800	3.07456100	0.01435600
H	-4.63118400	-0.25433100	0.11411600
H	-3.43949800	-2.41091200	-0.08587100
H	-1.01666300	-2.48928100	-0.37524800
Li	-0.00019600	-1.29193700	1.59441100

Li-Chrysene 2

C	-3.81299100	1.14292700	0.04877600
C	-4.67925600	0.08949000	-0.13876200
C	-4.17132600	-1.19896100	-0.31640200
C	-2.80693500	-1.41228800	-0.28727600
C	-1.90233000	-0.36290400	-0.07501000
C	-2.41977400	0.94935000	0.07680400
C	-1.52660200	2.04853000	0.24955400
C	-0.45682400	-0.57570200	-0.00787900
C	0.40854100	0.58278800	0.05140100
C	-0.17132500	1.85863000	0.20973100
C	3.79624900	-1.09275300	-0.01708900
C	4.64612800	-0.01487800	-0.18019100
C	4.12307200	1.26649700	-0.31772200
C	2.74788700	1.46041500	-0.27446700
C	0.11705500	-1.84980900	0.07284400
C	1.50752200	-2.02855200	0.20030900
C	2.39879200	-0.92229500	0.02952000
C	1.86007700	0.39744900	-0.07937700
H	-4.19563400	2.15341500	0.17201500
H	-5.75127600	0.26092100	-0.16036600
H	-4.84532100	-2.03286900	-0.48651100
H	-2.43416600	-2.41919800	-0.44870100
H	-1.94266600	3.04230400	0.38801500
H	0.47937800	2.72258600	0.31004700
H	4.19617700	-2.10043800	0.06794400
H	5.72001600	-0.17261300	-0.21631800
H	4.78300000	2.11459300	-0.47016400
H	2.35753700	2.46408400	-0.40988300
H	-0.51944600	-2.72884900	0.08769600
H	1.92452900	-3.02897500	0.26518900
Li	0.76004000	-0.76751600	1.81082100

Li-Pyrene 2

C	-3.52587600	0.05211100	-0.05002600
C	-2.85661900	-1.16274000	-0.08449800

C	1.35468600	1.24428900	-0.08203200
C	0.64328100	0.00000100	-0.07343100
C	1.35468600	-1.24428800	-0.08203500
C	2.79670200	-1.21669300	-0.08825200
C	0.61766800	2.44267600	-0.05501700
C	-0.78221900	0.00000000	-0.03416500
C	-1.49403200	1.23486200	-0.01667600
C	-0.75678600	2.44228600	-0.02905300
C	-2.90398100	1.20715800	0.01780300
H	-3.44715100	2.14819100	0.02950500
C	-3.58301200	-0.00000100	0.03297600
C	-2.90398000	-1.20715900	0.01780300
C	-1.49403100	-1.23486300	-0.01667700
C	-0.75678400	-2.44228600	-0.02905300
C	0.61766900	-2.44267500	-0.05501800
H	1.16324100	-3.38359900	-0.06927400
H	-1.30314100	-3.38202700	-0.01899200
H	1.16323900	3.38360000	-0.06927200
H	4.55802000	0.00000200	-0.19494500
H	3.33986300	2.15574100	-0.12866900
H	3.33986300	-2.15573800	-0.12869000
H	-1.30314300	3.38202600	-0.01899400
H	-4.66955700	-0.00000100	0.05755700
H	-3.44715000	-2.14819300	0.02950400
Li	2.24625900	-0.00000900	1.63686900

Li-Picene 1

C	-3.71622800	-1.65682000	-0.01250200
C	-2.96147500	-0.46377100	-0.00645800
C	-5.08924900	-1.63716100	0.01036000
C	-3.67356400	0.76180000	0.02587200
C	-1.51920500	-0.44342400	-0.03117700
C	-5.08183800	0.75769400	0.04939300
C	-2.94473300	1.98050800	0.03542800
C	-5.78504200	-0.41927600	0.04160300
C	-0.82865700	0.78296500	-0.02197500
C	-1.58891700	1.98870700	0.01273600
C	0.61529700	0.80753900	-0.04694600
C	-0.75879100	-1.64614300	-0.07182000
C	0.59936000	-1.63070600	-0.08503000
C	1.34121600	-0.42141200	-0.06216800
C	2.77398900	-0.42950500	-0.05092600

C	-1.44162600	-1.20614800	-0.09011400
C	-0.71756500	0.04055600	-0.06175100
C	-1.42825900	1.27021200	-0.01483100
C	-2.84407400	1.25391000	-0.01076100
C	-0.70135700	-2.41393500	-0.08984900
C	0.71756500	0.04055600	-0.06175000
C	1.44162600	-1.20614800	-0.09011400
C	0.70135700	-2.41393500	-0.08984800
C	2.85661900	-1.16274100	-0.08449800
H	3.40793200	-2.09833700	-0.12314000
C	3.52587600	0.05211100	-0.05002600
C	2.84407500	1.25391000	-0.01076100
C	1.42825900	1.27021200	-0.01483100
C	0.68252700	2.47481100	0.02152300
C	-0.68252600	2.47481100	0.02152300
H	-1.22866700	3.41476700	0.04845800
H	1.22866800	3.41476700	0.04845800
H	-1.24407500	-3.35532300	-0.11363200
H	-4.61278900	0.05618600	-0.05506500
H	-3.40793200	-2.09833700	-0.12314000
H	-3.38037800	2.19798100	0.01629600
H	1.24407500	-3.35532300	-0.11363100
H	4.61278900	0.05618500	-0.05506600
H	3.38037800	2.19798100	0.01629600
Li	-0.00000100	-1.37862300	1.67261400

Li-Picene 2

C	-3.68800500	-1.63520800	0.16664300
C	-2.91912700	-0.46147300	0.01911500
C	-5.06057100	-1.60260400	0.14585900
C	-3.61313400	0.76354800	-0.15631500
C	-1.47359100	-0.46675200	0.04306100
C	-5.02321900	0.77182900	-0.17744700
C	-2.87335100	1.96203300	-0.32082000
C	-5.73962600	-0.38662100	-0.02843700
C	-0.77849700	0.75378600	-0.07942100
C	-1.51307100	1.94921100	-0.28443900
C	0.67801400	0.77986500	0.00055700
C	-0.73287700	-1.66872700	0.18526700
C	0.64235800	-1.66102800	0.14462400
C	1.38566100	-0.47933200	0.02042600
C	2.85262100	-0.48169900	-0.09730900

C	1.34525700	2.00885300	-0.06541700
C	3.46816300	0.81771900	-0.06797600
C	2.71993600	2.01148100	-0.08709800
C	4.90302100	0.83004400	-0.01777100
C	3.55645000	-1.62905700	0.01987300
C	4.96905900	-1.58683900	-0.13306100
C	5.63401400	-0.37342800	-0.15442400
H	-3.21273200	-2.61689800	-0.03579800
H	-5.63994400	-2.57304500	0.00410000
H	-5.60131600	1.71276100	0.07350200
H	-3.49901000	2.91557700	0.06170800
H	-6.87043200	-0.41229100	0.05919500
H	-1.07760700	2.94413500	0.02351700
H	-1.26595200	-2.60370800	-0.09995300
H	1.12362200	-2.57931400	-0.12776800
H	0.83177400	2.96302400	-0.07246600
H	3.25939200	2.95537300	-0.11328300
H	5.41320600	1.78821300	-0.03747400
H	3.07030300	-2.59625400	0.04481200
H	5.52415100	-2.51711600	-0.20809200
H	6.71586100	-0.34265500	-0.24528200
Li	4.45343400	-0.49879900	1.66339300

Li-Picene 3

C	-3.66155600	-1.60438100	-0.28981400
C	-2.89836200	-0.44663000	-0.07731700
C	-5.03978800	-1.56835400	-0.31388100
C	-3.57803600	0.78893100	0.08533800
C	-1.43839800	-0.47530100	-0.02625000
C	-4.98783000	0.80059200	0.06337200
C	-2.83430500	1.98591700	0.26369600
C	-5.70851000	-0.35313300	-0.12761600
C	-0.72964100	0.77608800	0.04238500
C	-1.46207600	1.96556400	0.22165400
C	0.74046200	0.77040100	-0.07673200
C	-0.70677300	-1.66532500	0.03003900
C	0.70734000	-1.66724800	0.11933000
C	1.44493900	-0.46518600	0.00486600
C	2.89708500	-0.44377100	-0.01357900
C	1.46798400	1.96661200	-0.24245400
C	3.58008200	0.79562800	-0.14228500
C	2.83757200	1.99263700	-0.27104700

C	1.41366300	1.96670000	0.13358500
C	3.55665000	0.75190900	0.06263300
C	2.81847600	1.95600000	0.26744800
C	4.96740400	0.73597300	0.02683300
C	3.59135600	-1.64498000	-0.32834700
C	4.97990300	-1.63494300	-0.36157000
C	5.66566200	-0.43741300	-0.17451500
H	-3.19390000	-2.59094700	0.30152000
H	-5.62321400	-2.52376600	0.26355000
H	-5.53191900	1.72288800	-0.31605900
H	-3.41339400	2.89037900	-0.48788700
H	-6.82499900	-0.36741500	-0.04583700
H	-0.97843100	2.88070100	-0.43840900
H	-1.24400400	-2.61653500	0.30051400
H	1.16625400	-2.60983200	0.21662500
H	0.90086700	2.92132100	0.18214000
H	3.36168600	2.89068700	0.36883300
H	5.49725100	1.67756800	0.15008500
H	3.07089600	-2.58183500	-0.50123700
H	5.52376700	-2.55592300	-0.54486600
H	6.75134400	-0.42201300	-0.20258500
Li	1.90587300	0.76809300	1.83634100

Li-Coronene 1

C	3.62759000	-0.72378300	-0.04603400
C	2.41684900	-1.44404900	-0.07788300
C	1.17528000	-0.72716700	-0.06238600
C	1.18081400	0.71780200	-0.06185300
C	2.42822000	1.42509300	-0.07912100
C	3.63281800	0.69580400	-0.04868200
C	-0.05146900	-1.42592400	-0.03519800
C	-0.04048700	1.42603800	-0.03453400
C	-1.27498700	0.71551500	-0.01092900
C	-1.28047000	-0.70584800	-0.01124000
C	-2.49842700	1.42677800	0.01469000
C	-2.46934600	2.85541700	0.01164500
C	-1.28869300	3.53178500	-0.01632400
C	-0.04613800	2.84984000	-0.04110400
C	1.19274200	3.52468000	-0.07398100
C	2.38235700	2.85313000	-0.08938100
H	3.32302900	3.39704900	-0.12164000
H	1.18668000	4.61268900	-0.08953000

C	4.99202100	0.80699800	-0.15327800	H	4.56536000	-1.27168300	-0.06343700
C	3.66899000	-1.61704600	0.09182300	H	4.57471600	1.23667700	-0.06645700
C	5.04281300	-1.57993800	0.08179600	H	-3.41479700	3.39111400	0.02893300
C	5.71308500	-0.35256800	-0.04173000	H	-1.27905900	4.61957700	-0.02280600
H	-3.16245900	-2.55405700	-0.45588000	C	2.36026600	-2.87116000	-0.08842500
H	-5.60301500	-2.48018400	-0.48592100	C	1.16528600	-3.53389800	-0.07350400
H	-5.49714700	1.75239700	0.19439000	C	-0.06798500	-2.84965400	-0.04117000
H	-3.36940300	2.91918200	0.41307400	H	3.29685000	-3.42212100	-0.11996300
H	-6.79389000	-0.32176200	-0.14485300	H	1.15110500	-4.62181800	-0.08895400
H	-0.92672900	2.90316500	0.33474400	C	-1.31609700	-3.52206500	-0.01672400
H	-1.22014500	-2.62059900	0.03203600	C	-2.49119800	-2.83651900	0.01091300
H	1.21735600	-2.62135100	0.16458500	C	-2.50931900	-1.40755000	0.01426100
H	0.92723500	2.89859400	-0.36906900	H	-1.31477100	-4.60989400	-0.02308600
H	3.37019700	2.92980700	-0.40601900	H	-3.44073900	-3.36496200	0.02801200
H	5.49792700	1.76421000	-0.25463600	C	-3.70359900	0.70108200	0.04000500
H	3.17749900	-2.58014600	0.18171000	H	-4.64118800	1.25136800	0.05802600
H	5.60971100	-2.50205900	0.16460100	C	-3.70883300	-0.67267500	0.03983900
H	6.79853300	-0.32535600	-0.05198800	H	-4.65054400	-1.21591000	0.05773600
Li	-0.10275100	-0.54158700	1.77110800	Li	2.58410500	-0.00603900	1.69529300

Li-Coronene 2

C	3.61166700	0.98929100	-0.02585600
C	2.85095600	-0.20725400	-0.03459000
C	1.42427300	-0.10287200	-0.05655200
C	0.80264200	1.17981000	-0.05946800
C	1.59872900	2.36402200	-0.03269000
C	3.02504000	2.21799400	-0.02434000
C	0.62376000	-1.28331500	-0.05997700
C	-0.62476100	1.28347700	-0.05638100
C	-1.42555800	0.10296100	-0.05137000
C	-0.80362600	-1.18003500	-0.05524900
C	-2.85114000	0.20716100	-0.03698800
C	-3.43005400	1.49493100	-0.02621900
C	-2.67127700	2.63064100	-0.02109000
C	-1.24229300	2.56914800	-0.03333600
C	-0.42738700	3.70651400	-0.02510600
C	0.95744300	3.60442500	-0.02274200
H	1.56760200	4.50415000	-0.01476900
H	-0.90060500	4.68492500	-0.01808600
H	4.69646700	0.90521500	-0.02003400
H	3.63243000	3.11911400	-0.01823400
H	-4.51563700	1.56871900	-0.02042500

H	-3.14323300	3.60934700	-0.01387500
C	3.42951000	-1.49510200	-0.02594700
C	2.67063400	-2.63091000	-0.02447700
C	1.24140400	-2.56896900	-0.03273200
H	4.51510600	-1.56896600	-0.01990600
H	3.14240100	-3.60968800	-0.01823400
C	0.42605000	-3.70618600	-0.02210700
C	-0.95874600	-3.60455900	-0.02518900
C	-1.59971200	-2.36408300	-0.03366500
H	0.89937800	-4.68457200	-0.01404000
H	-1.56875500	-4.50436200	-0.01816800
C	-3.61219100	-0.98913100	-0.02586800
H	-4.69696200	-0.90493500	-0.01996100
C	-3.02564300	-2.21784900	-0.02151500
H	-3.63317400	-3.11888200	-0.01432500
Li	0.02222100	-0.00024300	1.73693000

N₂-Li-Naphthalene

C	-2.66386900	0.05488900	0.69351600
C	-1.47083500	-0.20664500	1.40628900
C	-0.26805000	-0.55938800	0.72049500
C	-0.26805500	-0.55951200	-0.72039500
C	-1.47084000	-0.20687800	-1.40624200
C	-2.66387500	0.05477100	-0.69350800
H	0.93315500	-0.84052000	2.47942000
H	-3.57932500	0.26736600	1.23764200
H	-1.46928900	-0.20425000	2.49247900
C	0.93739500	-0.83678500	1.39170200
C	0.93738300	-0.83703900	-1.39156300
H	-1.46929800	-0.20466000	-2.49243300
H	-3.57933400	0.26715900	-1.23766300
C	2.11131600	-1.09607600	-0.69550100
C	2.11132300	-1.09594800	0.69567800
H	0.93313400	-0.84097100	-2.47927900
H	3.02757600	-1.30457400	-1.23964600
H	3.02758800	-1.30434400	1.23985400
Li	-1.08935500	1.49208800	-0.00014200
N	2.09558500	2.30424400	-0.00022200
N	1.00334500	2.18435500	-0.00017500

CH₄-Li-Naphthalene

C	2.43044800	-0.41570100	0.76413100
C	1.20899600	-0.21981000	1.45031900
C	-0.04744200	-0.39262900	0.78222800
C	-0.04544800	-0.63749700	-0.63655300
C	1.21290800	-0.69312700	-1.32082600
C	2.43263900	-0.64952000	-0.60468200
H	-1.27977300	-0.09313600	2.51392200
H	3.36826000	-0.36621400	1.30963400
H	1.20643200	-0.03479700	2.52069400
C	-1.28143700	-0.27226700	1.44092900
C	-1.27774600	-0.74831800	-1.29993300
H	1.21378600	-0.87715500	-2.39140000
H	3.37210100	-0.78310700	-1.13293500
C	-2.48510400	-0.61763000	-0.61648300
C	-2.48737700	-0.38011600	0.75009600
H	-1.27356000	-0.93993600	-2.37070500
H	-3.42304300	-0.70714500	-1.15649800
H	-3.42689900	-0.28301500	1.28603700
Li	1.37268000	1.21980700	-0.22247600
C	-0.17984400	3.05181000	-0.41544800
H	-0.78537700	2.26012000	0.03697900
H	-0.79535600	3.94226000	-0.53579000
H	0.65954400	3.32261700	0.23623800
H	0.16227900	2.74891900	-1.41141200

N₂-Li-Anthracene 1

C	4.24875200	-0.94409100	0.35170500
C	3.09775600	-1.43932800	-0.21659700
C	1.92042700	-0.66514000	-0.27488300
C	1.93935700	0.65556800	0.27262000
C	3.13479700	1.13282400	0.84866200
C	4.26750200	0.35279300	0.88855000
C	0.72619100	-1.14867700	-0.85155700
C	0.76256000	1.43350800	0.22061700
C	-0.41508700	0.95828600	-0.34512700
C	-0.43376300	-0.38394900	-0.90363200
C	-1.66092700	-0.86732000	-1.45612000
H	-1.67559800	-1.87219500	-1.87030500
C	-2.79986200	-0.06038700	-1.53661500
C	-2.78278500	1.23355000	-0.99521500
C	-1.62584000	1.71844500	-0.37764100
H	0.71554700	-2.15245900	-1.27334600
H	5.14565700	-1.55537300	0.38448600
H	3.07932500	-2.44293700	-0.63571300
H	3.14534100	2.13905700	1.26174000
H	5.17883800	0.73995800	1.33437000
H	0.78008400	2.44065600	0.63405500
H	-3.70118600	-0.44045100	-2.00762000
H	-3.67056700	1.85622300	-1.04801200
H	-1.61363300	2.71986200	0.04488300
Li	-2.33693400	-0.19586000	0.57768500
N	-4.94640700	-1.04029300	2.22684400
N	-4.00323000	-0.77417200	1.72941300

N₂-Li-Anthracene 2

C	4.01402400	0.69938200	0.16697200
C	2.83210900	1.39230500	-0.00434900
C	1.60659500	0.71918100	-0.18711200
C	1.60656600	-0.71902000	-0.18757300
C	2.83203600	-1.39230900	-0.00515400
C	4.01398700	-0.69954500	0.16658100
C	0.36467700	1.40072500	-0.32067800
C	0.36462400	-1.40045000	-0.32159300
C	-0.84905700	-0.72042600	-0.59676600

CH₄-Li-Anthracene 1

C	3.84731400	-0.68630700	-0.14823300
C	2.65852700	-1.35526300	-0.34288000
C	1.42884000	-0.66799800	-0.36883600
C	1.43112900	0.75070900	-0.18741200
C	2.66350800	1.40482800	0.01009500
C	3.84968000	0.70415100	0.02982100
C	0.19412000	-1.33006300	-0.56024000
C	0.19965000	1.44449800	-0.20644000
C	-1.01721600	0.79527900	-0.39864800
C	-1.01981300	-0.64790500	-0.58509200
C	-2.27903000	-1.30579600	-0.72063700
H	-2.28163200	-2.38480900	-0.85343700
C	-3.48802900	-0.59667500	-0.72696800
C	-3.48586600	0.79133900	-0.54414300
C	-2.27394000	1.47026200	-0.35612400
H	0.19397100	-2.40983200	-0.70201200
H	4.78412000	-1.23544700	-0.13551600
H	2.65225100	-2.43386100	-0.48499200
H	2.66138900	2.48439000	0.14460300
H	4.78847700	1.22881400	0.18059300
H	0.20431000	2.52481800	-0.06939600
H	-4.42547700	-1.12537600	-0.86960800
H	-4.42115600	1.34255700	-0.54409000
H	-2.27187500	2.54740700	-0.20860200
Li	-2.50779200	-0.14213800	1.17871300
C	-1.06572600	-0.47334300	3.05662000
H	-1.30640400	0.59239500	2.97287600
H	-0.48454800	-0.60660900	3.96791500
H	-1.96887000	-1.08805400	3.15691400
H	-0.46007100	-0.79627000	2.20330300

CH₄-Li-Anthracene 2

C	3.47354000	-0.57987200	-0.84764100
C	2.28719200	-1.28721500	-0.80347400
C	1.05207100	-0.64065200	-0.58401400
C	1.04856500	0.78732800	-0.40009500
C	2.27976700	1.47493800	-0.45144700
C	3.46950600	0.80806400	-0.67132100
C	-0.17604900	-1.34573100	-0.46272700
C	-0.18237200	1.43149400	-0.10077300
C	-1.42929900	0.74725200	-0.14087600

C	-0.84906100	0.72091800	-0.59617500
C	-2.07518300	1.39350500	-0.79966500
H	-2.06991500	2.48128600	-0.80609900
C	-3.25267400	0.70140700	-0.98871600
C	-3.25267900	-0.70055900	-0.98927000
C	-2.07519900	-1.39282500	-0.80075800
H	0.36304000	2.48888900	-0.31002800
H	4.94536700	1.24176700	0.29825400
H	2.82903200	2.48000300	-0.01129200
H	2.82890700	-2.48000200	-0.01271400
H	4.94529900	-1.24205300	0.29757000
H	0.36298900	-2.48862200	-0.31174700
H	-4.18035100	1.24300900	-1.14675400
H	-4.18036100	-1.24202800	-1.14773800
H	-2.06995500	-2.48060100	-0.80802400
Li	0.00507400	-0.00067800	1.38993300
N	-1.98982100	-0.00092400	2.25710700
N	-3.07787400	-0.00098500	2.39636700

N₂-Li-Tetracene 1

C	4.66169400	0.70958300	-0.57875300
C	3.45286900	1.40428500	-0.54973200
C	2.19497700	0.73536000	-0.54612800
C	2.19510500	-0.72370300	-0.55775000
C	3.45317200	-1.39211300	-0.57017200
C	4.66182600	-0.69674400	-0.58864000
C	0.97903000	1.40730000	-0.46477500
C	0.97924300	-1.39716100	-0.48907300
C	-0.26048800	-0.71977300	-0.40703200
C	-0.26053800	0.72831500	-0.39389000
C	-1.47563500	1.39858700	-0.29537900
H	-1.47797400	2.48767500	-0.28774200
C	-2.69925500	0.71850900	-0.21108600
C	-2.69924200	-0.71352800	-0.22449400
C	-1.47556700	-1.39184600	-0.32116600
H	0.97875800	2.49620900	-0.45664600
H	5.60026900	1.25449800	-0.59706100
H	3.45302100	2.49172200	-0.53548800
H	3.45371600	-2.47964300	-0.57161700

C	-1.42604200	-0.67993900	-0.32758600
C	-2.66053700	-1.36257900	-0.31595900
H	-2.65463400	-2.44008100	-0.46514700
C	-3.85326100	-0.68985200	-0.13743300
C	-3.85636200	0.69706900	0.04419400
C	-2.66667900	1.39836100	0.04542600
H	-0.17210900	-2.42610800	-0.59343500
H	4.40870400	-1.10186300	-1.02652700
H	2.28537700	-2.36559600	-0.94704500
H	2.27227800	2.55467500	-0.31899100
H	4.40169200	1.36325700	-0.71308700
H	-0.18415500	2.50963700	0.04746100
H	-4.79017000	-1.23854800	-0.14275900
H	-4.79568000	1.22449300	0.17987900
H	-2.66570600	2.47798100	0.17858700
Li	0.02630500	-0.18342200	1.41986900
C	1.76013900	-0.45536400	3.03983200
H	1.38322400	0.57215900	3.09084800
H	2.50560100	-0.57029400	3.82521100
H	0.96650500	-1.18609800	3.23549500
H	2.23907800	-0.64315800	2.07328300

CH₄-Li-Tetracene 1

C	4.63314300	0.77495500	-0.53137300
C	3.42321300	1.45942100	-0.41831300
C	2.16752700	0.78593800	-0.43628900
C	2.17196200	-0.66857500	-0.55402800
C	3.43157700	-1.32814600	-0.64431500
C	4.63723400	-0.62703700	-0.64483800
C	0.95167600	1.44467400	-0.28628100
C	0.96043000	-1.35085500	-0.51004600
C	-0.28131600	-0.68553100	-0.36718300
C	-0.28529200	0.75743100	-0.25081900
C	-1.50161000	1.41551900	-0.10139600
H	-1.50690800	2.50131900	-0.01684400
C	-2.72276700	0.72747100	-0.06005300
C	-2.71887700	-0.69995800	-0.17537800
C	-1.49381500	-1.36581100	-0.32549600
H	0.94780000	2.53016900	-0.20023300
H	5.56929100	1.32435000	-0.53381500
H	3.42026700	2.54294800	-0.32478700
H	3.43552500	-2.41267700	-0.72485800

H	5.60053700	-1.24114500	-0.61414500
H	0.97926500	-2.48605400	-0.49927900
H	-1.47780300	-2.48088900	-0.33360600
C	-3.93897400	1.39626600	-0.11211000
C	-5.11863200	0.70678300	-0.03026500
C	-5.11863400	-0.70527600	-0.04365100
C	-3.93895500	-1.39307100	-0.13843300
H	-3.93409200	2.48401100	-0.10388100
H	-6.05971200	1.24357000	0.04394500
H	-6.05970200	-1.24339500	0.02032600
H	-3.93403500	-2.48077700	-0.15077100
N	1.82649800	-0.02800800	2.59041100
N	0.84168200	-0.03756900	3.06615200
Li	3.54950600	-0.00579600	1.20839900

N₂-Li-Tetracene 2

C	-4.42754000	-0.70289900	-0.88561200
C	-3.24877000	-1.39383700	-0.74768000
C	-2.01139500	-0.72014800	-0.59592000
C	-2.01127400	0.72196200	-0.59450900
C	-3.24857600	1.39610500	-0.74492200
C	-4.42743900	0.70559400	-0.88420300
C	-0.79123400	-1.39914500	-0.38155500
C	-0.79100700	1.40037500	-0.37893800
C	0.45862300	0.72828700	-0.29411200
C	0.45848900	-0.72736300	-0.29548600
C	1.67399700	-1.39711000	-0.16497900
H	1.67645400	-2.48601200	-0.17137200
C	2.89570500	-0.71608000	-0.04190300
C	2.89582300	0.71614200	-0.04056100
C	1.67422500	1.39760000	-0.16232400
H	-0.79531200	-2.48761600	-0.37056600
H	-5.36199100	-1.24225800	-1.00657900
H	-3.24353300	-2.48159700	-0.75673600
H	-3.24320200	2.48387800	-0.75188000
H	-5.36181400	1.24532500	-1.00409500
H	-0.79495700	2.48882600	-0.36599300
H	1.67685100	2.48651100	-0.16671700
C	4.13118200	-1.39453900	0.08286500

H	5.57666100	-1.16325200	-0.73536200
H	0.96375500	-2.43610100	-0.59983700
H	-1.49309300	-2.45112300	-0.41662600
C	-3.96411200	1.39266800	0.09171300
C	-5.14152900	0.69565800	0.12850800
C	-5.13772400	-0.71191000	0.01440900
C	-3.95651600	-1.38759500	-0.13331300
H	-3.96213800	2.47708900	0.17740600
H	-6.08379900	1.22294200	0.24427600
H	-6.07706800	-1.25605200	0.04315400
H	-3.94864000	-2.47164400	-0.22331700
Li	3.59193600	-0.07298100	1.21948800
C	2.13892300	-0.39540300	3.08031100
H	1.54738900	-0.73079200	2.22163100
H	1.54252000	-0.52151000	3.98262900
H	3.04305800	-1.00476800	3.20244300
H	2.37680300	0.67055100	2.99074700

CH₄-Li-Tetracene 2

C	4.61756300	0.76259900	-0.67075300
C	3.43159300	1.44324000	-0.52818000
C	2.19224600	0.76154000	-0.46159000
C	2.19602900	-0.67714900	-0.54204400
C	3.43903700	-1.34077100	-0.68293000
C	4.62153800	-0.64181800	-0.74857400
C	0.96213500	1.42654600	-0.24823900
C	0.96926700	-1.36831100	-0.40652100
C	-0.28359300	-0.70391400	-0.32208800
C	-0.28743200	0.75029100	-0.23976500
C	-1.50875400	1.40974600	-0.10452000
H	-1.51400500	2.49725900	-0.04843800
C	-2.73178700	0.72145600	-0.05502300
C	-2.72821700	-0.70859100	-0.13636400
C	-1.50177100	-1.38065200	-0.26283700
H	0.96315500	2.51263800	-0.17448400
H	5.55334400	1.30988900	-0.72987200
H	3.42389500	2.52969200	-0.47367400
H	3.43703700	-2.42658800	-0.74981900
H	5.56025600	-1.17402700	-0.86834700
H	0.97614500	-2.45582100	-0.45433200
H	-1.50142800	-2.46752800	-0.33035600
C	-3.97197100	1.38996500	0.07490400

C	5.30973500	-0.70545800	0.20221600
C	5.30985200	0.70466900	0.20352800
C	4.13141200	1.39416500	0.08547300
H	4.12660800	-2.48223000	0.07855200
H	6.24829700	-1.24372800	0.29399100
H	6.24850300	1.24261100	0.29630500
H	4.12701600	2.48186200	0.08319000
N	-4.10757900	-0.00391200	2.48764600
N	-3.02610000	-0.00329700	2.30917800
Li	-1.08600500	-0.00167500	1.36528900

N₂-Li-Pentacene 2

C	-3.64051900	-0.72046400	-0.34190100
C	-4.88820600	-1.39569200	-0.32219200
C	-6.07182800	-0.70498400	-0.31352900
C	-6.07182400	0.70586000	-0.31258500
C	-4.88818500	1.39654800	-0.32026600
C	-3.64052000	0.72131300	-0.34077900
C	-1.15539300	-0.73093700	-0.38126700
C	-2.40339800	-1.39863500	-0.32003300
C	-2.40338800	1.39940400	-0.31781500
C	-1.15539800	0.73179600	-0.38003300
C	1.30173700	-0.72325000	-0.34891800
C	0.06581500	-1.40096600	-0.36503100
C	0.06581200	1.40180300	-0.36267300
C	1.30173100	0.72405700	-0.34765400
C	3.74360400	-0.71750100	-0.28778200
C	4.99089600	-1.39678200	-0.25724800
C	6.16880600	-0.70827100	-0.22704900
C	6.16879400	0.70894000	-0.22575300
C	4.99087400	1.39748200	-0.25471100
C	3.74359500	0.71823600	-0.28649600
C	2.52435300	-1.39589800	-0.31817400
C	2.52433600	1.39666800	-0.31571300
H	-4.88397100	-2.48332600	-0.33131300
H	-7.01439700	-1.24349900	-0.31191100
H	-7.01438800	1.24437900	-0.31029600
H	-4.88389500	2.48419200	-0.32786400
H	-2.40663900	-2.48734600	-0.30557600

C	-5.15196200	0.69403900	0.12211500
C	-5.14851400	-0.71353300	0.04177100
C	-3.96509300	-1.39372400	-0.08380000
H	-3.97010400	2.47614500	0.13360600
H	-6.09399600	1.22534100	0.21918800
H	-6.08787900	-1.25707100	0.07730900
H	-3.95775900	-2.47950900	-0.14905400
Li	1.19183100	-0.06675700	1.40625200
C	2.86808900	-0.26733100	3.07868400
H	2.51761300	0.77045000	3.04736000
H	3.58959700	-0.34389600	3.89056800
H	2.05103300	-0.96277300	3.30437800
H	3.36718800	-0.53570100	2.14173900

CH₄-Li-Pentacene 2

C	-3.59069100	-0.68392000	-0.37388900
C	-4.83968100	-1.35637000	-0.41990600
C	-6.02248400	-0.66518400	-0.39096600
C	-6.02144100	0.74304100	-0.30172500
C	-4.83748700	1.43035300	-0.24291400
C	-3.58970000	0.75529500	-0.28197200
C	-1.10523700	-0.69710800	-0.36810600
C	-2.35505600	-1.36457200	-0.37127700
C	-2.35277200	1.42780400	-0.19170400
C	-1.10399600	0.76272000	-0.27415100
C	1.35159300	-0.69546300	-0.30353100
C	0.11423200	-1.36932400	-0.37435000
C	0.11667300	1.42783400	-0.19619700
C	1.35241200	0.74839200	-0.21084300
C	3.79293100	-0.69551300	-0.23191800
C	5.03973700	-1.37613000	-0.23926400
C	6.21804600	-0.69176900	-0.16053500
C	6.21871300	0.72233900	-0.06950400
C	5.04100000	1.41204400	-0.05989000
C	3.79365100	0.73708800	-0.13985700
C	2.57320200	-1.36964800	-0.31101400
C	2.57467000	1.41687000	-0.13235400
H	-4.83619900	-2.44130200	-0.49727700
H	-6.96538400	-1.20080300	-0.44128400
H	-6.96347600	1.28221200	-0.28409200
H	-4.83213000	2.51633200	-0.18204400
H	-2.35967900	-2.45205600	-0.42508800

H	-2.40659400	2.48809200	-0.30162200
H	0.06649100	-2.48987200	-0.36740000
H	0.06648700	2.49071000	-0.36317800
H	4.98610000	-2.48441300	-0.26000400
H	7.11319400	-1.24372600	-0.20509100
H	7.11317500	1.24436500	-0.20280200
H	4.98605800	2.48511600	-0.25547700
H	2.52611100	-2.48492300	-0.32197300
H	2.52607700	2.48569800	-0.31757500
Li	-2.37745800	-0.00165100	1.45673500
N	-0.59274800	-0.00346300	2.74667200
N	0.41109000	-0.00408900	3.18154200

N₂-Li-Pentacene 3

C	-3.90441400	-0.71090800	-0.17022000
C	-5.14806700	-1.39255800	-0.13807700
C	-6.32830700	-0.70688300	-0.06572000
C	-6.32989500	0.70694100	-0.02169600
C	-5.15131000	1.39864700	-0.05112400
C	-3.90599200	0.72339300	-0.12550600
C	-1.45833600	-0.71481300	-0.27982800
C	-2.68273600	-1.38768600	-0.24038600
C	-2.68586000	1.40622500	-0.15295600
C	-1.45980600	0.74015500	-0.23395300
C	1.02795000	-0.70844600	-0.41094800
C	-0.21016800	-1.38519000	-0.30826400
C	-0.21285000	1.41347300	-0.21786600
C	1.02685600	0.74692100	-0.36264400
C	3.47632700	-0.69349600	-0.50961700
C	4.72256700	-1.36918400	-0.57602300
C	5.90172800	-0.67819100	-0.59444500
C	5.90075900	0.73571400	-0.54659200
C	4.72065900	1.42229900	-0.48144300
C	3.47536600	0.74197800	-0.46076000
C	2.25642300	-1.37519300	-0.48139500
C	2.25449100	1.41859000	-0.38689300
H	-5.14212400	-2.47954700	-0.17499100
H	-7.27088500	-1.24536800	-0.04396600
H	-7.27375300	1.24080700	0.03339400

H	-2.35526200	2.51343800	-0.10807400
H	0.11379500	-2.45587500	-0.44617700
H	0.11861200	2.51455600	-0.12790100
H	5.03452000	-2.46141200	-0.31113900
H	7.16203800	-1.22835400	-0.16860000
H	7.16320100	1.25466600	-0.00880800
H	5.03658200	2.49758200	0.00802700
H	2.57447300	-2.45619900	-0.38480700
H	2.57687000	2.50386900	-0.06600800
Li	-2.38713000	-0.07874400	1.48410900
C	-0.85660600	-0.38568500	3.27909300
H	-0.30223600	-0.71350700	2.39316100
H	-0.21774500	-0.50933400	4.15213700
H	-1.10890400	0.67816800	3.20552500
H	-1.74794100	-1.00431400	3.44076900

CH₄-Li-Pentacene 3

C	3.58705400	0.75486100	-0.30910000
C	4.83180500	1.43516400	-0.29029200
C	6.01336500	0.75066200	-0.35748000
C	6.01521100	-0.66072700	-0.44804500
C	4.83553700	-1.35153200	-0.46899000
C	3.58895400	-0.67776600	-0.40092000
C	1.13708300	0.75916600	-0.26045300
C	2.36414700	1.42997800	-0.23798200
C	2.36742100	-1.35960700	-0.41621900
C	1.13869300	-0.69392000	-0.35375600
C	-1.35207400	0.75105500	-0.18362800
C	-0.10581100	1.42193600	-0.11983600
C	-0.10215800	-1.37213600	-0.29961200
C	-1.35006900	-0.70209700	-0.27613600
C	-3.80042300	0.73343900	-0.12653200
C	-5.04694100	1.40731900	-0.05796300
C	-6.22622100	0.71650100	-0.07719600
C	-6.22425500	-0.69523900	-0.16668500
C	-5.04301200	-1.37959200	-0.23460000
C	-3.79842900	-0.69885900	-0.21720900
C	-2.57988900	1.41536900	-0.10591400
C	-2.57602000	-1.37444600	-0.28262700
H	4.82560000	2.52083800	-0.22467100
H	6.95629000	1.28884600	-0.34479100
H	6.95958000	-1.19360000	-0.50433100

H	-5.14812400	2.48583000	-0.02028100
H	-2.68329000	-2.47592400	-0.27964900
H	-2.68924200	2.49477900	-0.12384400
H	-0.20818500	-2.47364000	-0.32697700
H	-0.21302700	2.50089300	-0.16679300
H	4.71868500	-2.45608400	-0.61667600
H	6.84543200	-1.21241200	-0.64829100
H	6.84369300	1.27369700	-0.56424500
H	4.71529200	2.50944800	-0.44832800
H	2.25860400	-2.46353400	-0.52144100
H	2.25521000	2.50715700	-0.35391200
Li	-0.08273000	-0.03404400	1.49743100
N	1.73890800	-0.13042800	2.71537500
N	2.76503400	-0.16881300	3.09345800

N₂-Li-Phenanthrene 1

C	4.07147300	-0.54099500	0.71652200
C	3.45289600	0.67992700	0.68308100
C	2.11441700	0.81276300	0.25390500
C	1.39333800	-0.34910600	-0.15176600
C	2.06521800	-1.59170300	-0.10930500
C	3.36593700	-1.69048500	0.31294700
C	1.48196400	2.07597800	0.21662300
C	0.02383100	-0.22568400	-0.57628900
C	-0.57469500	1.06500900	-0.59126000
C	0.18415000	2.19414500	-0.19780500
C	-1.95361400	1.19532100	-0.96643500
H	-2.39726400	2.18635500	-0.97182600
C	-2.66671800	0.09433100	-1.46576000
C	-2.08651800	-1.16907100	-1.45015700
C	-0.77589500	-1.34468300	-0.95927300
H	2.04825000	2.95266400	0.52004400
H	5.10135100	-0.62527900	1.04945900
H	3.98648200	1.57734100	0.98772800
H	1.54950700	-2.49379500	-0.42163800
H	3.85550400	-2.65943100	0.33238800
H	-0.29689600	3.16885400	-0.22795100
H	-3.68180600	0.22311300	-1.82932300
H	-2.64268300	-2.02774700	-1.81340700

H	4.83242500	-2.43668300	-0.54332800
H	2.36464100	2.51695700	-0.17103000
H	2.37018000	-2.44624000	-0.48931100
H	-0.10673800	2.50723800	-0.03423400
H	-0.10002200	-2.45957300	-0.35108700
H	-5.04391900	2.49297000	0.00777900
H	-7.17082100	1.24947700	-0.02621400
H	-7.16732600	-1.23305400	-0.18356300
H	-5.03682000	-2.46483600	-0.30658700
H	-2.58338500	2.50247400	-0.04230200
H	-2.57634300	-2.46084900	-0.35732000
Li	-0.03561600	-0.08309000	1.54832300
C	1.54888500	-0.37857400	3.29999300
H	1.25671900	0.67668600	3.25588500
H	2.21658900	-0.49622000	4.15200900
H	0.68500000	-1.03164000	3.47292300
H	2.08808700	-0.66924900	2.39230500

CH₄-Li-Phenanthrene 1

C	3.69019600	-0.34400400	-0.06157600
C	3.00142200	0.83384900	-0.16625900
C	1.59474500	0.85556500	-0.29771200
C	0.87704300	-0.38110900	-0.32664400
C	1.62411300	-1.57865700	-0.21779900
C	2.98820600	-1.56645500	-0.08766400
C	0.88802000	2.07113100	-0.39872700
C	-0.55623600	-0.37817700	-0.43777600
C	-1.23091500	0.87475300	-0.52316500
C	-0.47845400	2.07393700	-0.51367100
C	-2.66712500	0.90114800	-0.54213400
H	-3.16846800	1.86186100	-0.60811200
C	-3.40498500	-0.30227000	-0.64862100
C	-2.75564700	-1.51961000	-0.57374800
C	-1.34413000	-1.57131600	-0.39244500
H	1.44472200	3.00467500	-0.38659300
H	4.77135700	-0.34076800	0.03815100
H	3.52941700	1.78489600	-0.15167700
H	1.11215000	-2.53503600	-0.24647800
H	3.53218900	-2.50319000	-0.01101100
H	-1.01938700	3.01436400	-0.59288800
H	-4.48420100	-0.26494600	-0.76659400
H	-3.31909400	-2.44561000	-0.63781900

H	-0.35279800	-2.34185700	-0.95373500
Li	-2.17454200	-0.39331800	0.59260000
N	-4.85808500	-0.42506400	2.21394400
N	-3.88773200	-0.43418400	1.68038400

N₂-Li-Phenanthrene 2

C	-3.87049000	0.20083300	0.31479800
C	-3.12979500	-0.90453100	-0.03693400
C	-1.73744300	-0.81271100	-0.28263900
C	-1.10722600	0.46835300	-0.15676600
C	-1.89592300	1.56676300	0.19078500
C	-3.25774500	1.44932300	0.43148100
C	-0.96753300	-1.95527900	-0.63490900
C	0.34601000	0.56995900	-0.38394300
C	1.05853500	-0.58643500	-0.85360100
C	0.40102400	-1.83471200	-0.94122800
C	2.44117700	-0.44605900	-1.15813100
H	2.97092900	-1.31278600	-1.54681900
C	3.09943600	0.73864700	-0.95717000
C	2.41820500	1.85145600	-0.44028200
C	1.06379100	1.75255300	-0.17083200
H	-1.47339900	-2.91040200	-0.74394000
H	-4.93742700	0.10083600	0.49305000
H	-3.60716800	-1.87593200	-0.14253900
H	-1.44031300	2.54898700	0.26697700
H	-3.84018500	2.32534300	0.69691500
H	0.96299300	-2.69597000	-1.29243800
H	4.15684900	0.81501000	-1.19473600
H	2.94263000	2.78488900	-0.26631500
H	0.54682900	2.62799500	0.21020300
Li	0.13349100	-1.33784100	1.14307400
N	1.91462000	-0.91467200	2.09837800
N	2.96333100	-0.62010200	2.26828500

N₂-Li-Chrysene 1

C	4.32079800	-1.34664800	0.13536400
C	5.22462400	-0.40991900	0.57515400

H	-0.86336700	-2.53978000	-0.33237800
Li	-2.22786200	-0.36374100	1.21974700
C	-0.82399500	0.22224600	3.10954100
H	-0.06901200	0.10657800	2.32635400
H	-0.33039300	0.49200800	4.04228200
H	-1.51525700	1.03381600	2.85494100
H	-1.35062800	-0.72383100	3.28298400

CH₄-Li-Phenanthrene 2

C	3.68030800	-0.34802500	-0.04285200
C	2.98299100	0.82687100	-0.17979200
C	1.56560600	0.84161900	-0.30621100
C	0.87499600	-0.42090000	-0.30170800
C	1.62495300	-1.58989700	-0.15139900
C	3.00667800	-1.57371500	-0.02113000
C	0.84009400	2.05164100	-0.39885700
C	-0.59716100	-0.42870500	-0.43924200
C	-1.28664800	0.82636700	-0.58269300
C	-0.56983100	2.04289500	-0.54063800
C	-2.70504400	0.79695200	-0.70500100
H	-3.22671200	1.74310400	-0.83022800
C	-3.40591500	-0.38358300	-0.67036700
C	-2.73607300	-1.60200400	-0.51424700
C	-1.35099100	-1.60365700	-0.40601000
H	1.38789800	2.98949000	-0.41411300
H	4.76310500	-0.32353600	0.04525400
H	3.50795700	1.77912000	-0.20272200
H	1.11934600	-2.55075500	-0.15049600
H	3.55543700	-2.50343300	0.08501200
H	-1.11504300	2.97486700	-0.66043200
H	-4.48802700	-0.36921800	-0.76924600
H	-3.28675900	-2.53629400	-0.49062600
H	-0.84493100	-2.55829000	-0.29866400
Li	-0.04513100	1.12436100	1.32642300
C	-1.27447700	0.13893900	3.11969900
H	-1.62914000	-0.41227200	2.24296800
H	-0.20239600	-0.02905700	3.27653100
H	-1.50889200	1.20608500	3.02777900
H	-1.79337100	-0.23168500	4.00240600

CH₄-Li-Chrysene 1

C	-3.99673000	1.15544200	0.01800500
C	-4.87481500	0.09943000	0.08422700

C	4.79261400	0.89987200	0.81460400
C	3.47729300	1.24861000	0.61151700
C	2.52649900	0.31241900	0.16071100
C	2.97208200	-1.01144800	-0.07777800
C	2.03990200	-1.98869800	-0.53748700
C	1.13433300	0.64669100	-0.06299300
C	0.23125900	-0.36298800	-0.50545700
C	0.73748400	-1.67508600	-0.73914100
C	-2.99655400	1.58788900	-0.65242900
C	-3.89454200	0.63158900	-1.14788600
C	-3.46199400	-0.67377200	-1.36087900
C	-2.12821300	-1.03489500	-1.08824200
C	0.64162100	1.94628800	0.13737700
C	-0.68110100	2.25421400	-0.07390400
C	-1.60868200	1.27751700	-0.48519400
C	-1.15485200	-0.05892300	-0.70522500
H	4.63583000	-2.36958300	-0.05710900
H	6.26350200	-0.68057400	0.73593100
H	5.49878500	1.64756600	1.16308100
H	3.17814500	2.27226300	0.80886500
H	2.39995500	-2.99643400	-0.72897600
H	0.06834600	-2.44911500	-1.09864900
H	-3.32122100	2.60958500	-0.47826200
H	-4.92759300	0.90322100	-1.34272800
H	-4.15590400	-1.42485600	-1.72550300
H	-1.83119900	-2.06310700	-1.25366300
H	1.31040600	2.73651700	0.45948300
H	-1.03543900	3.27040700	0.08075200
Li	-3.16112600	-0.19075900	0.73740000
N	-4.68143700	-0.84560700	1.94165100
N	-5.55223000	-1.20294700	2.52062100

N₂-Li-Chrysene 2

C	-3.61092900	1.28772300	-0.31230400
C	-4.47799500	0.28082600	-0.67326500
C	-3.97329100	-0.97830100	-1.00342300
C	-2.61278200	-1.21169100	-0.95316800
C	-1.70750300	-0.21114600	-0.57122100
C	-2.22169100	1.07326500	-0.25842100

C	-4.37861100	-1.20719300	0.02470400
C	-3.02624100	-1.43477900	-0.09799000
C	-2.10157100	-0.37525100	-0.16723300
C	-2.61290500	0.94488300	-0.10762800
C	-1.70934600	2.04816700	-0.18295600
C	-0.67127900	-0.58235300	-0.29309000
C	0.20066800	0.54955000	-0.35741000
C	-0.37390500	1.85310500	-0.30426300
C	3.56713200	-1.15133900	-0.50773200
C	4.44910000	-0.05332500	-0.60522400
C	3.94668300	1.23610700	-0.56655400
C	2.55185200	1.45752900	-0.43146100
C	-0.10744800	-1.86252600	-0.35299100
C	1.25546400	-2.04480600	-0.45859000
C	2.14845400	-0.95703000	-0.49801300
C	1.62027500	0.37362200	-0.45216100
H	-4.36187900	2.17911400	0.05954400
H	-5.94174800	0.27557600	0.17978400
H	-5.06248400	-2.04940700	0.07388200
H	-2.67662700	-2.46073800	-0.14293200
H	-2.11907700	3.05462400	-0.14969800
H	0.27097400	2.72265800	-0.37285100
H	3.94925900	-2.16750800	-0.53646200
H	5.51821800	-0.22307100	-0.69243900
H	4.61738200	2.08782300	-0.62672700
H	2.19709200	2.47988700	-0.39035900
H	-0.74345600	-2.74017000	-0.31800400
H	1.66693400	-3.05033400	-0.50577500
Li	3.25201300	0.19090700	1.23766300
C	1.76441400	-0.09657000	3.11755600
H	1.04483000	0.04016600	2.30464500
H	1.22160500	-0.23289900	4.05189800
H	2.36328900	-0.99927800	2.95032600
H	2.39251000	0.79486300	3.23498800

CH₄-Li-Chrysene 2

C	-3.73894700	1.17828900	-0.24624800
C	-4.60352400	0.13778100	-0.50396100
C	-4.09398500	-1.13901700	-0.74646200
C	-2.72926700	-1.35448400	-0.71327100
C	-1.82642000	-0.31950600	-0.43368400
C	-2.34599200	0.98249800	-0.21099800

C	-1.32845000	2.11868400	0.12224000
C	-0.27413600	-0.45475900	-0.45040300
C	0.59846200	0.65595000	-0.15767600
C	0.02367100	1.90822900	0.14716400
C	3.95494000	-1.07650300	-0.22933700
C	4.83184900	-0.01096200	-0.14937700
C	4.33819000	1.28886400	-0.11045000
C	2.96801500	1.51194300	-0.13861400
C	0.27813700	-1.74376100	-0.52423200
C	1.64575600	-1.97184500	-0.34548600
C	2.56290300	-0.87542900	-0.25984900
C	2.05144500	0.45579100	-0.19268700
H	-3.99017300	2.27597300	-0.06294100
H	-5.54714000	0.46669800	-0.70874400
H	-4.64693000	-1.77418400	-1.30569400
H	-2.24481800	-2.19448800	-1.23116600
H	-1.74169200	3.09018300	0.37809700
H	0.67416700	2.73404100	0.41956000
H	4.33087200	-2.09562200	-0.28085900
H	5.90281600	-0.18925100	-0.13126700
H	5.02026300	2.13224000	-0.06933800
H	2.60617600	2.53509300	-0.13276700
H	-0.37064900	-2.59884000	-0.68520800
H	2.04356300	-2.98076900	-0.40275200
Li	0.74891000	-0.97906200	1.45554700
N	-1.07868200	-0.85637500	2.48379500
N	-2.14456700	-0.67864600	2.68899000

N₂-Li-Pyrene 1

C	3.49580000	0.00075900	-0.42317600
C	2.81924200	1.21674300	-0.39132600
C	1.38023900	1.24368600	-0.43175800
C	0.66847500	0.00115600	-0.46066800
C	1.37984700	-1.24161100	-0.43482800
C	2.81879200	-1.21516700	-0.39359900
C	0.64261700	2.44271100	-0.39522100
C	-0.75721300	0.00133700	-0.44327200
C	-1.46959900	1.23569900	-0.41202300
C	-0.73186200	2.44312600	-0.39255000

C	-1.45467400	2.06674100	0.04465900
C	-0.38333300	-0.53968700	-0.34969100
C	0.48229700	0.60881700	-0.19767800
C	-0.09724300	1.87370900	0.02209200
C	3.86301100	-1.08045100	-0.20324900
C	4.72334500	-0.00095400	-0.27307400
C	4.21134200	1.28885100	-0.36811200
C	2.83642500	1.48812900	-0.37570300
C	0.18279700	-1.81896100	-0.31507300
C	1.56423000	-2.01289800	-0.14135400
C	2.46562800	-0.90429900	-0.21060100
C	1.93697800	0.42185700	-0.27498300
H	-4.12309200	2.18056000	-0.07080400
H	-5.67511400	0.31157600	-0.52968400
H	-4.76588500	-1.96168000	-0.97109500
H	-2.35506500	-2.35094200	-0.92773600
H	-1.87097100	3.05272500	0.23077400
H	0.55282100	2.72799200	0.18898700
H	4.25502200	-2.09356900	-0.15193700
H	5.79723800	-0.16284200	-0.26955300
H	4.88041600	2.13976200	-0.44796900
H	2.45591400	2.49973500	-0.47629400
H	-0.45709700	-2.69420800	-0.36918200
H	1.97460500	-3.01779000	-0.11122100
Li	0.73137600	-0.83772900	1.53255000
C	-0.87584500	-0.33930800	3.22297600
H	-0.71373700	0.58615200	2.65925700
H	-1.32117700	-1.10303900	2.57709200
H	0.04981800	-0.69649700	3.69092600
H	-1.57874500	-0.12738800	4.02727900

CH₄-Li-Pyrene 1

C	-3.40391900	0.00464300	-0.56549900
C	-2.73099700	-1.21195600	-0.49373200
C	-1.29169500	-1.23971900	-0.44633600
C	-0.58014700	0.00299200	-0.41324800
C	-1.29065800	1.24648800	-0.43860200
C	-2.72999600	1.22025000	-0.48680900
C	-0.55802500	-2.43891200	-0.38008200
C	0.84156300	0.00204400	-0.30421100
C	1.55131900	-1.23320000	-0.24650100
C	0.81421900	-2.44000300	-0.28915300

C	-2.87987400	1.20861400	-0.37736900
H	-3.42248600	2.14985100	-0.35771000
C	-3.55924200	0.00160300	-0.36555600
C	-2.88025700	-1.20553600	-0.38147500
C	-1.46996500	-1.23289300	-0.41602500
C	-0.73258200	-2.44058700	-0.40004900
C	0.64187700	-2.44056900	-0.40207200
H	1.18785700	-3.38128400	-0.38766600
H	-1.27903200	-3.38019700	-0.38124500
H	1.18884200	3.38324800	-0.37834500
H	4.58337700	0.00052400	-0.42261300
H	3.36327100	2.15620700	-0.40220700
H	3.36260800	-2.15473100	-0.40617000
H	-1.27802600	3.38283300	-0.37066000
H	-4.64575500	0.00173200	-0.33901100
H	-3.42312300	-2.14668700	-0.36497800
N	-0.68869600	-0.01035200	2.94372600
N	0.35376800	-0.00729800	2.60969700
Li	2.16973200	-0.00079100	1.35414500

N₂-Li-Pyrene 2

C	-3.09269300	0.72428700	-0.93525800
C	-2.57481800	-0.55363700	-1.08569100
C	-1.20607300	-0.80704600	-0.83873300
C	-0.36080100	0.29217800	-0.45620700
C	-0.91728000	1.58903000	-0.29655000
C	-2.29749500	1.78473000	-0.53843500
C	-0.63308000	-2.10118000	-0.90941000
C	1.03575900	0.07708000	-0.21477800
C	1.59815000	-1.24093200	-0.34738900
C	0.72772300	-2.31422100	-0.67770600
C	2.97870400	-1.41217200	-0.11031500
H	3.41068800	-2.40259200	-0.22606400
C	3.77277200	-0.33258300	0.25430800
C	3.24226800	0.93407200	0.40353400
C	1.86594500	1.16350300	0.17146300
C	1.27521300	2.44529900	0.31030500
C	-0.05584100	2.64754200	0.09035400
H	-0.48388000	3.64071900	0.20384800

C	2.95821300	-1.20656400	-0.13967400
H	3.49946100	-2.14806700	-0.10159700
C	3.63611900	0.00018300	-0.08714100
C	2.95918700	1.20780900	-0.13148600
C	1.55232600	1.23628700	-0.23821300
C	0.81620800	2.44395700	-0.27295100
C	-0.55597700	2.44461800	-0.36425500
H	-1.10081900	3.38580400	-0.39014300
H	1.36107800	3.38358600	-0.22641700
H	-1.10365100	-3.37946100	-0.41191400
H	-4.48939700	0.00527300	-0.63338700
H	-3.27346700	-2.15092800	-0.54613200
H	-3.27165000	2.15996900	-0.53395600
H	1.35834300	-3.38035800	-0.24899700
H	4.72009800	-0.00051200	-0.00770600
H	3.50117200	2.14861200	-0.08706300
Li	-2.20937200	-0.00019500	1.28210300
C	-0.65550700	-0.02557000	3.10567800
H	-1.68614400	-0.02943900	3.48254200
H	0.00015700	-0.03783100	3.97515700
H	-0.44132600	-0.91684300	2.50641500
H	-0.43913300	0.88070100	2.53017100

CH₄-Li-Pyrene 2

C	-3.44859300	0.01092000	-0.50886600
C	-2.77186100	-1.20011700	-0.48628800
C	-1.35669900	-1.23402200	-0.43560100
C	-0.64107000	0.01600700	-0.41197700
C	-1.35935000	1.24252600	-0.42238300
C	-2.77496000	1.21806300	-0.47410200
C	-0.61312000	-2.43611200	-0.35699300
C	0.79004800	0.02433000	-0.32974200
C	1.51940400	-1.21751900	-0.27705500
C	0.78545200	-2.42843600	-0.27965100
C	2.93179200	-1.16715000	-0.18769700
H	3.48737800	-2.10082900	-0.16715800
C	3.59319400	0.05124000	-0.14203800
C	2.90530000	1.25023500	-0.17124700
C	1.49196600	1.25899000	-0.26253000
C	0.74039400	2.45972900	-0.28962800
C	-0.62362100	2.45163900	-0.36661000
H	-1.17509200	3.38881400	-0.38493000

H	1.91403200	3.27569900	0.60132800
H	-1.27287300	-2.93537900	-1.18672800
H	-4.14802200	0.89391400	-1.13209900
H	-3.21221200	-1.37682100	-1.39756400
H	-2.71571600	2.78045800	-0.42286700
H	1.14739600	-3.31230500	-0.77341800
H	4.83411700	-0.49062700	0.42630600
H	3.87263200	1.77028700	0.69216100
N	-3.03355900	-0.91286100	2.24241600
N	-1.97045400	-1.18366600	2.15936600
Li	-0.15625900	-1.51445100	1.16188700

N₂-Li-Picene 1

C	-4.23470500	-1.69589000	0.11856600
C	-3.50265500	-0.48930400	0.10237200
C	-5.59221900	-1.70800600	0.32580700
C	-4.21957300	0.71581400	0.30981100
C	-2.07660000	-0.43587900	-0.11104900
C	-5.61184800	0.67947700	0.51941400
C	-3.51165100	1.94714500	0.30336500
C	-6.29358900	-0.51006900	0.52841500
C	-1.40613700	0.80185900	-0.10736800
C	-2.17079100	1.98660100	0.10545900
C	0.02178200	0.85658600	-0.31315900
C	-1.31399200	-1.61570000	-0.33266900
C	0.03038900	-1.57088900	-0.52449900
C	0.75202000	-0.35031800	-0.51409200
C	2.17531500	-0.32402400	-0.69448900
C	0.73087600	2.07384500	-0.32795300
C	2.84628700	0.93333500	-0.69197200
C	2.08948400	2.10994300	-0.51716500
C	4.27131200	0.97354700	-0.82794600
C	2.96898500	-1.50227500	-0.85027200
C	4.35128100	-1.42357300	-1.11081600
C	4.99868700	-0.19233000	-1.11014300
H	-3.72634100	-2.64148000	-0.03334600
H	-6.12613200	-2.65348900	0.33260700
H	-6.13620400	1.61929300	0.67510200
H	-4.06990600	2.86640900	0.46291300

H	1.27976700	3.40316200	-0.24799300
H	-1.15087500	-3.38065700	-0.37446100
H	-4.53464600	0.00814900	-0.55548400
H	-3.31628100	-2.14001300	-0.51838000
H	-3.31681600	2.15929200	-0.49150900
H	1.33255000	-3.36692000	-0.24053800
H	4.67843800	0.06101700	-0.08110800
H	3.43528900	2.19754100	-0.13244400
Li	-0.01776500	-1.32979300	1.43678500
C	-0.76516600	0.19028700	3.12274100
H	-0.49929400	-0.77945900	3.56219400
H	-1.08559100	0.83027000	3.94356400
H	0.09599500	0.66551300	2.64050400
H	-1.59618100	0.09984300	2.41538700

CH₄-Li-Picene 1

C	-3.89352700	-1.65651800	-0.02090300
C	-3.13942900	-0.46369200	-0.06852000
C	-5.26255300	-1.63607000	0.08508900
C	-3.84874400	0.76251400	-0.00250600
C	-1.70166000	-0.44457500	-0.17866000
C	-5.25302500	0.75903200	0.10541200
C	-3.12068400	1.98062100	-0.04731500
C	-5.95545400	-0.41767700	0.14918600
C	-1.01112000	0.78133400	-0.21613600
C	-1.76828400	1.98754600	-0.14923900
C	0.43009000	0.80561100	-0.31722300
C	-0.94513000	-1.64891700	-0.25643200
C	0.41005500	-1.63407900	-0.35279200
C	1.15359700	-0.42611400	-0.37927900
C	2.58638600	-0.43780700	-0.44578900
C	1.16053200	2.00461600	-0.35590100
C	3.28221400	0.81046300	-0.47139200
C	2.53483200	2.00526100	-0.43806800
C	4.71419400	0.82081500	-0.45495600
C	3.36581100	-1.63592600	-0.41458600
C	4.78035800	-1.59613600	-0.53153000
C	5.44646700	-0.38364100	-0.55285400
H	-3.39247200	-2.61700700	-0.06773500
H	-5.81256100	-2.57180700	0.11872000
H	-5.77017500	1.71451800	0.15308500
H	-3.67245900	2.91632800	0.00106100

H	-7.36669200	-0.52810800	0.69107300
H	-1.67587300	2.95053600	0.11225500
H	-1.80811700	-2.58008000	-0.35734200
H	0.55561000	-2.50378300	-0.69782400
H	0.20777200	3.01308300	-0.19359900
H	2.61106300	3.06387400	-0.52850800
H	4.76397000	1.94132100	-0.81987300
H	2.50019500	-2.47873900	-0.84842800
H	4.91116400	-2.33293100	-1.30664300
H	6.06725100	-0.13748100	-1.29470100
Li	4.11576400	-0.51192300	0.85910700
N	5.64117600	-0.43488700	2.20540300
N	6.52011200	-0.36825700	2.87335400

N₂-Li-Picene 2

C	-3.91026500	-1.54686800	0.73059200
C	-3.10030200	-0.57684700	0.10433400
C	-5.27971900	-1.44359300	0.73603100
C	-3.74816600	0.51453600	-0.52713100
C	-1.65650700	-0.65658000	0.08524300
C	-5.15512700	0.59946300	-0.51003200
C	-2.96427400	1.50254800	-1.17774500
C	-5.91311800	-0.35938200	0.10999700
C	-0.91315700	0.35911800	-0.55059400
C	-1.60765700	1.42155000	-1.18800800
C	0.54090700	0.31070800	-0.55142500
C	-0.96285200	-1.73371800	0.69014600
C	0.40487800	-1.82265800	0.62339800
C	1.19321300	-0.84589100	-0.00497000
C	2.65208300	-0.97909700	-0.11573700
C	1.33529700	1.37166700	-1.03527000
C	3.41085400	0.12799400	-0.60143500
C	2.73365100	1.31815900	-0.99864100
C	4.81600800	0.01627500	-0.66770800
C	3.33798800	-2.14317700	0.24752800
C	4.71989700	-2.23029300	0.17295200
C	5.45963800	-1.14023500	-0.28293600
H	-3.45296500	-2.39835700	1.22197500
H	-5.87527000	-2.20712900	1.22710700

H	-7.03781800	-0.41011300	0.23203900
H	-1.25736700	2.94278400	-0.18100200
H	-1.45312100	-2.60639700	-0.24821600
H	0.92945400	-2.58391700	-0.42238500
H	0.65018200	2.96002600	-0.32377900
H	3.07457100	2.94893100	-0.46973800
H	5.22562100	1.77861100	-0.47203100
H	2.87907500	-2.60295000	-0.38736500
H	5.33579800	-2.52725300	-0.59043600
H	6.52969600	-0.35458800	-0.62533400
Li	4.20470600	-0.47730300	1.27297600
C	2.74043400	0.04063600	3.12800000
H	3.42995500	0.87062300	2.93616400
H	2.19605900	0.27156300	4.04264500
H	2.02540500	-0.05888700	2.30566800
H	3.27388900	-0.90232000	3.29807300

CH₄-Li-Picene 2

C	-3.70038000	-1.65642800	0.05995000
C	-2.93279500	-0.49398200	-0.16398900
C	-5.07313800	-1.62269600	0.06036600
C	-3.62864400	0.72085300	-0.39570500
C	-1.48675300	-0.50104200	-0.16184000
C	-5.03902800	0.73044500	-0.39299700
C	-2.89072900	1.90655100	-0.63970000
C	-5.75396400	-0.41660000	-0.16825600
C	-0.79189800	0.70837000	-0.37274300
C	-1.52929100	1.89159200	-0.63019300
C	0.66526400	0.73841100	-0.30955100
C	-0.74497700	-1.69113500	0.05242200
C	0.63212300	-1.68523100	0.00010600
C	1.37275600	-0.51554800	-0.20735300
C	2.84065100	-0.52283500	-0.30544200
C	1.39909500	1.93151400	-0.24733400
C	3.54179700	0.71884700	-0.21327900
C	2.80094100	1.93265800	-0.09994400
C	4.95300600	0.70239000	-0.22729200
C	3.58310500	-1.69720200	-0.45381400
C	4.97172200	-1.68769600	-0.46910100
C	5.65453500	-0.47995400	-0.34634800
H	-3.20480400	-2.60467400	0.23614800
H	-5.63453000	-2.53532600	0.23621100

H	-5.62797000	1.44559300	-1.00282600
H	-3.47137100	2.32332800	-1.67841100
H	-6.99608800	-0.28411800	0.11693600
H	-1.04735400	2.18675200	-1.71366800
H	-1.50917500	-2.51740300	1.20055500
H	0.88652800	-2.68108000	1.08078900
H	0.86592300	2.27014400	-1.41900800
H	3.32059500	2.14985400	-1.37713100
H	5.38382700	0.86564200	-1.03972100
H	2.78109600	-3.01163300	0.58382500
H	5.21961400	-3.14983300	0.45997000
H	6.54180600	-1.20521700	-0.34670200
Li	1.90383100	1.19666200	1.03595500
N	1.80592600	3.06254800	1.82299900
N	1.75260200	4.11479400	2.15513100

N₂-Li-Picene 3

C	3.65127600	1.05573800	-1.04422200
C	2.88618000	0.04009100	-0.44452800
C	5.02687300	1.01821700	-1.04422400
C	3.57173100	-1.04778600	0.15483300
C	1.43047500	0.07013100	-0.42332000
C	4.98215000	-1.06435900	0.14431500
C	2.82973000	-2.09940400	0.74989600
C	5.70025600	-0.05223300	-0.43982200
C	0.72308700	-1.03692700	0.13891000
C	1.46139800	-2.08770500	0.72652600
C	-0.74807700	-1.04981900	0.10249700
C	0.69706300	1.16956000	-0.90851500
C	-0.70798200	1.18730300	-0.87946400
C	-1.44861500	0.08107100	-0.40752400
C	-2.90187700	0.06796600	-0.41299300
C	-1.48977600	-2.15655100	0.57102900
C	-3.59392800	-1.06596200	0.08694900
C	-2.85779200	-2.17389300	0.57226800
C	-5.00508000	-1.07213100	0.08344100
C	-3.66453800	1.14615400	-0.89990400
C	-5.03903800	1.11881500	-0.89135300
C	-5.71824400	-0.00329300	-0.39340400

H	-5.54917000	1.67327000	-0.57577900
H	-3.43234300	2.82568000	-0.84774800
H	-6.83947300	-0.39636300	-0.16874700
H	-0.99688100	2.81166600	-0.84784400
H	-1.25424300	-2.62957500	0.23407500
H	1.15714400	-2.62676000	0.13430900
H	0.88521700	2.88687000	-0.26228500
H	3.34230400	2.87280600	-0.05321100
H	5.48070300	1.65053400	-0.15511400
H	3.06539600	-2.64372300	-0.57532100
H	5.51843100	-2.61754100	-0.58829600
H	6.74053500	-0.46508400	-0.36021700
Li	1.85434300	0.85550400	1.56456400
C	0.21609800	0.51735500	3.26291400
H	-0.10605100	1.37887100	2.66874300
H	-0.50453000	0.37647900	4.06710200
H	0.22043400	-0.38884000	2.64688100
H	1.19185700	0.69336000	3.73213700

CH₄-Li-Picene 3

C	-3.53938500	-1.57775500	-0.66916200
C	-2.77923300	-0.42599500	-0.41864700
C	-4.91810900	-1.54252100	-0.70634900
C	-3.46201400	0.80438800	-0.22682800
C	-1.32035100	-0.45766800	-0.33977700
C	-4.87170500	0.81545200	-0.26485700
C	-2.72074700	1.99473900	-0.00002800
C	-5.58957100	-0.33327900	-0.49507600
C	-0.61220500	0.78935900	-0.21931400
C	-1.34581000	1.97314700	-0.02046300
C	0.86015600	0.78116400	-0.27924100
C	-0.59403200	-1.64983400	-0.28360700
C	0.81318900	-1.65889300	-0.13428600
C	1.55774900	-0.45671500	-0.18912200
C	3.00887500	-0.43907500	-0.14367800
C	1.59625400	1.97807500	-0.39575600
C	3.69954000	0.80018600	-0.22446300
C	2.96565100	2.00091700	-0.36708200
C	5.11069700	0.80809700	-0.17504400
C	3.77348900	-1.61573600	-0.02157300
C	5.14649800	-1.58197000	0.02769100
C	5.82410500	-0.35475800	-0.04972800

H	3.15641600	1.89018700	-1.52992600
H	5.58961400	1.81613200	-1.51853700
H	5.49119700	-1.90499300	0.60962100
H	3.36626500	-2.92237700	1.21352400
H	6.78567400	-0.08126300	-0.44033400
H	0.93425100	-2.91942500	1.18060100
H	1.21204200	2.02809500	-1.32301300
H	-1.21800500	2.05603800	-1.27723300
H	-0.96530400	-3.03389100	0.93251500
H	-3.39776800	-3.04382100	0.93547500
H	-5.51738100	-1.95037100	0.46882900
H	-3.16783800	2.02532800	-1.29619000
H	-5.59887300	1.96629400	-1.27449100
H	-6.80382100	-0.02354600	-0.38930400
Li	0.05085000	1.06898500	1.15748400
N	0.08442800	2.94615300	1.93260500
N	0.09690600	3.99967000	2.26563200

N₂-Li-Coronene 1

C	-3.49483000	0.68332700	-0.61519500
C	-2.28936300	1.42876400	-0.50804100
C	-1.06303100	0.71558700	-0.42429200
C	-1.05504800	-0.69630100	-0.42685900
C	-2.28757700	-1.42987900	-0.51708500
C	-3.50354800	-0.67616200	-0.61828500
C	0.15929500	1.43445300	-0.29258800
C	0.19216900	-1.40893500	-0.30929600
C	1.40453200	-0.69160500	-0.18739100
C	1.39080900	0.73247500	-0.18325400
C	2.64004200	-1.38736300	-0.06517500
C	2.61966800	-2.79342700	-0.05391900
C	1.44673000	-3.49841200	-0.13910100
C	0.19389300	-2.83671700	-0.25796900
C	-1.04189700	-3.52892100	-0.28534100
C	-2.25945200	-2.82703900	-0.43305800
H	-3.19713800	-3.37391500	-0.49095500
H	-1.03694300	-4.61419400	-0.24717300
H	-4.43169500	1.23108500	-0.69429100
H	-4.43983100	-1.22255700	-0.70275500

H	-3.03760100	-2.52211400	-0.85672900
H	-5.47846300	-2.44986900	-0.90890300
H	-5.38351900	1.76304100	-0.11377000
H	-3.25731500	2.92462500	0.16510700
H	-6.67475500	-0.30171900	-0.52362100
H	-0.81168200	2.90618100	0.13133300
H	-1.10943100	-2.60358400	-0.32132600
H	1.31878500	-2.61536200	-0.08755000
H	1.06262800	2.91311300	-0.53085300
H	3.50561000	2.93845200	-0.46607200
H	5.62233700	1.76541700	-0.24073300
H	3.27645700	-2.57863200	0.03398900
H	5.70751300	-2.50663700	0.12187900
H	6.90907600	-0.33031500	-0.01336000
Li	-0.09098500	-0.57819700	1.53801200
C	-1.69350800	-0.14858800	3.25101200
H	-1.72055200	0.72717900	2.59311700
H	-2.39794800	0.01412400	4.06533500
H	-2.01189400	-1.04383300	2.70622100
H	-0.70348600	-0.28190500	3.70416300

CH₄-Li-Coronene 1

C	2.08192000	-3.00750900	-0.40645500
C	0.70309800	-2.72049300	-0.31661600
C	0.29655600	-1.35509000	-0.29517200
C	1.25797300	-0.32349100	-0.36321200
C	2.65417500	-0.63917300	-0.43037000
C	3.02418400	-2.01909400	-0.45935600
C	-1.08701500	-1.03328000	-0.18989100
C	0.83721000	1.05557800	-0.31637900
C	-0.53549100	1.37028700	-0.21077900
C	-1.50225800	0.32582500	-0.15081700
C	-0.96096600	2.72895100	-0.16460600
C	0.02105700	3.74102400	-0.22112300
C	1.35369000	3.45134800	-0.30225200
C	1.81806500	2.10065100	-0.34318100
C	3.18383100	1.76076500	-0.36755200
C	3.59739600	0.40566400	-0.40996400
H	4.65429300	0.15975300	-0.46302000
H	3.92296800	2.55663800	-0.39022300
H	2.39064100	-4.05064200	-0.43415400
H	4.08033500	-2.26677900	-0.53012100

H	3.56526400	-3.32464100	0.03068600	H	-0.30573600	4.77867800	-0.19768000
H	1.45551800	-4.58533400	-0.12344300	H	2.09081800	4.24921700	-0.34574600
C	-2.26862000	2.84052300	-0.48058700	C	-0.28697800	-3.73311000	-0.24665900
C	-1.09819300	3.53457200	-0.36589200	C	-1.60993800	-3.42780500	-0.15270800
C	0.14708800	2.85010500	-0.26321200	C	-2.05038400	-2.06846400	-0.11808100
H	-3.21511900	3.37179200	-0.55470100	H	0.03619400	-4.77162100	-0.27165600
H	-1.09668200	4.62096800	-0.34668000	H	-2.35836200	-4.21429200	-0.10199900
C	1.37305500	3.53546900	-0.13390800	C	-3.40973700	-1.72289200	-0.01468700
C	2.56085400	2.85612400	-0.03521500	C	-3.81139300	-0.40872600	0.02029300
C	2.60311800	1.44928400	-0.05392900	C	-2.87834600	0.64168000	-0.04404200
H	1.36033100	4.62239900	-0.11528300	H	-4.14649100	-2.52094900	0.03644100
H	3.49618800	3.40221600	0.06222500	H	-4.86731600	-0.16144900	0.09917800
C	3.84166200	-0.63632900	0.05083900	C	-2.34642700	3.01118800	-0.06329100
H	4.78068000	-1.17825600	0.13771500	H	-2.65833400	4.05303000	-0.03398700
C	3.82834900	0.72230600	0.05673300	C	-3.27222800	2.01502600	-0.00492100
H	4.75448800	1.28400600	0.14837300	H	-4.33129900	2.24669600	0.07193000
N	-1.51979600	-0.24580200	2.54290500	Li	2.43888200	0.72597800	1.41148100
N	-1.67139700	0.79283300	2.86763200	C	1.17557300	-0.30952900	3.16859700
Li	-1.29830800	-2.09805700	1.42487800	H	2.05611700	0.20375600	3.57516800
				H	0.63858500	-0.73500400	4.01512400
				H	0.50079500	0.38631200	2.65787100
				H	1.45874300	-1.12726300	2.49777400