

Electronic Supplementary Information for

On the Mechanism of the Shapiro Reaction: Understanding the Regioselectivity

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1. Cartesian coordinates and calculated potential energies (atomic units) of the optimized structures

THF

E= -232.449958 H

C	-2.92235300	1.62350400	0.00000000
O	-1.49345000	1.64020100	0.00000000
C	-0.97622900	2.97235200	0.00000000
C	-2.16065300	3.96095600	-0.00000100
C	-3.43237800	3.07938100	-0.00000100
H	-3.26722600	1.07184300	-0.88565900
H	-3.26722700	1.07184300	0.88565800
H	-0.33898300	3.10203800	0.88568000
H	-0.33898200	3.10203700	-0.88567900
H	-2.12792200	4.60997200	0.88025800
H	-2.12792200	4.60997100	-0.88026100
H	-4.05134100	3.27673600	0.88022100
H	-4.05134100	3.27673500	-0.88022300

Tosyl

E= -819.668544 H

C	-2.49923400	-0.89392300	-0.30002500
C	-2.88264100	0.44471000	-0.42134200
C	-3.84795200	0.98521400	0.42900700
C	-4.45307200	0.20272700	1.42644900
C	-4.06333300	-1.13923900	1.53710800
C	-3.09579600	-1.68098700	0.68512500
C	-5.48752600	0.80000800	2.35241100
S	-1.12132300	-1.57714800	-1.35389500
O	-1.31477300	-0.80083800	-2.65880500
O	-1.49521800	-3.05906800	-1.43427600
H	-2.43024300	1.05086900	-1.20284100
H	-4.14487400	2.02759900	0.31748000
H	-4.52849000	-1.76717100	2.29586600
H	-2.80936100	-2.72707900	0.76535500
H	-5.94193700	0.03572200	2.99209600
H	-5.04778000	1.56205100	3.01011200
H	-6.29392100	1.29172700	1.79344100

Butane

E= -158.4612146 H

C	-4.42193100	-1.37518000	-0.01386100
H	-4.08473100	-2.41937500	-0.04916800
H	-4.08110500	-0.88675000	-0.93601400
H	-5.51893100	-1.38079500	-0.02740400
C	-3.88050500	-0.65904800	1.22685100
H	-4.26518100	0.37088900	1.25178100
H	-4.26789200	-1.15128000	2.13090100
C	-2.34822300	-0.62544200	1.28920500

H	-1.96083400	-0.13320300	0.38515900
H	-1.96354900	-1.65537900	1.26426700
C	-1.80679800	0.09067100	2.52992800
H	-2.14771800	-0.39770300	3.45207700
H	-0.70979900	0.09618600	2.54353000
H	-2.14390600	1.13489700	2.56518700

TS_{Inv}

E= -1244.080595 H

C	1.17258800	4.96399600	-2.05364400
C	1.16593400	4.07710600	-0.80157300
C	1.37421500	2.58983000	-1.11639600
C	1.36319800	1.69049200	0.13558300
C	1.61290300	0.22253300	-0.20351100
N	0.67431200	-0.56563100	-0.48914300
N	-0.27457400	-1.40281300	-0.70709000
C	-2.65148500	-0.57452300	0.53312600
C	-2.83666200	0.72075700	1.01521200
C	-3.39121600	0.89671700	2.28400600
C	-3.75879900	-0.20007600	3.07392200
C	-3.56037500	-1.49360800	2.55940700
C	-3.00972600	-1.69031800	1.29802500
C	-4.35196700	-0.00912700	4.44707600
S	-1.92727200	-0.82371700	-1.08038300
O	-1.85906200	0.47901300	-1.76040800
O	-2.54180700	-1.99546200	-1.72902200
H	2.12504400	4.82861300	-2.58802100
H	0.38568800	4.62317800	-2.74293700
H	0.21199300	4.20571600	-0.26864500
H	1.95163800	4.41687900	-0.11024900
H	2.32773000	2.46313100	-1.64892300
H	0.58647300	2.24434300	-1.79915100
H	0.39474700	1.78069200	0.64175600
H	2.13530700	2.03564200	0.83730700
H	-0.09693800	-2.21563200	-1.31124100
H	-2.56560600	1.57509100	0.40470600
H	-3.54233700	1.90437100	2.66202500
H	-3.84521600	-2.35660700	3.15623800
H	-2.86825800	-2.69389700	0.90982800
H	-3.67869700	-0.39424400	5.22371100
H	-4.54049900	1.04763000	4.65903700
H	-5.29904800	-0.55270000	4.54748200
C	3.06732800	-0.22597600	-0.22726900
H	3.49793900	-0.19092600	0.78310900
H	3.15840300	-1.24688800	-0.60946400
H	3.67665300	0.43993100	-0.85277100
C	0.97095100	6.45622200	-1.75856300
H	0.01790500	6.59690500	-1.22838100
H	1.75722700	6.80062000	-1.07120600
C	0.98369800	7.32477800	-3.01978900
H	0.18402400	7.03252400	-3.71246100
H	0.84111400	8.38517300	-2.77799800
H	1.93634600	7.23175100	-3.55703300

1a

E= -1244.133148 H

C	0.98152100	5.18970800	-0.69771400
C	1.93387200	4.06973000	-0.25920000
C	1.32826600	2.66649000	-0.39639200
C	2.30997900	1.56431700	0.00917200
C	1.80983600	0.14340000	-0.10544400
N	0.58600800	-0.04438400	-0.44570800
N	0.13779100	-1.36474400	-0.49865600
C	-2.53352300	-0.88259000	-0.29796500
C	-2.93540600	0.44880500	-0.43195400
C	-3.89448500	0.95401700	0.44212100
C	-4.45907900	0.15076500	1.44587400
C	-4.03911600	-1.18318100	1.55079600
C	-3.07837100	-1.70714700	0.68784700
C	-5.48720900	0.71862000	2.39177700
S	-1.30386900	-1.54930600	-1.40610200
O	-1.29221600	-0.73637000	-2.62922300
O	-1.45033400	-3.00940100	-1.49888700
H	0.68704000	5.02559900	-1.74508300
H	0.05443700	5.13205700	-0.10792400
H	2.23379000	4.23716100	0.78615500
H	2.85743800	4.12791300	-0.85443600
H	1.00784700	2.50101400	-1.43347100
H	0.42085800	2.59305900	0.21654700
H	2.64131700	1.71620100	1.04883100
H	3.22866800	1.63998400	-0.59271100
H	0.81220300	-2.07081100	-0.81225200
H	-2.50936700	1.07273600	-1.20972400
H	-4.21311400	1.98857600	0.34176800
H	-4.47216100	-1.82236100	2.31568200
H	-2.76634000	-2.74276900	0.77315200
H	-5.94897000	-0.06550100	2.99951000
H	-5.03130800	1.44703300	3.07500500
H	-6.28157300	1.24331000	1.84813800
C	2.78421700	-0.96808100	0.19997600
H	2.38481200	-1.63984000	0.97072600
H	2.98504500	-1.57912600	-0.69179700
H	3.73973800	-0.56962500	0.54989100
C	1.58214900	6.59444400	-0.55715400
H	1.86958500	6.76261800	0.49078100
H	2.51196100	6.65098100	-1.14133200
C	0.63187700	7.70736800	-1.00767300
H	-0.29765200	7.69922500	-0.42392000
H	1.08899100	8.69730900	-0.88807100
H	0.35865600	7.59428400	-2.06467600

2

E= -1260.655053H

C	-2.80711100	0.10406700	0.93189700
H	-1.98806100	-0.28145700	1.55422800
H	-3.03303100	1.12015800	1.28275700
H	-3.69083300	-0.51635300	1.13066300
C	-2.42450300	0.10071500	-0.55315100
H	-2.24625400	-0.93544700	-0.88024700
H	-3.27642900	0.46155700	-1.15005200

C	-1.18054700	0.95131900	-0.88880200
H	-0.35457600	0.59282600	-0.24966000
H	-1.38115900	1.97868600	-0.53485700
C	-0.72637900	0.99075600	-2.36187400
H	-1.59549900	1.35706500	-2.95347700
H	-0.62203600	-0.06307300	-2.70568200
C	2.33018000	2.28994300	-4.15441900
H	1.94398900	3.03424900	-4.88620600
H	2.52780900	1.39966200	-4.79146300
C	3.69737600	2.81923900	-3.67604000
H	4.15803000	2.09925000	-2.97598300
H	3.55715700	3.73903400	-3.08016600
C	4.74848900	3.13268200	-4.76302900
H	4.33024000	3.87619900	-5.45922400
H	4.92177000	2.22493300	-5.36127800
C	6.08690400	3.64452000	-4.21683800
H	6.55111700	2.90786700	-3.54709200
H	6.80506200	3.85756800	-5.01954300
H	5.95326100	4.57061500	-3.64123600
Li	1.53700200	1.10577000	-2.40703700
O	2.31186200	1.63061100	-0.59340400
C	3.57159200	1.17626300	-0.04445000
C	1.97610600	2.92946200	-0.04787700
C	4.18038000	2.38593000	0.66526400
H	3.37205300	0.35808300	0.66027100
H	4.18598100	0.79064800	-0.86216100
C	2.92863200	3.14555400	1.12798900
H	2.12085900	3.68621000	-0.82916100
H	0.92056700	2.91751200	0.23688500
H	4.75675100	2.99461500	-0.04119900
H	4.84205600	2.09379200	1.48644500
H	3.11123600	4.20650100	1.32371300
H	2.52154200	2.69304000	2.04034000
O	2.29255400	-0.80671500	-2.46285400
C	2.64290200	-1.44815300	-3.71455300
C	1.82357300	-1.79852900	-1.51594200
C	2.67606400	-2.94742900	-3.41876700
H	1.87923700	-1.20183500	-4.46287100
H	3.60289600	-1.04427400	-4.04845000
C	1.60759900	-3.07796200	-2.32347100
H	2.59092000	-1.93514000	-0.74275300
H	0.91313300	-1.42032900	-1.04355800
H	3.65907900	-3.24172700	-3.03191600
H	2.46317200	-3.54951200	-4.30716400
H	1.71869500	-3.97832900	-1.71188000
H	0.60505900	-3.08426400	-2.76708000
O	-0.76958200	2.29450400	-5.54434600
C	-2.13864300	2.70240100	-5.77317900
C	-0.47117600	1.10811600	-6.32151600
C	-2.60475600	1.92149100	-7.00185000
H	-2.73746800	2.45106400	-4.88747100
H	-2.15509200	3.78713200	-5.91273600

C	-1.81248900	0.61312000	-6.86374900
H	0.21576100	1.38678200	-7.13079000
H	0.03049400	0.38720300	-5.66973500
H	-2.31926000	2.44798800	-7.92049300
H	-3.68892000	1.77453700	-7.01252200
H	-1.70178200	0.06918500	-7.80668400
H	-2.29682800	-0.05061100	-6.13786200
O	-0.36729200	4.45465800	-3.32659500
C	0.38143900	5.59422900	-3.81803400
C	-1.40192700	4.89460400	-2.41761100
C	-0.36375800	6.83398300	-3.31629600
H	1.39912200	5.53830400	-3.41399500
H	0.43424900	5.53284200	-4.90936100
C	-1.01959700	6.32005000	-2.02577900
H	-2.37031000	4.86767900	-2.93586900
H	-1.43363300	4.19544100	-1.57797000
H	-1.13134300	7.13933100	-4.03735000
H	0.30819700	7.68189500	-3.15427300
H	-1.88451500	6.91201500	-1.71180900
H	-0.29263900	6.30768100	-1.20501400
Li	0.14539800	2.53467000	-3.72797600

3a

E= -1948.554599H

C	-1.61918700	5.97786300	-2.66739200
C	-2.47165700	4.71494900	-2.48878800
C	-1.72807500	3.57109700	-1.78595900
C	-2.59188300	2.31791400	-1.62252600
C	-1.93881700	1.12727700	-0.94978200
N	-0.72349800	1.23620800	-0.54047700
N	-0.17156100	0.11043500	0.08546700
C	2.05654600	0.21913000	-1.57866400
C	2.28019200	1.41336200	-2.26856500
C	2.70533200	1.37276800	-3.59571200
C	2.91355800	0.15184300	-4.25568600
C	2.68416600	-1.03377800	-3.54298300
C	2.25598400	-1.00706800	-2.21543200
C	3.35849600	0.12195700	-5.69797000
S	1.46459900	0.25511800	0.12929500
O	1.97481900	1.53139600	0.69429400
O	1.93674500	-1.00106100	0.76902400
H	-1.27281800	6.32494800	-1.68231900
H	-0.71212200	5.72560400	-3.23690900
H	-2.82040700	4.37229400	-3.47482400
H	-3.37756700	4.96868400	-1.91731100
H	-1.37886300	3.90767100	-0.80090400
H	-0.82397700	3.31568400	-2.35373200
H	-2.95324100	1.99079900	-2.61133100
H	-3.50774700	2.57275500	-1.06337500
H	2.13927700	2.36229500	-1.76257200
H	2.88543200	2.30520800	-4.12649800

H	2.84871100	-1.99139200	-4.03172600
H	2.09324700	-1.93145300	-1.67053400
H	3.71207100	-0.87279000	-5.98828800
H	2.53384000	0.38881000	-6.37263400
H	4.16740900	0.83840700	-5.88290600
O	-0.91298500	-2.74915500	1.82465500
O	0.37990300	-0.31667700	3.58533000
C	-0.51023000	-3.48338900	0.64970200
C	-1.25686400	-4.82660900	0.73804200
C	-1.61032200	-4.96166200	2.24545800
C	-0.96317700	-3.72250000	2.88140200
C	0.64454700	1.07751500	3.89429000
C	2.10603800	1.13856800	4.33489400
C	2.31310700	-0.24557100	4.96644500
C	1.48155500	-1.14141300	4.04899900
H	-0.76690600	-2.87568900	-0.21885800
H	0.57788600	-3.62207100	0.67391700
H	-0.62893700	-5.64826500	0.38125200
H	-2.16408300	-4.81117800	0.12692900
H	-2.69483100	-4.94436500	2.39157800
H	-1.22724000	-5.88477200	2.69007800
H	0.05839600	-3.94027100	3.22455400
H	-1.53181700	-3.29287800	3.70841300
H	0.44595400	1.67045400	2.99842900
H	-0.03590000	1.38962700	4.69737700
H	2.29469400	1.96462700	5.02751500
H	2.75096300	1.26287900	3.45915100
H	3.36283100	-0.55295700	4.99913500
H	1.91732400	-0.26522300	5.98920100
H	1.06146700	-2.01263600	4.56118400
H	2.04963300	-1.47009400	3.17379700
C	-2.35617700	7.12244900	-3.37480700
H	-3.26287400	7.37571600	-2.80633000
H	-2.70072200	6.77691300	-4.36030500
C	-1.49893000	8.37956700	-3.54836900
H	-0.60278500	8.17123000	-4.14701800
H	-2.05595800	9.17866700	-4.05288500
H	-1.16401200	8.76978600	-2.57865200
C	-2.76869100	-0.12975900	-0.82841500
H	-2.22220800	-0.98794700	-1.24051500
H	-2.98872700	-0.36905400	0.21898600
H	-3.71794900	-0.03050400	-1.36579900
Li	-0.66618000	-0.75955100	1.91653500
O	-2.47333100	-0.06010300	2.58157500
C	-3.18608300	-0.78275800	3.61619300
C	-2.85182500	1.34023600	2.61046400
C	-4.25582800	0.17715600	4.13748800
H	-3.59614300	-1.69690000	3.17706500
H	-2.47267400	-1.05467900	4.40387800
C	-3.58386500	1.54315500	3.93565600
H	-1.94693200	1.94344700	2.50461000
H	-3.51014200	1.54181400	1.75618600

H	-4.52179400	-0.02814600	5.17863100
H	-5.16504300	0.10557800	3.52925000
H	-2.87044600	1.74261100	4.74401000
H	-4.29414100	2.37410600	3.89193500

4a

E= -1715.530965 H

C	-1.93573000	5.95205200	-0.97001800
C	-2.43183800	4.55731300	-1.37359500
C	-1.58013000	3.41322100	-0.80636800
C	-2.08078200	2.02953000	-1.23552900
C	-1.31423600	0.81277900	-0.71718500
C	-1.95628800	-0.47443100	-0.83061600
N	-0.14467800	1.06472600	-0.17271500
N	0.46496700	-0.13880900	0.32317400
C	3.08739100	0.62348900	-0.12689200
C	3.08322900	1.91855400	-0.66030700
C	4.00255800	2.26509200	-1.64820000
C	4.94761300	1.34039300	-2.12204900
C	4.94060700	0.05209400	-1.57150200
C	4.01791500	-0.30934900	-0.58688200
C	5.94079900	1.73240300	-3.19038400
S	1.84145200	0.14703000	1.10298700
O	1.83574000	1.28500300	2.06632500
O	2.29657200	-1.16425100	1.65183400
H	-1.91641100	6.02796400	0.12770400
H	-0.89345800	6.07565400	-1.30075100
H	-2.45160300	4.48692500	-2.47220700
H	-3.47529000	4.43577500	-1.04406600
H	-1.56474400	3.47375100	0.29056200
H	-0.53841200	3.53840800	-1.12692900
H	-2.09882200	1.98312100	-2.33708600
H	-3.13331100	1.91763000	-0.93169800
H	-1.28318600	-1.29180900	-1.11905400
H	2.36873600	2.64765700	-0.29507400
H	3.99089500	3.27413900	-2.05621300
H	5.66826200	-0.68025000	-1.91551400
H	4.02155000	-1.30941600	-0.16551600
H	6.61635200	0.90510200	-3.43190600
H	5.43511600	2.03187900	-4.11758000
H	6.55595400	2.58533700	-2.87525900
Li	-1.01250500	-1.35719900	0.97912100
O	-0.78561100	-3.34905900	0.90332500
O	-1.59335500	-1.05212800	2.86639400
C	0.52567700	-3.90984800	0.69096700
C	0.51030900	-4.34278800	-0.77335400
C	-0.94417900	-4.83035300	-0.97694400
C	-1.72541600	-4.18096100	0.19081200
C	-1.86802900	0.32766500	3.22890800
C	-0.96571700	0.63279300	4.42460400
C	-0.84631800	-0.74199500	5.09863500

C	-0.77899600	-1.67766800	3.89235800
H	1.25252600	-3.13230200	0.93494200
H	0.66425800	-4.77172000	1.36243600
H	1.25287400	-5.11766500	-0.98825700
H	0.72162500	-3.47866800	-1.41157500
H	-1.34030400	-4.52448700	-1.94932200
H	-1.00934000	-5.92167300	-0.91968100
H	-2.12391300	-4.93921300	0.87836400
H	-2.54581100	-3.53473900	-0.13131400
H	-1.66264600	0.95811300	2.35983600
H	-2.93252700	0.40768800	3.48620600
H	-1.39017600	1.40167700	5.07788600
H	0.01352400	0.97187900	4.07086300
H	0.03454400	-0.83420000	5.74150300
H	-1.73770000	-0.95640200	5.70128300
H	-1.18494300	-2.67515700	4.08611700
H	0.24556400	-1.77397200	3.51349700
C	-2.78335300	7.09717000	-1.53959700
H	-3.82328500	6.98174500	-1.20117200
H	-2.80923300	7.01793400	-2.63628300
C	-2.27219500	8.48540700	-1.14388900
H	-1.24713100	8.64872700	-1.50098900
H	-2.90035000	9.28037700	-1.56484000
H	-2.26470500	8.61106800	-0.05342700
H	-2.85478900	-0.47590700	-1.45661700

TS (4-5)a

E= -1715.510142 H

C	-1.63148600	2.33899100	-6.06451400
C	-2.48253800	1.34608700	-5.26156500
C	-2.06346700	1.22633600	-3.79073700
C	-2.92109200	0.23226600	-2.98437700
C	-2.46737600	0.05832100	-1.54131500
C	-3.08554300	0.74707100	-0.53583600
N	-1.35432600	-0.75790000	-1.43170500
N	-1.02192900	-1.22057800	-0.22455500
Li	0.03807400	-2.67392700	0.56238300
H	-1.69599900	3.33344500	-5.59732100
H	-0.57366600	2.04220100	-6.00258600
H	-2.42449600	0.35443000	-5.73577600
H	-3.53992800	1.64805800	-5.31711000
H	-2.11752700	2.21465600	-3.31111200
H	-1.01403600	0.90909600	-3.72898400
H	-2.87840300	-0.74653900	-3.48553300
H	-3.96922500	0.56062600	-3.00732600
H	-2.73855200	0.68054800	0.49030400
C	1.30924800	0.85706400	0.17105100
C	0.90868300	1.98772500	-0.54618700
C	1.84862600	2.71187900	-1.28287700
C	3.19539300	2.32573300	-1.32077200
C	3.57566800	1.17910000	-0.60324600

C	2.64355100	0.44182400	0.12589600
C	4.21588900	3.11546900	-2.10626100
S	0.02587100	-0.11601900	1.03244800
O	-0.54780200	0.83148900	2.06058400
O	0.80047900	-1.27678700	1.68689800
H	-0.13023700	2.30860900	-0.51894600
H	1.53042800	3.59301500	-1.83651100
H	4.61769500	0.86322100	-0.61542900
H	2.94128700	-0.44637800	0.67550900
H	4.98661900	3.54057600	-1.44958500
H	4.73515000	2.48506900	-2.83932500
H	3.74866600	3.94358500	-2.64935700
O	1.08045700	-3.85231000	-0.67825100
C	1.93082900	-3.09395300	-1.58609700
C	1.61388600	-3.59878400	-2.99856300
C	0.18572500	-4.14335800	-2.84271000
C	0.24442300	-4.75179100	-1.44649800
H	1.68090400	-2.03575500	-1.46751400
H	2.97476000	-3.25053900	-1.29402700
H	2.30073100	-4.40406100	-3.28579900
H	1.69193800	-2.80082500	-3.74245900
H	-0.54066500	-3.32282300	-2.86296200
H	-0.08509500	-4.87682600	-3.60873200
H	0.70772200	-5.74894400	-1.45901500
H	-0.72112000	-4.81929700	-0.93955400
O	-1.01244800	-4.01953600	1.63003100
C	-2.33294600	-3.57167100	2.03336200
C	-2.27698000	-3.48488700	3.55469300
C	-1.35370000	-4.66273600	3.90359200
C	-0.33688400	-4.63457400	2.75680100
H	-2.51757400	-2.61945500	1.52830400
H	-3.07405400	-4.31125500	1.69892100
H	-3.26715700	-3.56066000	4.01437800
H	-1.82369200	-2.53552900	3.86202900
H	-0.87272800	-4.56275500	4.88122700
H	-1.91692500	-5.60353600	3.89456700
H	0.00498500	-5.63110200	2.45690600
H	0.53909000	-4.02320900	3.00535100
H	-3.93399800	1.39678800	-0.74092100
C	-2.03816800	2.44836600	-7.53991100
H	-3.09538900	2.74435000	-7.60410000
H	-1.97066000	1.45574300	-8.00855100
C	-1.18440800	3.44235200	-8.33293100
H	-0.12404200	3.15885500	-8.31581000
H	-1.49727800	3.49149700	-9.38334000
H	-1.26150900	4.45496900	-7.91618200

5a

E= -1128.318321 H

C	-2.22439900	4.08525700	-3.45197900
C	-2.36892200	2.61848500	-3.87803200

C	-2.58988500	1.66036000	-2.70109700
C	-2.72381400	0.18620900	-3.13148400
C	-2.87193000	-0.75394200	-1.96453200
N	-1.61227500	-0.96724600	-1.21643600
N	-1.65780300	-1.11522600	0.02014800
H	-3.12425100	4.39328300	-2.89857300
H	-1.38658400	4.17559100	-2.74413700
H	-1.46855300	2.31107900	-4.43107000
H	-3.20705500	2.52671000	-4.58523800
H	-3.49374000	1.95515100	-2.14943100
H	-1.75412400	1.75162700	-1.99333200
H	-1.82009900	-0.09653500	-3.69171900
H	-3.57387200	0.07855400	-3.81753900
Li	0.17204000	-1.54728600	0.68456400
O	0.82872700	-3.35845400	0.05786400
O	0.03888600	-1.80552400	2.66310200
C	1.59974200	-3.68164000	-1.11331100
C	0.56459400	-4.07242000	-2.17240400
C	-0.60307100	-4.66222000	-1.33670300
C	-0.21002300	-4.35904600	0.12364200
C	-1.22940600	-1.80122100	3.35000600
C	-1.01082100	-0.86648600	4.53397500
C	0.42669700	-1.22341600	4.95712600
C	1.10045000	-1.64004900	3.63275600
H	2.20208600	-2.80749200	-1.36854500
H	2.27293800	-4.51951600	-0.87849300
H	0.97328300	-4.78343300	-2.89673000
H	0.23158800	-3.18284100	-2.71528700
H	-1.54860100	-4.17846900	-1.59535700
H	-0.72068500	-5.73886400	-1.49179500
H	0.18989300	-5.25031700	0.62678900
H	-1.02320800	-3.94986400	0.72633400
H	-1.98352700	-1.47234800	2.63199200
H	-1.47062100	-2.82098100	3.68598400
H	-1.74228400	-1.01901300	5.33323000
H	-1.07410300	0.17654700	4.20272200
H	0.94736800	-0.39052900	5.43854100
H	0.41735100	-2.06308000	5.66043200
H	1.65261200	-2.58273100	3.72808100
H	1.78210900	-0.87937000	3.24042900
C	-3.97183100	-1.45994000	-1.68112300
H	-3.98544800	-2.12350600	-0.81747400
H	-4.87702100	-1.39973000	-2.28165600
C	-1.99947200	5.04905100	-4.62414000
H	-2.83861800	4.96477500	-5.32974300
H	-1.10193400	4.74118500	-5.17995300
C	-1.84937700	6.50933500	-4.18813200
H	-0.99488500	6.63784400	-3.51120500
H	-1.69130500	7.16994900	-5.04939700
H	-2.74480700	6.86150800	-3.65993600
O	1.53256100	-0.10081200	0.49035200
C	2.51777700	0.04325200	-0.56701400

C	1.10616500	1.20901800	0.93512700
C	2.72036400	1.55129400	-0.76744300
H	3.43478400	-0.45768200	-0.23596100
H	2.14647000	-0.45497800	-1.46803100
C	2.25967200	2.13828900	0.57554500
H	0.18221300	1.48747300	0.41122500
H	0.89885900	1.14532800	2.00641700
H	2.08108700	1.91752700	-1.57829300
H	3.75742100	1.79609300	-1.01469600
H	1.94684500	3.18422600	0.50474900
H	3.05544000	2.06304300	1.32652700

TS (5-6)a

E= -1128.310118 H

C	-3.86885800	-4.86777800	-0.08487000
O	-3.22280300	-3.57127800	0.02035300
C	-2.66446400	-3.40142300	1.35243800
C	-2.70767100	-4.78654600	1.99313200
C	-3.95728600	-5.40041600	1.34461700
Li	-2.45007900	-2.60560300	-1.49687600
N	-0.39666000	-2.66226200	-1.46705400
N	0.30721300	-2.55413800	-0.54852600
C	2.30871100	-2.72667800	-1.09270400
C	3.42461500	-2.62138000	-0.09980400
C	4.64984300	-1.08374000	1.56415300
C	4.79428000	0.33006700	2.14310700
C	5.88091600	0.44502700	3.22000700
C	6.02146300	1.85779700	3.79445600
C	2.40298400	-2.97698500	-2.38744300
H	-4.84208000	-4.72722600	-0.56430500
H	-3.25181300	-5.51647300	-0.71875200
H	-1.65490100	-2.99453500	1.24948900
H	-3.28783000	-2.68310700	1.90002300
H	-2.76564900	-4.73450500	3.08431800
H	-1.81368100	-5.36022400	1.72195400
H	-3.97052100	-6.49379800	1.37618300
H	-4.86467600	-5.02986700	1.83583000
H	4.40516600	-2.91554400	-0.52684800
H	3.24203900	-3.31834900	0.73629100
H	5.61360600	-1.39945400	1.13683000
H	4.43426200	-1.78895200	2.38126800
H	3.83031800	0.64977000	2.56706600
H	5.01692800	1.03548300	1.32824800
H	6.84477400	0.12662400	2.79733100
H	5.65849600	-0.25894600	4.03506900
H	6.80394400	1.90133000	4.56200600
H	5.08471100	2.19561700	4.25637400
H	6.28362400	2.58196100	3.01235300
H	3.32668800	-3.15666400	-2.95429600
H	1.47366100	-3.01973900	-2.98496300
O	-3.11492600	-3.38916400	-3.17680700

C	-3.80372600	-2.57760400	-4.16089600
C	-3.04288800	-2.79927400	-5.46327300
C	-2.64401900	-4.27801800	-5.34309200
C	-2.33467300	-4.41944300	-3.84963600
H	-4.84480900	-2.91946500	-4.23883500
H	-3.79271500	-1.54577800	-3.80178800
H	-2.15209700	-2.16099500	-5.49549000
H	-3.65485500	-2.58605500	-6.34470000
H	-3.48478700	-4.92204100	-5.62550600
H	-1.78481800	-4.54565700	-5.96464000
H	-1.27830700	-4.23475900	-3.62758700
H	-2.62012600	-5.39357200	-3.44032000
C	3.55730100	-1.20304900	0.49427300
H	3.76398300	-0.49511800	-0.32153500
H	2.59027100	-0.90222100	0.92146500
C	-4.22476200	-0.22614100	-0.86526900
O	-2.98175200	-0.72071900	-1.42563900
C	-2.04045500	0.37479600	-1.59797100
C	-2.85019400	1.64996800	-1.36759200
C	-3.91271200	1.18134700	-0.36191100
H	-4.98632700	-0.21312500	-1.65600000
H	-4.54294500	-0.91941700	-0.08195300
H	-1.23784000	0.26108100	-0.86095700
H	-1.60966600	0.30049300	-2.60062200
H	-2.22908400	2.46825400	-0.99229700
H	-3.32492500	1.97795900	-2.29976000
H	-3.49121600	1.14044400	0.64925300
H	-4.80104200	1.81919900	-0.33924600

6a

E= -1018.824106 H

C	-2.12017000	4.45816100	-3.03500400
C	-2.24741300	2.99788100	-3.48838900
C	-2.13162400	1.98204100	-2.34347000
C	-2.27349000	0.51526100	-2.79331900
C	-2.16157400	-0.48820700	-1.64819700
H	-2.88378000	4.66771800	-2.27060500
H	-1.14766100	4.60332600	-2.54029900
H	-1.47506900	2.78411100	-4.24323700
H	-3.21371300	2.86203900	-3.99721100
H	-2.90456600	2.19778900	-1.58992400
H	-1.16555600	2.11356500	-1.83339000
H	-1.48328100	0.32340200	-3.54029700
H	-3.23494700	0.42283700	-3.34240700
Li	-0.54784600	-1.18399200	-0.38571000
O	0.18579800	-3.03543300	-0.88398500
O	-1.06082400	-1.46246400	1.55877000
C	0.34134400	-3.31112700	-2.29237000
C	-0.71197900	-4.36851300	-2.59844300
C	-0.65545700	-5.23942200	-1.33181600
C	-0.31841300	-4.22574800	-0.22312200

C	-2.30825500	-1.05075700	2.15850500
C	-1.89878400	-0.31331100	3.42768600
C	-0.71207900	-1.16379900	3.91223800
C	-0.07206500	-1.65449300	2.60085800
H	0.20103300	-2.37006300	-2.83022000
H	1.35734600	-3.68686400	-2.48379800
H	-0.49705900	-4.92708100	-3.51465900
H	-1.69250300	-3.89028900	-2.69844600
H	-1.59354400	-5.76608000	-1.13341000
H	0.13922600	-5.98865400	-1.42086900
H	0.44764500	-4.60113800	0.46551500
H	-1.19452000	-3.92783400	0.35951500
H	-2.83797200	-0.44291300	1.42322900
H	-2.91486900	-1.93842800	2.39052400
H	-2.71060500	-0.25218200	4.15878700
H	-1.57659000	0.70562600	3.18236300
H	-0.00469800	-0.60260100	4.52973600
H	-1.07352500	-2.01310600	4.50230300
H	0.20365100	-2.71457500	2.64310000
H	0.81266200	-1.07686900	2.31837700
C	-3.28042300	-1.21820800	-1.43599600
H	-3.35903900	-1.96762400	-0.63953400
H	-4.20568500	-1.12532400	-2.03655800
C	-2.26179600	5.47309100	-4.17689700
H	-3.23271700	5.32644600	-4.67187700
H	-1.49692800	5.26997000	-4.94052800
C	-2.14271600	6.92769100	-3.71345600
H	-1.16716000	7.11885900	-3.24786800
H	-2.25225400	7.62678400	-4.55167900
H	-2.91525800	7.17366100	-2.97348100
O	1.21920400	-0.20360800	-0.17877600
C	2.55402900	-0.72692100	-0.38658100
C	1.28775600	1.18319400	0.22571900
C	3.50140200	0.46893000	-0.25208700
H	2.74965300	-1.48920600	0.37732600
H	2.59554500	-1.20202000	-1.37095900
C	2.72554100	1.39885400	0.69242600
H	1.04472300	1.82087100	-0.63430100
H	0.53656200	1.34643100	1.00378000
H	3.64783500	0.95307000	-1.22453900
H	4.48220000	0.17606600	0.13434400
H	3.03353400	2.44614400	0.62025600
H	2.84392900	1.07603500	1.73383900

1b

E= -1244.130748H

C	5.91016100	3.34796200	0.08717500
C	4.38369500	3.21077200	0.02252300
C	3.90600600	1.75271800	-0.00501900
C	2.37752700	1.64347500	-0.09458700
C	1.79885800	0.24120200	-0.11447600

N	0.56698500	-0.01218800	-0.38643600
N	-0.25184800	1.07158100	-0.71261700
C	-2.16536300	-0.35876200	-2.02015100
C	-2.10609600	-1.74641800	-1.86688200
C	-2.29992700	-2.55589800	-2.98267700
C	-2.55472400	-2.00240000	-4.24809500
C	-2.61281800	-0.60651000	-4.36816600
C	-2.41805900	0.22176600	-3.26389000
C	-2.76345000	-2.89716600	-5.44437000
S	-1.92093900	0.69419200	-0.60076000
O	-2.22956300	-0.08095200	0.60826700
O	-2.57062200	1.99478600	-0.81948700
H	6.28637800	2.81730200	0.97464300
H	6.35715200	2.84359700	-0.78258200
H	4.00996000	3.73310700	-0.87062400
H	3.93498200	3.72277100	0.88680400
H	4.26580200	1.23819500	0.89528600
H	4.36097100	1.23861000	-0.86223600
H	2.02947400	2.16914200	-0.99620000
H	1.92965300	2.18886900	0.75331500
H	-0.08575500	1.94709500	-0.20527300
H	-1.91689400	-2.18079200	-0.89153300
H	-2.25563600	-3.63623600	-2.86938800
H	-2.81520000	-0.16000600	-5.33809400
H	-2.47051500	1.30063900	-3.36665400
H	-2.95475800	-2.31597300	-6.35148900
H	-1.88338200	-3.52711200	-5.62414300
H	-3.61395300	-3.57239900	-5.28850800
C	2.65930400	-0.94887900	0.21136500
H	2.07083800	-1.86719100	0.14047800
H	3.51539900	-1.02250500	-0.47015200
H	3.06623200	-0.87005700	1.22768200
C	6.39237500	4.80385400	0.12867700
H	6.00684300	5.33871100	-0.75125400
H	5.95708600	5.30459800	1.00547500
C	7.91728600	4.93514300	0.17449100
H	8.38382600	4.48190100	-0.70967600
H	8.22733700	5.98668600	0.20950800
H	8.33371600	4.43698600	1.05950000

3b

E= -1948.552055 H

C	-2.46594900	1.87840400	-1.98104500
C	-1.72280700	0.78197300	-1.25563900
N	-0.46503500	0.98745300	-1.05135100
N	0.24443200	0.01353300	-0.33461300
C	2.06944300	-0.33817100	-2.39881300
C	1.97037500	0.62087100	-3.41164100
C	2.09658000	0.23062600	-4.74327400
C	2.32367500	-1.11079800	-5.09055000
C	2.42489400	-2.05350300	-4.05847600

C	2.29522900	-1.67694200	-2.72040500
C	2.45734900	-1.51727900	-6.53834000
S	1.84693900	0.14595100	-0.67094700
O	2.40556500	1.51956600	-0.57651200
O	2.49689800	-0.90688800	0.15202500
H	-2.86983200	1.53221300	-2.94173300
H	-3.32152700	2.24349400	-1.39494300
H	1.80841300	1.66239900	-3.15545700
H	2.02206900	0.98097400	-5.52774600
H	2.61002600	-3.09683000	-4.30380100
H	2.38106700	-2.41371200	-1.92821100
H	2.66108900	-2.58837900	-6.63618600
H	1.54066300	-1.29784100	-7.10092300
H	3.27189500	-0.97329600	-7.03297800
O	-0.02173400	-2.17137600	2.30036300
O	1.47157000	0.62190100	2.94659100
C	0.20209800	-3.27378400	1.39894300
C	-0.54544200	-4.45582800	2.03443000
C	-0.58131100	-4.10338000	3.54803000
C	0.10469100	-2.72723900	3.62080400
C	1.73934400	2.04351500	2.83719800
C	3.25937200	2.17752200	2.83306500
C	3.68436100	1.01575800	3.74319400
C	2.67516300	-0.07354200	3.37337500
H	-0.16559800	-2.97565000	0.41638600
H	1.28045600	-3.46753200	1.33025900
H	-0.03531000	-5.40261600	1.83454700
H	-1.56002500	-4.53054000	1.63128300
H	-1.61234300	-4.04444300	3.90963200
H	-0.05434100	-4.83852900	4.16318000
H	1.17028500	-2.82896700	3.86951000
H	-0.35669800	-2.03008500	4.32340000
H	1.27212800	2.40714400	1.91937300
H	1.29077200	2.55393600	3.70029000
H	3.58970500	3.15595900	3.19567600
H	3.63662900	2.03187300	1.81618300
H	4.71562700	0.69072500	3.57515800
H	3.58258600	1.29730900	4.79833000
H	2.41549300	-0.72188700	4.21618700
H	3.02084600	-0.68414200	2.53476600
C	-3.55629200	-0.94859600	-1.79846200
H	-4.31010400	-0.16876900	-1.97077600
H	-3.08866500	-1.14741000	-2.77335700
C	-4.26059100	-2.22101700	-1.30767100
H	-3.50990800	-3.00446300	-1.12517400
H	-4.73391400	-2.01918300	-0.33465900
C	-5.31729100	-2.75162200	-2.28485300
H	-6.06301700	-1.96548900	-2.47692100
H	-4.84134700	-2.96309400	-3.25402100
C	-6.03386900	-4.01469800	-1.78935200
H	-5.28959600	-4.79965400	-1.59189400
H	-6.51682700	-3.80244300	-0.82449600

C	-7.07934100	-4.54406400	-2.77474800
H	-6.62318700	-4.80102600	-3.73939700
H	-7.57165000	-5.44586600	-2.39068300
H	-7.86007700	-3.79703300	-2.96769700
H	-1.79385800	2.71972500	-2.17416300
C	-2.48820100	-0.44856700	-0.81025400
H	-2.96591000	-0.23714800	0.15856400
H	-1.76171300	-1.24615100	-0.61880000
Li	0.12989100	-0.26348400	1.72287600
O	-1.59356800	0.59521600	2.38874100
C	-1.86658400	2.00787700	2.34022700
C	-2.39910700	0.07696800	3.46208500
C	-3.37795500	2.13171000	2.58709500
H	-1.29540000	2.51761500	3.12909100
H	-1.53675200	2.37404900	1.36649100
C	-3.73005500	0.84815300	3.38876200
H	-2.49821700	-0.99893700	3.30738100
H	-1.88879900	0.25648500	4.41960700
H	-3.92290200	2.15654100	1.63890600
H	-3.61705700	3.04881400	3.13331900
H	-4.49182000	0.26108700	2.86767000
H	-4.11009100	1.07173500	4.38977500

4b

E= -1715.526146 H

C	-2.06545600	1.95833300	-1.01571000
C	-1.27419800	0.70254000	-0.68699600
C	-1.84536600	-0.58817900	-0.94277700
N	-0.11356500	0.97450800	-0.10842200
N	0.58011800	-0.22761500	0.27639700
C	3.15579200	0.68163400	-0.17555300
C	3.02378000	1.96529900	-0.72249600
C	3.92558700	2.40220400	-1.69024300
C	4.97898800	1.58324300	-2.12984300
C	5.09598800	0.30487900	-1.56935100
C	4.19297900	-0.14772500	-0.60410900
C	5.95439600	2.07624000	-3.17233300
S	1.95492000	0.08328800	1.04638300
O	1.91643300	1.16892200	2.06855000
O	2.48639600	-1.22868600	1.51898700
H	-2.28272700	2.04259400	-2.09013200
H	-3.03539200	1.97598100	-0.49886800
H	-1.09219900	-1.35836200	-1.15915000
H	2.21775900	2.61118600	-0.39215400
H	3.81477500	3.40067600	-2.10952000
H	5.90710400	-0.34638800	-1.88900100
H	4.29062300	-1.13869900	-0.17258500
H	6.72582600	1.32826000	-3.38375500
H	5.44806900	2.31032200	-4.11784200
H	6.45910600	2.99494700	-2.84655400
Li	-0.86911700	-1.43952100	0.96516300

O	-0.57622000	-3.41185600	1.10129100	Li	0.01390200	-2.65946700	0.56967200
O	-1.51052400	-1.02499700	2.80521500	H	-1.97280500	-0.12016000	-3.70005400
C	0.72542500	-4.01226700	0.95192600	H	-3.71097600	-0.25757100	-3.36732800
C	0.58128500	-4.88559900	-0.29163800	H	-2.90806700	0.35799500	0.40965700
C	-0.86279000	-5.42689000	-0.16397200	C	1.22283400	0.84260400	0.18734600
C	-1.54947900	-4.43388600	0.80541600	C	0.82247300	1.94555600	-0.57228000
C	-1.80366800	0.37779000	3.05516600	C	1.76738800	2.65505000	-1.31761600
C	-0.96710000	0.76968900	4.27365800	C	3.11816000	2.28309600	-1.32093800
C	-0.85904000	-0.55906400	5.03686000	C	3.49911800	1.16568800	-0.55854200
C	-0.71843800	-1.56322400	3.89464200	C	2.56206300	0.44148900	0.17725000
H	1.45047100	-3.19962000	0.88101400	C	4.14242200	3.05529200	-2.11893200
H	0.94709000	-4.62117400	1.84286700	S	-0.06035700	-0.11378300	1.06322700
H	1.33175000	-5.68111600	-0.33557500	O	-0.63278600	0.85285200	2.07498600
H	0.68508800	-4.26686200	-1.18952800	O	0.70729600	-1.26561600	1.74220700
H	-1.36953200	-5.46658900	-1.13242400	H	-0.21777500	2.26170000	-0.56600100
H	-0.87093500	-6.43764800	0.25647900	H	1.44935700	3.51412000	-1.90507800
H	-1.84781700	-4.92699700	1.74063500	H	4.54494100	0.86279500	-0.54100400
H	-2.42278400	-3.93467600	0.38026700	H	2.85991600	-0.42621400	0.75876700
H	-1.54797700	0.94465600	2.15567500	H	4.93110300	3.46319200	-1.47311300
H	-2.88034500	0.46909700	3.24909900	H	4.63838200	2.41711000	-2.86171300
H	-1.43553700	1.56920300	4.85639300	H	3.68344300	3.89324100	-2.65398500
H	0.02392800	1.10213700	3.94816500	O	1.10060200	-3.81751400	-0.65088200
H	-0.00953400	-0.59543300	5.72602100	C	1.96567200	-3.03993900	-1.52844400
H	-1.77561300	-0.75463400	5.60745300	C	1.68805700	-3.53005600	-2.95430000
H	-1.10288800	-2.55934500	4.13324800	C	0.26170200	-4.08945000	-2.83969200
H	0.32296900	-1.65317800	3.56155900	C	0.29314700	-4.71572000	-1.45058800
C	-3.06799900	-0.71380400	-1.84316500	H	1.70225500	-1.98597200	-1.40283400
H	-3.84271600	0.01064800	-1.54873300	H	3.00364300	-3.19053000	-1.21288500
H	-2.85182000	-0.47344400	-2.90739900	H	2.38919600	-4.32542900	-3.23458900
C	-3.70870700	-2.11095400	-1.82863500	H	1.77658400	-2.72205200	-3.68605100
H	-2.94109600	-2.86015700	-2.07925000	H	-0.47082400	-3.27459900	-2.86600800
H	-4.03628200	-2.34183600	-0.80359700	H	0.01551400	-4.81493400	-3.62146600
C	-4.89202500	-2.27064800	-2.79339500	H	0.76773200	-5.70755100	-1.46513300
H	-5.66564600	-1.52669100	-2.54770600	H	-0.68339100	-4.80060900	-0.96779300
H	-4.56112200	-2.03657500	-3.81680200	O	-1.02210900	-4.03848800	1.61101800
C	-5.51981500	-3.67048500	-2.77813300	C	-2.33747200	-3.60434500	2.04385200
H	-4.74762000	-4.41497200	-3.02099900	C	-2.25587700	-3.53445800	3.56493800
H	-5.85809300	-3.90521200	-1.75835800	C	-1.31596100	-4.70734600	3.88419100
C	-6.69389200	-3.82365800	-3.74996700	C	-0.32040000	-4.65813400	2.71944300
H	-6.38298700	-3.62604800	-4.78413500	H	-2.53915500	-2.64800900	1.55372200
H	-7.11320000	-4.83707500	-3.71770100	H	-3.07975200	-4.34467200	1.71386800
H	-7.50376500	-3.12233700	-3.51028900	H	-3.23745100	-3.62521500	4.04016200
H	-1.50174800	2.84460400	-0.70663700	H	-1.80657900	-2.58462200	3.87610100

TS (4-5)b

E= -1715.508344 H

C	-2.78769000	0.26411400	-3.07593500
C	-2.44573400	0.04401500	-1.61380100
C	-3.20801300	0.57724400	-0.61341600
N	-1.27400000	-0.69458000	-1.45343300
N	-1.01473200	-1.20081900	-0.24334200

H	-1.97280500	-0.12016000	-3.70005400
H	-3.71097600	-0.25757100	-3.36732800
H	-2.90806700	0.35799500	0.40965700
C	1.22283400	0.84260400	0.18734600
C	0.82247300	1.94555600	-0.57228000
C	1.76738800	2.65505000	-1.31761600
C	3.11816000	2.28309600	-1.32093800
C	3.49911800	1.16568800	-0.55854200
C	2.56206300	0.44148900	0.17725000
C	4.14242200	3.05529200	-2.11893200
S	-0.06035700	-0.11378300	1.06322700
O	-0.63278600	0.85285200	2.07498600
O	0.70729600	-1.26561600	1.74220700
H	-0.21777500	2.26170000	-0.56600100
H	1.44935700	3.51412000	-1.90507800
H	4.54494100	0.86279500	-0.54100400
H	2.85991600	-0.42621400	0.75876700
H	4.93110300	3.46319200	-1.47311300
H	4.63838200	2.41711000	-2.86171300
H	3.68344300	3.89324100	-2.65398500
O	1.10060200	-3.81751400	-0.65088200
C	1.96567200	-3.03993900	-1.52844400
C	1.68805700	-3.53005600	-2.95430000
C	0.26170200	-4.08945000	-2.83969200
C	0.29314700	-4.71572000	-1.45058800
H	1.70225500	-1.98597200	-1.40283400
H	3.00364300	-3.19053000	-1.21288500
H	2.38919600	-4.32542900	-3.23458900
H	1.77658400	-2.72205200	-3.68605100
H	-0.47082400	-3.27459900	-2.86600800
H	0.01551400	-4.81493400	-3.62146600
H	0.76773200	-5.70755100	-1.46513300
H	-0.68339100	-4.80060900	-0.96779300
O	-1.02210900	-4.03848800	1.61101800
C	-2.33747200	-3.60434500	2.04385200
C	-2.25587700	-3.53445800	3.56493800
C	-1.31596100	-4.70734600	3.88419100
C	-0.32040000	-4.65813400	2.71944300
H	-2.53915500	-2.64800900	1.55372200
H	-3.07975200	-4.34467200	1.71386800
H	-3.23745100	-3.62521500	4.04016200
H	-1.80657900	-2.58462200	3.87610100
H	-0.81807900	-4.61290800	4.85387900
H	-1.87055900	-5.65323100	3.87566100
H	0.02536400	-5.64819700	2.40325800
H	0.55399700	-4.04059800	2.95826900
H	-2.93514800	1.32413900	-3.32463500
C	-4.47406100	1.38254100	-0.79044800
H	-5.35683400	0.73331300	-0.95676500
H	-4.41975600	2.01299700	-1.69269000
C	-4.78594500	2.27946400	0.42010500

H	-4.84483800	1.65036300	1.32122200
H	-3.94147300	2.96402000	0.58726500
C	-6.08411800	3.08523500	0.28524300
H	-6.92015700	2.39734300	0.08470500
H	-6.01637100	3.74429500	-0.59409400
C	-6.41653800	3.92846300	1.52318300
H	-5.58251900	4.61468800	1.72912500
H	-6.48982400	3.26821200	2.39949000
C	-7.71366900	4.73102700	1.38422700
H	-8.57306500	4.07084200	1.20846800
H	-7.92406900	5.31477100	2.28906900
H	-7.66042500	5.43360000	0.54232400

5b

E=-1128.324486 H

C	-2.73343600	-0.15523700	-3.41867200
C	-2.99329000	-0.70520000	-2.04699700
N	-1.72547400	-1.10539900	-1.37025800
N	-1.65534600	-1.02826600	-0.12957200
H	-2.08745800	-0.83925100	-3.98514600
H	-3.64580800	0.01266800	-3.99814400
Li	0.13001000	-1.55876400	0.57923000
O	1.06213100	-3.17660900	-0.13402500
O	-0.01016800	-1.90528600	2.55235400
C	0.84950100	-3.52343400	-1.52912000
C	0.34442700	-4.98384600	-1.55016000
C	0.13673200	-5.32594600	-0.06071300
C	1.13514400	-4.39928700	0.62423900
C	-1.32059600	-1.88678900	3.17434000
C	-1.16573900	-0.99392300	4.40127400
C	0.26846100	-1.31946300	4.84621200
C	0.99671400	-1.48620100	3.50933100
H	0.12423000	-2.80731400	-1.92548600
H	1.79782100	-3.41425100	-2.06964300
H	1.09754200	-5.64329700	-1.99428600
H	-0.57599000	-5.08769600	-2.13164400
H	-0.88130500	-5.07395800	0.25758700
H	0.31764300	-6.38148000	0.16456300
H	2.15786900	-4.80239400	0.57598600
H	0.89372600	-4.15142100	1.65971600
H	-2.03229100	-1.51801500	2.43164400
H	-1.59377600	-2.91305100	3.45643100
H	-1.91585800	-1.20502500	5.16918700
H	-1.25135900	0.06142100	4.11548200
H	0.71988100	-0.53911300	5.46603700
H	0.28547600	-2.25807500	5.41219100
H	1.78680200	-2.24422000	3.53846200
H	1.42926500	-0.54386500	3.15520600
C	-4.17900000	-0.94961000	-1.47378300
H	-4.13167600	-1.36730000	-0.46334100
O	1.41429000	-0.04366000	0.41689100

C	2.73582400	-0.04709000	-0.17779000
C	0.89733500	1.30908800	0.47139300
C	2.97099200	1.37740100	-0.68556200
H	3.46124700	-0.32805200	0.59650600
H	2.75870000	-0.80112100	-0.96981900
C	2.11163700	2.21285500	0.27559700
H	0.15913100	1.43981800	-0.32906300
H	0.39442400	1.44007500	1.43416500
H	2.60256300	1.48269100	-1.71253100
H	4.03027100	1.65055000	-0.67204600
H	1.83854000	3.19274300	-0.12688800
H	2.63500400	2.36293800	1.22750700
H	-2.19164900	0.80096200	-3.36014200
C	-5.55887100	-0.73354200	-2.03202300
H	-5.51710200	-0.22741100	-3.00467000
H	-6.11562300	-0.05946700	-1.36099200
C	-6.36379300	-2.04100000	-2.17608700
H	-5.82326200	-2.72029700	-2.85070700
H	-6.40660200	-2.54781600	-1.20080700
C	-7.78813800	-1.82207600	-2.70190300
H	-7.74117300	-1.30867000	-3.67433900
H	-8.32544500	-1.14171600	-2.02396300
C	-8.59205000	-3.11937400	-2.85727400
H	-8.04960600	-3.80286600	-3.52623800
H	-8.65150500	-3.62806700	-1.88434100
C	-10.00588400	-2.89333200	-3.40095800
H	-10.55251400	-3.83883400	-3.50308000
H	-10.58987200	-2.24298100	-2.73691700
H	-9.97993800	-2.41698700	-4.38957100

TS (5-6)b

E= -1128.312937 H

C	-4.33707300	-4.72712500	-0.02246500
O	-3.52176200	-3.53484200	0.11648400
C	-3.20411800	-3.31037800	1.51717900
C	-3.62577300	-4.58613300	2.24438200
C	-4.80760000	-5.06839400	1.38997400
Li	-2.40460700	-2.73074400	-1.28535400
N	-0.41888400	-2.89039500	-0.87457200
N	0.39827600	-3.05948800	-0.07546400
C	2.35803000	-2.98066000	-0.94771000
C	3.61626900	-3.17237600	-0.16358500
C	2.21422400	-2.76410600	-2.24563800
H	-5.15129700	-4.50520100	-0.71815200
H	-3.71897200	-5.52996700	-0.44349000
H	-2.13531100	-3.09328900	1.59302000
H	-3.77170600	-2.43816600	1.86497400
H	-3.89284100	-4.39634800	3.28801000
H	-2.81405400	-5.32258500	2.22450300
H	-5.02065100	-6.13501300	1.50649300
H	-5.71563800	-4.50617000	1.63812000

H	4.55655300	-3.13040300	-0.74904600	H	-1.42644000	0.23022900	-3.09845800
H	3.61480900	-4.14253900	0.35868800	H	-3.13368400	0.66952100	-2.98343100
H	1.16163200	-2.65786900	-2.59629300	Li	-0.61995500	-1.34540900	-0.20627700
O	-2.82393800	-3.60476600	-2.99084100	O	0.08908800	-3.20276000	-0.67586100
C	-2.99177200	-2.80494500	-4.19064200	O	-0.87275400	-1.53339700	1.80733200
C	-2.00459800	-3.37976000	-5.20132000	C	0.22573700	-3.52225500	-2.08122500
C	-2.01952700	-4.87334600	-4.84269700	C	-0.66888200	-4.73653100	-2.30896500
C	-2.12871400	-4.84238100	-3.31712200	C	-0.50172300	-5.49549000	-0.98410700
H	-4.02923200	-2.90372700	-4.53659400	C	-0.42593700	-4.35738300	0.03870700
H	-2.80382600	-1.76193500	-3.92394900	C	-2.10175100	-1.14705200	2.46733400
H	-1.00655700	-2.95699400	-5.03878000	C	-1.66464300	-0.29225200	3.65226400
H	-2.30364300	-3.17869000	-6.23425500	C	-0.36907000	-0.99804400	4.07933500
H	-2.89675900	-5.36282300	-5.28171900	C	0.23547100	-1.41922700	2.73463000
H	-1.12518900	-5.40663400	-5.17721500	H	-0.06793300	-2.63987900	-2.65620500
H	-1.14364000	-4.81284100	-2.83777100	H	1.27827500	-3.75486800	-2.29573200
H	-2.70272400	-5.67761000	-2.90451900	H	-0.36823600	-5.31979200	-3.18454800
C	-4.12464200	-0.26191800	-1.26601700	H	-1.70883300	-4.41733000	-2.44230900
O	-2.78803400	-0.81695800	-1.37733200	H	-1.32486800	-6.18394600	-0.77152700
C	-1.79645900	0.23095300	-1.20561100	H	0.43177600	-6.07045100	-0.99060300
C	-2.56524800	1.53960000	-1.36674600	H	0.24374300	-4.57536600	0.87706100
C	-3.93749200	1.17565300	-0.78011400	H	-1.41340100	-4.10107500	0.43747300
H	-4.59643300	-0.29871100	-2.25601500	H	-2.71868300	-0.62595100	1.73266000
H	-4.69993000	-0.88876800	-0.57856900	H	-2.63042100	-2.05098600	2.80161600
H	-1.35765800	0.14073000	-0.20439500	H	-2.41978500	-0.25513200	4.44328300
H	-1.01012700	0.07787500	-1.94904700	H	-1.45627900	0.73294600	3.32276300
H	-2.07841900	2.37022200	-0.84753000	H	0.30770100	-0.35669700	4.65189200
H	-2.65762900	1.80124700	-2.42746100	H	-0.60111700	-1.87849600	4.68978500
H	-3.90421300	1.20816200	0.31510000	H	0.75857900	-2.38054400	2.78204200
H	-4.74351000	1.83303800	-1.11883800	H	0.92571200	-0.66543500	2.34146200
C	3.23738300	-2.66224000	-3.36105900	C	-3.53322800	-1.19236800	-1.07114100
H	4.25652600	-2.69967600	-2.95008800	H	-3.59214200	-1.96043000	-0.28187900
H	3.14684100	-1.68559300	-3.86690100	O	1.10462700	-0.28039200	-0.31151700
C	3.08282300	-3.76564700	-4.42480800	C	2.45741400	-0.78081100	-0.43402100
H	2.04817200	-3.75737200	-4.80111800	C	1.11369500	1.16495800	-0.23971900
H	3.22259500	-4.74545800	-3.94504700	C	3.34414200	0.44969500	-0.64018000
C	4.04969800	-3.63039600	-5.60854800	H	2.71362300	-1.31917700	0.48737000
H	5.08544500	-3.63306600	-5.23624700	H	2.49442100	-1.48573600	-1.26926800
H	3.90195100	-2.65033100	-6.08759700	C	2.55531100	1.54724400	0.08970100
C	3.89261100	-4.73385600	-6.66293100	H	0.80119600	1.57283200	-1.20950800
H	2.85515800	-4.74093500	-7.02780000	H	0.38756900	1.47236500	0.51847700
H	4.05594500	-5.71290300	-6.18977200	H	3.42550900	0.68725000	-1.70730900
C	4.84771400	-4.57759000	-7.84999200	H	4.35358200	0.30254000	-0.24486100
H	5.89531900	-4.59850500	-7.52273000	H	2.80372500	2.55797500	-0.24734600
H	4.71427100	-5.38259800	-8.58322200	H	2.72999400	1.49261400	1.17102800
H	4.68467500	-3.62488000	-8.37057800	C	-4.89806000	-0.98595600	-1.71971900
H	3.70933400	-2.41617800	0.63232500	H	-5.62334100	-0.64990900	-0.95775200

6b

E= -1018.822839H

C	-2.22894200	0.46569600	-2.38066700	H	-5.48058100	-3.07122600	-1.62204100
C	-2.32627900	-0.61286900	-1.30178900	C	-6.86473300	-2.09350300	-2.96604300
				H	-7.55446700	-1.75358400	-2.17832800

H	-6.84463000	-1.29043800	-3.71850600
C	-7.42481300	-3.36898400	-3.60925200
H	-6.73426700	-3.71228400	-4.39319100
H	-7.45474200	-4.17101300	-2.85748500
C	-8.82170300	-3.18270300	-4.20932100
H	-8.81908800	-2.41060900	-4.98956600
H	-9.19186100	-4.11061600	-4.66260200
H	-9.54621400	-2.87530600	-3.44411400
H	-1.93254900	1.43030700	-1.93644700

1c

E= -1244.131855 H

C	2.57864900	5.12245900	-2.22252000
C	2.44869900	4.24638300	-0.96976600
C	2.08444600	2.79031600	-1.28552400
C	1.96919600	1.91627700	-0.01654300
C	1.63760800	0.47143200	-0.32654800
N	0.47023700	0.01484900	-0.61370900
N	-0.59353300	0.91263500	-0.67334200
C	-2.38118400	-0.77306300	-1.85093500
C	-2.03203100	-2.12573800	-1.88289300
C	-2.24977700	-2.84965700	-3.05179700
C	-2.81228600	-2.24542500	-4.18783800
C	-3.15682200	-0.88758600	-4.12244100
C	-2.94372800	-0.14421900	-2.96270500
C	-3.03758800	-3.04674600	-5.44540900
S	-2.10949200	0.17309300	-0.36318100
O	-2.04105000	-0.75649400	0.77243300
O	-3.03259000	1.31642400	-0.31746100
H	3.33692800	4.68898800	-2.89170000
H	1.63079800	5.10173200	-2.78077100
H	1.68647600	4.67534600	-0.30249300
H	3.39518500	4.26980600	-0.40968800
H	2.84532300	2.35801500	-1.94932800
H	1.13646100	2.75805500	-1.83832400
H	2.91789100	1.94586000	0.53108500
H	1.21443700	2.34842300	0.65746900
H	-0.52435400	1.76181600	-0.10151300
H	-1.60334000	-2.60102100	-1.00770800
H	-1.98119500	-3.90279300	-3.08274000
H	-3.60033900	-0.40517500	-4.98948000
H	-3.21907100	0.90438900	-2.92042300
H	-3.51739100	-2.44555500	-6.22350400
H	-2.08888400	-3.42492700	-5.84668300
H	-3.67232100	-3.91975000	-5.24998200
C	2.77126800	-0.51675900	-0.34289800
H	2.42122600	-1.50910600	-0.63904800
H	3.55492100	-0.19266400	-1.04070400
H	3.23739000	-0.58401900	0.64897300
C	2.95188900	6.57828000	-1.91374500
H	2.19382200	7.01305700	-1.24645200

H	3.89839000	6.59813200	-1.35450700
C	3.08518000	7.44844800	-3.16665600
H	2.14379300	7.48387800	-3.73001700
H	3.35599100	8.47987800	-2.90987600
H	3.85917500	7.06061300	-3.84153800

3c

E= -1948.552512 H

C	-2.56176700	1.26515200	-1.88969400
C	-1.67079600	0.39523500	-1.03836600
N	-0.44481500	0.76996300	-0.90475000
N	0.38691300	-0.01977600	-0.09666000
C	2.25417000	-0.48474200	-2.09895600
C	1.99043900	0.24759900	-3.26100400
C	2.17167100	-0.34904800	-4.50686400
C	2.61803700	-1.67544900	-4.62132500
C	2.88073500	-2.38831300	-3.44377900
C	2.69822300	-1.80454700	-2.18865000
C	2.81989300	-2.30332600	-5.97943900
S	1.95677100	0.26230800	-0.47927900
O	2.33266900	1.69043400	-0.63855200
O	2.73197900	-0.53789800	0.50586200
H	-3.03477800	0.68132000	-2.69223400
H	-3.37991000	1.70083400	-1.29803900
H	1.65717600	1.27728100	-3.18682500
H	1.96661900	0.22593100	-5.40752300
H	3.23419200	-3.41494100	-3.50777800
H	2.91150400	-2.36432200	-1.28376200
H	3.07139800	-3.36561300	-5.89679900
H	1.91759100	-2.21657500	-6.59715100
H	3.63148000	-1.80990100	-6.53002100
O	0.68707600	-1.96734800	2.78049800
O	1.48731600	1.22256000	3.02078300
C	1.12326200	-3.09371200	1.99489100
C	0.65735200	-4.31557400	2.79414500
C	0.68596400	-3.82221000	4.26684100
C	0.97977700	-2.31207500	4.14665200
C	1.45916100	2.61378800	2.60424900
C	2.91567000	3.07022900	2.58675000
C	3.53091800	2.22736200	3.71331900
C	2.79953100	0.89428300	3.55137900
H	0.67707200	-2.99658900	1.00448400
H	2.21613400	-3.06389300	1.89556700
H	1.30449200	-5.18092400	2.62401100
H	-0.36010700	-4.59381300	2.50152600
H	-0.27398100	-4.00130200	4.76005700
H	1.45999900	-4.32227600	4.85626100
H	2.03724900	-2.09830000	4.35402200
H	0.36001800	-1.68169100	4.78789300
H	0.98223200	2.66405200	1.62285700
H	0.86278400	3.18326400	3.32913200

H	3.01356300	4.14813700	2.74852900	C	4.62202200	1.23495800	-2.61239400
H	3.36702200	2.81575700	1.62277000	C	4.73643500	-0.02194600	-2.00462600
H	4.61558400	2.11326400	3.62452400	C	3.91102400	-0.38875300	-0.93897900
H	3.31248500	2.67304900	4.69135700	C	5.51000500	1.63153000	-3.76825000
H	2.66108000	0.35964200	4.49628100	S	1.83488600	0.01727500	0.88398500
H	3.30046200	0.24007400	2.83158000	O	1.84923700	1.18882700	1.80661800
C	-2.09725500	-2.07932100	-1.41067400	O	2.39876400	-1.24979800	1.43354900
H	-2.54267000	-1.85142800	-2.38929900	H	-2.67015100	1.83565400	-1.89970000
H	-1.02520600	-2.23450100	-1.58645600	H	-3.37840800	1.58433500	-0.30677000
C	-2.71945500	-3.36799200	-0.85757100	H	-3.15223400	-0.72235400	-1.18058000
H	-2.28406500	-3.58378300	0.12983700	H	2.09233200	2.47113700	-0.67043300
H	-3.79539200	-3.21022900	-0.68851300	H	3.54728100	3.10638400	-2.56809600
C	-2.52092500	-4.58435400	-1.77163400	H	5.48343000	-0.72481200	-2.36821600
H	-2.96575000	-4.37682000	-2.75631000	H	4.00855700	-1.36366300	-0.47209600
H	-1.44511900	-4.73214200	-1.94859100	H	6.22246500	0.83746700	-4.01519800
C	-3.12099500	-5.87984100	-1.20971500	H	4.92195400	1.84462000	-4.67052900
H	-2.68356000	-6.08172900	-0.22119100	H	6.08523900	2.53880700	-3.54209600
H	-4.19874700	-5.73896000	-1.04333400	Li	-1.04179100	-1.51522000	1.03734300
C	-2.90110900	-7.09272000	-2.11832300	O	-0.80734100	-3.48849200	1.31487700
H	-1.83174800	-7.28175200	-2.27843900	O	-1.51383100	-0.99079200	2.92111500
H	-3.33746700	-8.00195900	-1.68683800	C	0.48748200	-4.11759800	1.36726600
H	-3.35988400	-6.94112400	-3.10388700	C	0.44780100	-5.13557200	0.23169200
H	-1.98815600	2.08021000	-2.34124600	C	-1.00441500	-5.65538600	0.30332200
C	-2.27965900	-0.86995200	-0.46796500	C	-1.78288900	-4.49316900	0.96432200
H	-3.35390100	-0.70801000	-0.30258800	C	-1.80234300	0.40758900	3.18675400
H	-1.83216600	-1.09296400	0.50402000	C	-0.80568400	0.84003500	4.26043000
Li	0.41859900	-0.15081500	1.99248500	C	-0.60691700	-0.45956100	5.05457900
O	-1.45278200	0.29295900	2.69387200	C	-0.62937500	-1.51332600	3.94697100
C	-2.02164800	1.61452200	2.69763400	H	1.23479300	-3.32788000	1.26244600
C	-2.20565000	-0.45690200	3.66098300	H	0.61487100	-4.61377700	2.34248700
C	-3.54002400	1.40745300	2.85107600	H	1.19122200	-5.92994600	0.35125500
H	-1.61316900	2.18170700	3.54608400	H	0.63249400	-4.63064500	-0.72248100
H	-1.72624800	2.10427600	1.76797800	H	-1.40421900	-5.90561600	-0.68358700
C	-3.66388500	-0.01613200	3.46124100	H	-1.06372900	-6.55558300	0.92421300
H	-2.02529600	-1.51622600	3.47151900	H	-2.30559000	-4.81995800	1.87286100
H	-1.85138300	-0.20742400	4.67246200	H	-2.50829900	-4.01885300	0.29831800
H	-4.04183200	1.45972900	1.88058600	H	-1.69751200	0.95827800	2.24883600
H	-3.97778300	2.17714400	3.49330400	H	-2.84036100	0.48464600	3.53792100
H	-4.17584200	-0.69043000	2.76840500	H	-1.18423600	1.66736900	4.86916800
H	-4.21533500	-0.02506000	4.40593400	H	0.13360200	1.14672800	3.78853700
				H	0.32813800	-0.48104900	5.62295600
				H	-1.43771900	-0.61686300	5.75355700
				H	-1.01766600	-2.48307100	4.27251800
				H	0.36503100	-1.65642600	3.50756400
				C	-1.38757700	-1.84691800	-1.72798800
				H	-0.45094100	-2.19482500	-1.27140900
				H	-2.02732100	-2.74010500	-1.82751200
				C	-1.04353000	-1.35318000	-3.15233200
				H	-1.96103400	-0.97866400	-3.63389500
				H	-0.36698900	-0.49056400	-3.06941000
				C	-0.40051600	-2.41718900	-4.05247800
				H	0.50564600	-2.80757500	-3.56396000

4c

E= -1715.520703H

C	-2.42206800	1.70060400	-0.83675800
C	-1.53216900	0.48656400	-0.61596700
C	-2.11216600	-0.82451500	-0.84026900
N	-0.33538300	0.79765300	-0.15903300
N	0.42108200	-0.36146900	0.21881600
C	2.95628700	0.50714900	-0.45567100
C	2.83021000	1.77087700	-1.04725100
C	3.65390500	2.12267700	-2.11440500

H	-1.08583600	-3.27428400	-4.15104800
C	-0.03273700	-1.90718000	-5.45269800
H	-0.93188400	-1.49847600	-5.93717900
H	0.66940900	-1.06679600	-5.35643200
C	0.58271300	-2.98187500	-6.35409900
H	-0.11109100	-3.81895400	-6.50730500
H	0.83956900	-2.58008400	-7.34243400
H	1.50156800	-3.39186900	-5.91488300
H	-1.94201100	2.61583600	-0.47304500

TS (4-5)c

E= -1715.502504 H

C	-2.82234700	0.07024800	-3.17245100
C	-2.70980200	-0.16836600	-1.67098800
C	-3.77200000	0.21937300	-0.89588600
N	-1.47428300	-0.74314100	-1.38745300
N	-1.22295000	-1.20768800	-0.15156400
Li	-0.04851600	-2.59518400	0.61167200
H	-2.03394400	0.75131300	-3.52224000
H	-2.68133100	-0.86836900	-3.72705700
H	-4.61630900	0.64123300	-1.44693400
C	1.04179200	0.88122400	0.26682700
C	0.68126600	1.99958100	-0.49083500
C	1.65552300	2.69426400	-1.21218900
C	2.99814100	2.29462200	-1.19139100
C	3.34008900	1.16439200	-0.42978000
C	2.37345000	0.45466100	0.28092900
C	4.05477000	3.05265000	-1.95987700
S	-0.26842700	-0.06591800	1.11565700
O	-0.89055000	0.93411400	2.06646500
O	0.49165700	-1.18601900	1.85223800
H	-0.34857000	2.34535000	-0.49776700
H	1.36743200	3.56583800	-1.79649000
H	4.37914500	0.84086400	-0.39130200
H	2.64204000	-0.42013700	0.86560900
H	4.55142800	2.41179500	-2.69987100
H	3.62516900	3.90654200	-2.49403900
H	4.83886500	3.43581200	-1.29371600
O	1.19674900	-3.63728400	-0.58473100
C	1.93492300	-2.78110200	-1.50597600
C	1.80857800	-3.42947900	-2.88766400
C	0.47789300	-4.18669600	-2.76908300
C	0.54308100	-4.69378100	-1.33266000
H	1.47496900	-1.78852100	-1.48388700
H	2.96845000	-2.70666600	-1.15253500
H	2.63350600	-4.13003000	-3.06576800
H	1.81230500	-2.68393900	-3.68800500
H	-0.36368400	-3.49355900	-2.88375500
H	0.37072500	-4.99820100	-3.49564300
H	1.14597800	-5.60982400	-1.25510300
H	-0.43124900	-4.87339600	-0.87240000

O	-0.88941500	-4.13287700	1.59902500
C	-2.17780400	-3.85042700	2.20150500
C	-1.94606000	-3.94259200	3.70616600
C	-0.90436900	-5.06945500	3.79428900
C	-0.03936900	-4.81657300	2.55456300
H	-2.49382200	-2.86617300	1.84711400
H	-2.90082400	-4.60366000	1.85854100
H	-2.86576100	-4.15950900	4.25810800
H	-1.52883100	-3.00148400	4.08191000
H	-0.31654400	-5.04622300	4.71677500
H	-1.39540600	-6.04752400	3.72677300
H	0.33500000	-5.73642300	2.09297000
H	0.81439400	-4.16622800	2.78075300
H	-3.79126600	0.49321200	-3.45963600
C	-4.00312800	0.14158100	0.59634400
H	-3.07272600	0.29664200	1.15063500
H	-4.35861100	-0.86261200	0.89600700
C	-5.04870700	1.16685800	1.07234200
H	-4.69262700	2.18037600	0.83209300
H	-5.98178200	1.03130300	0.50182700
C	-5.35969400	1.07905500	2.57168600
H	-4.43134700	1.22649100	3.14334800
H	-5.70452200	0.06106200	2.81081200
C	-6.41296700	2.08850000	3.04693400
H	-7.33745500	1.94678400	2.46782900
H	-6.06641600	3.10765800	2.82218500
C	-6.72951900	1.97921600	4.54153400
H	-5.83314000	2.15103200	5.15129900
H	-7.48477300	2.71378900	4.84823400
H	-7.11384500	0.98268300	4.79552200

5c

E= -1128.321859 H

C	-2.48772600	0.87590700	-3.02986900
C	-2.91442000	-0.05921500	-1.93251500
N	-1.77981000	-0.59593100	-1.18449500
N	-1.73458700	-0.45700800	0.05835000
H	-1.70609500	0.41575600	-3.64957000
H	-3.32377900	1.15788800	-3.67904100
Li	-0.03961700	-1.27856600	0.72038300
O	0.49443200	-3.13230900	0.16573600
O	-0.09282200	-1.40293500	2.72274700
C	0.23323800	-3.53177700	-1.20864700
C	-0.53195200	-4.87020000	-1.14192100
C	-0.91602500	-4.99609800	0.34414300
C	0.22876400	-4.25756800	1.02755400
C	-1.25234500	-0.91779100	3.44420800
C	-0.69103900	0.01388300	4.51298400
C	0.61855000	-0.69659900	4.88882500
C	1.09574700	-1.24850000	3.54061500
H	-0.34736500	-2.72603400	-1.66702300

H	1.18933000	-3.63180600	-1.73620200	O	-2.82742100	-3.88956200	0.00739900
H	0.11983600	-5.69933200	-1.43772500	C	-2.01864900	-4.07922100	1.19986300
H	-1.40260400	-4.87556500	-1.80372600	C	-2.27420200	-5.51988700	1.63237000
H	-1.86295900	-4.48210500	0.54593300	C	-3.73916800	-5.72192000	1.21663000
H	-1.00673000	-6.03464100	0.67698000	Li	-2.54426200	-2.38682300	-1.21102100
H	1.12788400	-4.88771200	1.09856200	N	-0.56518700	-1.80507300	-1.31788600
H	-0.00805500	-3.85859800	2.01581700	N	0.31677500	-2.37418500	-0.81419100
H	-1.91172300	-0.43525100	2.71943000	C	2.23464600	-1.80464000	-1.11346600
H	-1.77677000	-1.77283000	3.89334100	C	3.02813200	-2.38239400	0.01443400
H	-1.37384700	0.13932100	5.35857800	C	2.77042600	-1.45890300	-2.28971500
H	-0.48583800	1.00193500	4.08369100	H	-4.78942000	-4.50013300	-0.29243100
H	1.35792500	-0.03231400	5.34596100	H	-3.54313900	-5.58492200	-0.95654200
H	0.41703600	-1.51541100	5.58908200	H	-0.97954800	-3.86669700	0.93642200
H	1.59313500	-2.22091000	3.62549400	H	-2.34761400	-3.36350700	1.96491600
H	1.76933600	-0.55588300	3.02428700	H	-2.10312400	-5.66709700	2.70263600
C	-4.18155300	-0.47743900	-1.76562200	H	-1.61981000	-6.20502900	1.08062000
H	-4.92755600	-0.10064400	-2.47021300	H	-4.01493000	-6.77324300	1.09295700
O	1.52666300	-0.11340600	0.32375400	H	-4.41137200	-5.27584600	1.95900000
C	2.76155900	-0.47882000	-0.34070400	H	4.05202000	-2.70384900	-0.25542400
C	1.33482300	1.32152100	0.26317100	H	2.51015600	-3.25839500	0.43976600
C	3.27263400	0.79969200	-1.00866700	H	3.85965600	-1.55890700	-2.46337300
H	3.46217600	-0.85329400	0.41648100	O	-3.11002300	-2.97428800	-3.00015100
H	2.54998700	-1.28438300	-1.04949400	C	-3.70005200	-2.04887200	-3.94994700
C	2.70269800	1.89638000	-0.09607400	C	-2.91168800	-2.23070600	-5.24430300
H	0.58441500	1.54890900	-0.50379300	C	-2.55240200	-3.72299600	-5.18934900
H	0.95327400	1.65256800	1.23378600	C	-2.26705400	-3.93098900	-3.70209200
H	2.85805700	0.89388500	-2.01892200	H	-4.75801900	-2.31106900	-4.08116600
H	4.36401300	0.81860000	-1.08268000	H	-3.63454200	-1.04295000	-3.52699300
H	2.62695400	2.87168000	-0.58574400	H	-2.00315800	-1.61791500	-5.22705100
H	3.32039100	2.00758700	0.80322700	H	-3.49726800	-1.95722600	-6.12698000
H	-2.05295600	1.79704100	-2.61311500	H	-3.40597200	-4.33373500	-5.50608200
C	-4.70352900	-1.44420600	-0.73556900	H	-1.69227900	-3.98454500	-5.81217200
H	-3.87263100	-1.96212500	-0.24407700	H	-1.22108500	-3.71509800	-3.45410400
H	-5.30803200	-2.21279300	-1.24450500	H	-2.51695800	-4.93417900	-3.34389800
C	-5.58401000	-0.77947300	0.34152300	C	-4.97876200	-0.73670800	-0.43957600
H	-4.96948500	-0.05285600	0.89007900	O	-3.55273300	-0.78726900	-0.70663900
H	-6.38535900	-0.20411500	-0.14593100	C	-2.98624500	0.54693500	-0.63248600
C	-6.20526400	-1.78253900	1.32150400	C	-4.17496200	1.48885100	-0.79057800
H	-5.40341900	-2.35214200	1.81568800	C	-5.28713300	0.71603400	-0.06512200
H	-6.80052600	-2.51869500	0.75986500	H	-5.50689600	-1.04548500	-1.34999100
C	-7.09244300	-1.12980800	2.38963100	H	-5.21018800	-1.44748400	0.35983200
H	-6.49732000	-0.40308900	2.96104600	H	-2.49651900	0.67184600	0.34192700
H	-7.88744900	-0.55212400	1.89601800	H	-2.23215700	0.63456000	-1.41775300
C	-7.72387700	-2.13892000	3.35305400	H	-3.98259600	2.47568600	-0.35975500
H	-8.34922300	-1.63978900	4.10355500	H	-4.42155400	1.61648500	-1.85136300
H	-8.35822600	-2.85761300	2.81820600	H	-5.20345400	0.85815400	1.01836000
H	-6.95629000	-2.71194000	3.88926800	H	-6.29412100	1.01388400	-0.37164200
				C	1.99358400	-0.90325000	-3.46756200
				H	0.93172400	-0.85268100	-3.20004900
				H	2.30656800	0.13556400	-3.67254700
				C	2.14310300	-1.70717800	-4.77836300
				H	1.42089100	-1.32180100	-5.51476800

TS (5-6)c

E= -1128.305337 H

C -3.81037500 -4.95085000 -0.10243400

H	1.86225000	-2.75401800	-4.58905700
C	3.54534700	-1.66250700	-5.40083700
H	4.28044700	-2.06610700	-4.69088900
H	3.82938000	-0.61235600	-5.57081400
C	3.65560700	-2.43316900	-6.72331300
H	2.91929100	-2.03730100	-7.43816900
H	3.38137700	-3.48463600	-6.55403100
C	5.05286500	-2.36837600	-7.34690100
H	5.81030200	-2.78465000	-6.67028400
H	5.10079800	-2.93390100	-8.28580800
H	5.34211900	-1.33302400	-7.56897700
H	3.12912600	-1.66692000	0.84694600

6c

E= -1018.826321 H

C	-2.23618800	0.59607300	-2.04830900
C	-2.40641600	-0.58569100	-1.09537600
H	-1.48577200	0.38621900	-2.82865800
H	-3.16343700	0.90514200	-2.57517800
Li	-0.63308900	-1.33680400	-0.07344000
O	0.05680200	-3.20514600	-0.50552300
O	-0.68796600	-1.41412700	1.95947900
C	0.17274000	-3.56134900	-1.90384000
C	-0.71440000	-4.78883300	-2.08325300
C	-0.51536700	-5.51205500	-0.74259600
C	-0.42640000	-4.34766300	0.24967000
C	-1.79160600	-0.87313900	2.72274600
C	-1.14371800	0.00685000	3.78587700
C	0.12251500	-0.79683200	4.12132600
C	0.52173700	-1.37558000	2.75729000
H	-0.13908100	-2.69764000	-2.49733100
H	1.22329500	-3.79106900	-2.13003800
H	-0.42418100	-5.39167400	-2.94906600
H	-1.75987200	-4.48366200	-2.20548700
H	-1.32979000	-6.19938900	-0.49551400
H	0.42125700	-6.08175600	-0.75328900
H	0.26569800	-4.53861400	1.07625500
H	-1.40689800	-4.09109900	0.66513400
H	-2.44208900	-0.34167700	2.02513200
H	-2.35529600	-1.69940700	3.17839200
H	-1.79536000	0.16851800	4.64976800
H	-0.88270900	0.98363100	3.36101400
H	0.91969100	-0.18935700	4.56004500
H	-0.11726800	-1.60222400	4.82490400
H	0.93343600	-2.38843600	2.82625200
H	1.24442300	-0.73929600	2.23609100
C	-3.66574200	-1.07288400	-1.03620400
H	-4.48228600	-0.62587700	-1.64184600
O	1.07738900	-0.27934100	-0.43528400
C	2.40826900	-0.81134700	-0.64400700
C	1.13158700	1.16311500	-0.32864700

C	3.31586900	0.40053800	-0.86943300
H	2.70076100	-1.37813200	0.24863900
H	2.38160100	-1.49511000	-1.49722200
C	2.59905100	1.49897000	-0.07023900
H	0.77922800	1.60517300	-1.26905700
H	0.45718700	1.46989900	0.47607800
H	3.34588400	0.66355000	-1.93328300
H	4.34088400	0.21653200	-0.53410200
H	2.85629800	2.51115300	-0.39619700
H	2.83194500	1.41245600	0.99794900
C	-4.15203000	-2.23065800	-0.18832000
H	-4.51600500	-3.05100300	-0.83323100
H	-3.30758700	-2.64233200	0.38352200
C	-5.29188600	-1.86547200	0.78211500
H	-4.94124500	-1.08296800	1.47120000
H	-6.12032700	-1.41725800	0.21260100
C	-5.82243800	-3.05841100	1.58835200
H	-6.18445900	-3.83182900	0.89371700
H	-4.99241100	-3.51821000	2.14695300
C	-6.94609700	-2.69686400	2.56832600
H	-6.58054900	-1.93790600	3.27530400
H	-7.77085000	-2.22473300	2.01524300
C	-7.48255300	-3.90052300	3.34890100
H	-6.68903400	-4.38113300	3.93594000
H	-8.27711800	-3.60583400	4.04562100
H	-7.89895000	-4.65977800	2.67431000
H	-1.85890600	1.49090100	-1.52633700

7a

E= -786.3575599 H

C	-2.14738300	4.44457700	-3.43875300
C	-2.78114200	3.04915100	-3.36322300
C	-2.11074700	2.12180100	-2.34046800
C	-2.76196000	0.72939200	-2.23551700
C	-2.04318100	-0.20395000	-1.27075300
H	-2.19987300	4.92103900	-2.44801900
H	-1.07634200	4.34572100	-3.67241000
H	-2.74136300	2.57889100	-4.35777400
H	-3.84907900	3.15133300	-3.11815100
H	-2.13151900	2.59949700	-1.34921400
H	-1.04750600	2.00319200	-2.59863100
H	-2.75990500	0.28863100	-3.24735700
H	-3.83024600	0.86972300	-1.96916100
Li	-0.17233700	-1.07984400	-1.01116300
O	0.27196800	-2.92619700	-1.46496700
C	0.71223300	-3.18077400	-2.82689000
C	-0.13757300	-4.34868900	-3.32135100
C	-0.37514400	-5.14191100	-2.02726800
C	-0.55908200	-4.02647600	-1.00054000
H	0.57748100	-2.26267000	-3.40820200
H	1.77969800	-3.43311700	-2.80442200

H	0.36911100	-4.92658600	-4.09970900	H	-2.55839200	-2.97155000	-2.37843400
H	-1.08883700	-3.98232700	-3.72391000	H	-1.01635400	-3.85272100	-2.23857200
H	-1.24658700	-5.80111000	-2.07689000	H	-2.57802000	-5.70602500	-2.04059600
H	0.50421900	-5.74894300	-1.78157400	H	-3.75240300	-4.70710600	-1.15725600
H	-0.23057400	-4.29511400	0.00794700	H	-2.59695900	-5.85290100	0.68956900
H	-1.59897100	-3.68121200	-0.95743800	H	-1.03199800	-5.69414800	-0.13258100
C	-2.78054300	-0.64557300	-0.22699000	H	-0.90420000	-3.71940800	1.24013400
H	-2.37867400	-1.31560800	0.54435900	H	-2.67156000	-3.49607600	1.22263100
H	-3.83888500	-0.37526200	-0.05473200	C	-3.40327200	-0.06919500	-2.24797800
C	-2.80486400	5.36488000	-4.47538700	H	-3.89509100	-0.97489500	-1.87922000
H	-3.87602900	5.46178900	-4.24646400	H	-3.93315700	0.41094900	-3.09050100
H	-2.74625600	4.89267700	-5.46674700	C	-0.40249100	6.59379800	-1.44304500
C	-2.17145300	6.75771100	-4.53800600	H	-0.97396400	6.88861100	-2.33515400
H	-1.10551500	6.69959900	-4.79378200	H	0.62103700	6.39061400	-1.79028400
H	-2.65916800	7.38709300	-5.29257500	C	-0.37933300	7.75762900	-0.44843200
H	-2.25143400	7.27499200	-3.57302300	H	0.21421000	7.51060400	0.44127900
O	1.38530300	-0.33180700	-0.16076000	H	0.05542400	8.65996800	-0.89604900
C	2.51414700	-1.08027200	0.36611600	H	-1.39183800	8.01149700	-0.10892800
C	1.50324900	1.06982100	0.20362700	O	0.70045700	-1.05943900	-0.28835300
C	3.48394000	-0.03434300	0.91779800	C	1.47398400	-2.17420200	-0.80584500
H	2.14664900	-1.74980700	1.15312000	C	1.53750000	0.12057200	-0.20479600
H	2.93660000	-1.68400300	-0.44162700	C	2.87555500	-1.62377600	-1.09403100
C	2.53975700	1.10751600	1.32245800	H	1.48917500	-2.95877600	-0.04073300
H	1.83617200	1.63309600	-0.67729400	H	0.97846700	-2.56555800	-1.69943300
H	0.51297800	1.42543400	0.49772500	C	2.96425000	-0.41503600	-0.15012200
H	4.17243500	0.30069300	0.13323000	H	1.37689800	0.73983200	-1.09731000
H	4.07694600	-0.42293200	1.75069500	H	1.22931100	0.67945200	0.67997800
H	3.03870100	2.07850700	1.39120900	H	2.94953700	-1.29396200	-2.13663100
H	2.06675200	0.89264700	2.28786500	H	3.65418100	-2.37199500	-0.91843700

TS (7-8)a

E= -2501.318325 H

C	-1.00355400	5.30751500	-0.86090500	O	-2.25927300	1.63137100	3.99547000
C	-1.04069900	4.14212000	-1.85828500	C	-1.00745900	-0.57077100	4.83313000
C	-1.63523800	2.85025400	-1.28099000	N	-2.38334700	-0.60608800	2.47951400
C	-1.70190000	1.69524900	-2.29849700	C	-0.11005100	-1.61532900	4.58473000
C	-2.25835100	0.40521500	-1.72062100	C	-1.54446700	-0.33417700	6.10051100
H	-2.02442500	5.51452200	-0.50609200	S	-4.13340400	-0.77521600	2.74346900
H	-0.42788300	5.00940200	0.02824000	F	-2.26506500	-0.07358000	1.04575300
H	-0.01979300	3.94096900	-2.21798700	C	0.24937900	-2.44638500	5.64310600
H	-1.61960600	4.44475600	-2.74407100	H	0.29790100	-1.77249700	3.59172700
H	-2.64898200	3.05126200	-0.90465200	C	-1.16771900	-1.17394300	7.14823800
H	-1.04550700	2.53224400	-0.40957000	H	-2.23445800	0.48593500	6.26187200
H	-0.67913400	1.52452400	-2.67492000	O	-4.20555700	-1.09393100	4.17170500
H	-2.29307900	2.04064200	-3.17196700	O	-4.53414300	-1.74810900	1.72923400
Li	-1.26790600	-0.98347900	-0.41806300	C	-4.94350300	0.77699800	2.41337700
O	-1.68992900	-2.91257700	-0.50610900	C	-0.27767700	-2.22592700	6.91972000
C	-1.96658700	-3.62703600	-1.73518200	H	0.94312000	-3.26385900	5.47171300
C	-2.68401200	-4.90272300	-1.30535300	H	-1.57119400	-1.00446600	8.14191500
C	-2.00070900	-5.20911300	0.03631600	C	-5.17358500	1.15581900	1.08682700
C	-1.80825400	-3.81144600	0.62906800	C	-5.37549000	1.54789100	3.49648600

H	0.00879600	-2.87742800	7.74033400
C	-5.85212000	2.35020100	0.84910300
H	-4.82840100	0.54549300	0.26020900
C	-6.06093300	2.73315000	3.23624500
H	-5.18520200	1.22460600	4.51286800
C	-6.29494200	3.13377600	1.91813000
H	-6.03561900	2.66315600	-0.17425300
H	-6.41077000	3.34249800	4.06417900
H	-6.82740300	4.06048300	1.72315900

8a

E= -413.7212653 H

C	-3.33152100	1.13004600	0.01651400
C	-3.44521200	-0.34685600	-0.38305600
C	-4.30326100	-1.17187600	0.58322600
C	-4.40410700	-2.65389000	0.17114800
C	-5.21643500	-3.47351300	1.12069900
H	-4.33904300	1.56737700	0.08251600
H	-2.90115700	1.20056900	1.02665200
H	-2.43838200	-0.78659500	-0.44014300
H	-3.86870500	-0.41803800	-1.39591100
H	-5.31495600	-0.74644800	0.63647700
H	-3.88370500	-1.11049000	1.59554300
H	-3.39176900	-3.08051200	0.11774500
H	-4.84473800	-2.74173900	-0.82804900
C	-6.33445500	-4.15745900	0.90008100
H	-6.82363600	-4.70970000	1.69631900
H	-6.77613400	-4.17518500	-0.08991200
C	-2.48303200	1.96265400	-0.95341400
H	-2.91827000	1.89946600	-1.96118900
H	-1.47826200	1.52203000	-1.02634500
C	-2.36366500	3.43312900	-0.54280100
H	-1.89038500	3.53439100	0.44239700
H	-1.75913900	4.00143000	-1.26024100
H	-3.34938000	3.91281200	-0.48637500
F	-4.68663300	-3.46923000	2.38187800

NTs₂F

E= -1714.955006 H

S	1.46918000	3.36474200	0.19466900
S	-1.30595900	4.74076700	-0.30003200
O	1.91695200	4.30468800	-0.83234200
O	1.90184500	1.97007800	0.20398600
O	-0.76533300	5.84409000	0.49623600
O	-2.65042900	4.22902200	-0.04551200
C	-1.06491700	5.05195400	-2.03370300
C	-1.61293100	4.15725900	-2.95889000
C	-0.38076600	6.20573300	-2.42252100
C	-1.45909900	4.43171500	-4.31576500
H	-2.14446800	3.27126100	-2.62844000

C	-0.24288100	6.46545900	-3.78559100
H	0.02993300	6.87997700	-1.67986500
C	-0.77706500	5.58154100	-4.72616800
H	-1.87355700	3.74899600	-5.05118900
H	0.28352100	7.35786600	-4.11011100
H	-0.66283600	5.78976500	-5.78618000
C	1.67736800	4.05167100	1.82354000
C	1.51672300	3.21759600	2.93572900
C	2.02720000	5.39938900	1.94547900
C	1.70340400	3.76244500	4.20457000
H	1.26286200	2.17075800	2.81509000
C	2.21975900	5.92187200	3.22329600
H	2.15259900	6.01751300	1.06456600
C	2.05303100	5.10832800	4.34696600
H	1.58075100	3.13312500	5.08074100
H	2.49969000	6.96455900	3.33871500
H	2.20038200	5.52396300	5.33969300
N	-0.28818700	3.23380900	-0.13483500
F	-0.82143600	2.56006900	0.99203100

NTs₂Li(THF)₂

E= -2087.791732 H

Li	-1.32516800	-1.14055500	1.13319800
O	-1.04430700	-2.91279600	0.39229000
C	-0.91585600	-3.13453300	-1.04020100
C	-1.66853400	-4.43351300	-1.33239500
C	-1.53588100	-5.19440000	-0.00494700
C	-1.67184900	-4.06874900	1.01441600
H	-1.32708700	-2.26684900	-1.56567700
H	0.15116000	-3.22008200	-1.27598500
H	-1.24302000	-4.96929900	-2.18578500
H	-2.72282900	-4.22529600	-1.54732700
H	-2.29934000	-5.96612800	0.12885800
H	-0.54883900	-5.66534500	0.07398100
H	-1.16163900	-4.25737000	1.96216900
H	-2.72353700	-3.83281600	1.21707600
O	-0.03826100	0.09693200	0.36927600
C	1.28173700	-0.32555800	-0.07654700
C	0.02730200	1.45818900	0.87830400
C	2.17111600	0.91639100	0.00876100
H	1.63140900	-1.12126300	0.59185000
H	1.19119700	-0.72678600	-1.08998300
C	1.50709300	1.71883100	1.13686200
H	-0.37696400	2.13579600	0.11530500
H	-0.59460500	1.51145500	1.77458500
H	2.13597000	1.47865500	-0.93145800
H	3.21379200	0.65858100	0.21532500
H	1.74980500	2.78515100	1.11136600
H	1.79551500	1.32008800	2.11606600
O	0.11231000	-0.56826500	4.61750900

S	-1.32625900	-0.88279000	4.66933800	H	-3.39710000	4.23482600	-2.12402000
O	-2.18653000	-0.12635400	5.59999200	H	-2.80197900	5.16440400	-0.75531600
C	-1.45080300	-2.62206300	5.12961400	H	-0.78268100	3.68802900	-0.59903500
N	-1.85242300	-0.75786700	3.10679000	H	-1.26395700	2.85345600	-2.05757400
C	-0.38110800	-3.47730800	4.85095800	H	-3.29658000	1.99212900	-0.94185700
C	-2.60285400	-3.08859900	5.76617500	H	-1.31086600	-0.89148000	-1.19327100
S	-3.42920400	-0.60213400	2.69581100	H	1.93525600	2.84391100	0.72602500
C	-0.47389000	-4.82324000	5.20981400	H	3.57352900	4.00467500	-0.72166200
H	0.51524300	-3.08912200	4.37870000	H	5.61454600	0.28393600	-1.39662400
C	-2.68491000	-4.43651200	6.11956800	H	3.95426600	-0.87887900	0.04313200
H	-3.41779000	-2.40775400	5.98265800	H	6.45631800	2.25446900	-2.45763700
O	-4.35595600	-1.51125400	3.39416900	H	5.22537300	3.45489700	-2.88273200
O	-3.32848200	-0.72812900	1.20513300	H	6.26015300	3.71862600	-1.48084600
C	-3.99213900	1.07846800	3.01618700	Li	-1.15451600	-1.51371300	0.82495700
C	-1.62491400	-5.30292000	5.84090900	O	-0.82480900	-3.40690600	0.27146800
H	0.35628100	-5.49324700	5.00366300	O	-1.84907200	-1.71970200	2.67130500
H	-3.57644700	-4.80752800	6.61749800	C	0.52764300	-3.90603100	0.15434700
C	-3.74112000	2.07695800	2.07120100	C	0.65947100	-4.30201200	-1.31130300
C	-4.67586100	1.35545400	4.20175200	C	-0.72758400	-4.90226700	-1.59941000
H	-1.69265400	-6.35049700	6.12159100	C	-1.66446400	-4.06106600	-0.71352100
C	-4.17976600	3.37687000	2.32603300	C	-2.29954700	-0.51239900	3.33723700
H	-3.22796500	1.83853100	1.14590600	C	-1.38969400	-0.35636200	4.55149600
C	-5.10948700	2.65918600	4.44426400	C	-1.13898800	-1.81996900	4.94669100
H	-4.86300300	0.56557200	4.91912300	C	-1.04578000	-2.51388000	3.58430900
C	-4.86095200	3.66830000	3.51057400	H	1.19654700	-3.10790000	0.48384400
H	-3.99497200	4.15902000	1.59502100	H	0.64974700	-4.77912700	0.81349200
H	-5.64372900	2.88417200	5.36304500	H	1.47772600	-5.00768800	-1.48574200
H	-5.20164100	4.68175700	3.70420700	H	0.83372200	-3.41040900	-1.92486200

9-NMe₂

E= -1849.484089 H

C	-1.69287700	5.48696000	-2.57786300	H	-1.00756500	-4.85044900	-2.65572800
C	-2.47782900	4.57516300	-1.62323300	H	-0.75486400	-5.95482200	-1.29480900
C	-1.66160700	3.35730500	-1.16460900	H	-2.41346000	-4.67153800	-0.19567200
C	-2.42039300	2.27957100	-0.34999100	H	-2.18394200	-3.27660300	-1.27301200
C	-1.55332200	1.01215000	-0.22285300	H	-2.23323800	0.31057900	2.62202000
C	-2.06037400	-0.21061700	-0.77483800	H	-3.35052700	-0.64650200	3.63020800
N	-0.42281000	1.17448700	0.43680900	H	-1.85646700	0.23281300	5.34752500
N	0.26029800	-0.08191600	0.59577200	H	-0.45391300	0.12714700	4.25158300
C	2.84019500	0.90482800	0.46907900	H	-0.22889000	-1.95927700	5.53842100
C	2.73548100	2.28518300	0.25383000	H	-1.98574700	-2.21315900	5.52250900
C	3.66306600	2.93202200	-0.55988800	H	-1.43717000	-3.53663600	3.59042800
C	4.71496500	2.22890100	-1.17002300	H	-0.01672000	-2.52844900	3.20766600
C	4.80523100	0.85014100	-0.93986200	C	-2.48385600	6.70842800	-3.06431500
C	3.87649800	0.18925900	-0.13204500	H	-2.81332600	7.29799700	-2.19648800
C	5.71685900	2.94743800	-2.04263200	H	-3.40074100	6.37000000	-3.56843200
S	1.59730300	0.04701400	1.47375200	C	-1.68469900	7.60623000	-4.01364600
O	1.50428600	0.87534900	2.71088500	H	-1.37273000	7.05808800	-4.91208500
O	2.12011300	-1.33877300	1.66137000	H	-2.27418300	8.47137400	-4.34181500
H	-0.77352800	5.82825600	-2.07840000	H	-0.77661600	7.98836800	-3.52956900
H	-1.36372400	4.90062400	-3.44902800	H	-2.93192400	-0.11278900	-1.42607300
				N	-2.97845000	2.70255200	0.96323200
				C	-4.32328800	3.25555900	0.92068100
				H	-4.74046100	3.27326900	1.93710500
				H	-4.39097300	4.28834900	0.52768300

H	-4.97214700	2.62025000	0.30733200
C	-2.09791300	3.48728100	1.81558600
H	-1.11899300	3.00708200	1.86057000
H	-1.96651000	4.53682600	1.48414900
H	-2.51523500	3.52171000	2.83131500

10-NMe₂

E= -1849.478312 H

C	-2.18734000	1.73526500	-0.96459000
C	-1.41988300	0.44468000	-0.65528500
C	-1.96911200	-0.74998700	-1.16620300
N	-0.34072400	0.75627000	0.08091100
N	0.55784700	-0.32608800	0.38182600
C	2.85823900	1.10001400	-0.15986200
C	2.45125000	2.38015700	-0.56147200
C	3.13263100	3.03616900	-1.58634300
C	4.23162300	2.44510900	-2.22896500
C	4.63101500	1.16843200	-1.80741900
C	3.95017700	0.49732200	-0.79018100
C	4.94772300	3.15767400	-3.35204200
S	1.90258200	0.18906100	1.08298900
O	1.74508700	1.16704500	2.20093100
O	2.71631200	-1.02257500	1.40116400
H	-2.10215700	2.02430600	-2.02272100
H	-3.25940400	1.66691300	-0.74029100
H	1.61057900	2.85427000	-0.06875800
H	2.80829600	4.03012400	-1.89008800
H	5.48879300	0.69383300	-2.28060600
H	4.26476600	-0.49102500	-0.46994100
H	5.92509100	2.70611000	-3.55453800
H	4.36917100	3.11743100	-4.28548100
H	5.10671300	4.21812200	-3.12193200
Li	-0.16907000	-2.08975900	0.74543700
O	0.78285200	-3.89757000	0.89341700
O	-1.23269400	-2.10301700	2.49654200
C	2.18126300	-4.07905900	0.60182700
C	2.24263200	-5.38960400	-0.19295700
C	1.01729200	-6.19143100	0.32643800
C	0.29542600	-5.19764000	1.25990800
C	-1.76208500	-0.79705100	2.85954700
C	-1.08649900	-0.44186000	4.18062200
C	-0.95505000	-1.81703700	4.85084400
C	-0.63952000	-2.72943700	3.66186000
H	2.52609600	-3.18974500	0.07660600
H	2.73562700	-4.16116300	1.54780800
H	3.19004300	-5.91370700	-0.03357300
H	2.14671500	-5.18997300	-1.26485600
H	0.37014500	-6.49738000	-0.50103800
H	1.30965500	-7.09495900	0.86983500
H	0.54600000	-5.39505500	2.31215400
H	-0.79127500	-5.19134900	1.15384300

H	-1.52833800	-0.10276900	2.04891500
H	-2.85178400	-0.88291100	2.97259300
H	-1.67333500	0.27133800	4.76849300
H	-0.10096600	-0.00526900	3.98408600
H	-0.17282400	-1.85673600	5.61541800
H	-1.90425100	-2.10721100	5.31735200
H	-1.05905700	-3.73565000	3.76931500
H	0.43970600	-2.81536400	3.49287900
C	-3.13267100	-0.71605500	-2.15407600
H	-3.12880000	0.21276800	-2.74379900
H	-2.99999400	-1.51160300	-2.90648700
C	-4.56119800	-0.87064900	-1.57215200
H	-4.63870200	-1.82628500	-1.03504000
H	-4.72424600	-0.08954100	-0.81544600
C	-5.67302100	-0.79195600	-2.62751600
H	-5.60256800	0.17005300	-3.15879800
H	-5.50877000	-1.56948800	-3.39028800
C	-7.08768900	-0.94510700	-2.05253700
H	-7.16255300	-1.90799100	-1.52630400
H	-7.25371800	-0.16973400	-1.29061300
C	-8.19142400	-0.85929100	-3.11112000
H	-8.08163600	-1.64745300	-3.86749000
H	-9.18750600	-0.96704200	-2.66362800
H	-8.16620400	0.10504900	-3.63503400
H	-1.76582600	2.54834000	-0.36600300
N	-1.26732200	-2.03997700	-1.04627300
C	-0.35392700	-2.30332000	-2.17154900
H	0.18997900	-3.24494500	-2.00831800
H	-0.88021800	-2.38458500	-3.14045500
H	0.37478900	-1.49286000	-2.24020000
C	-2.16388600	-3.18907100	-0.87602700
H	-2.79132600	-3.04204200	0.00894500
H	-2.82920800	-3.36850000	-1.73914900
H	-1.56907700	-4.10105000	-0.73822400

11-NMe₂

E= -1849.466719 H

C	-2.07332400	1.75347100	-1.41766000
C	-1.41373600	0.51700800	-0.81922900
C	-2.08095800	-0.80885500	-0.84002100
N	-0.22798900	0.77450300	-0.32063300
N	0.40596400	-0.34355000	0.29011700
C	2.96935100	0.52974900	-0.28743100
C	2.94046700	1.80786800	-0.85697200
C	3.81039500	2.12236800	-1.89920000
C	4.72711500	1.18018400	-2.39272200
C	4.74671200	-0.09108300	-1.80360200
C	3.87413100	-0.41997000	-0.76381700
C	5.65956800	1.53470400	-3.52693000
S	1.78514100	0.08673100	1.01211600
O	1.72844700	1.29671800	1.88128100

O	2.32456700	-1.14771400	1.65128900
H	-2.41805800	1.56830000	-2.44322000
H	-2.95327300	2.08992100	-0.85475900
H	2.24674600	2.54976900	-0.47741900
H	3.78027500	3.11869700	-2.33633200
H	5.45468400	-0.83553100	-2.16205400
H	3.89898000	-1.40638400	-0.31179700
H	6.35007800	0.71451800	-3.74930700
H	5.10261200	1.75965100	-4.44601000
H	6.25857100	2.42403500	-3.29272600
Li	-1.01706900	-1.57487900	1.03771600
O	-0.63114300	-3.53194900	1.33213000
O	-1.54852800	-1.08323200	2.93122000
C	0.70090900	-4.07701100	1.29658300
C	0.64619600	-5.10716700	0.17147500
C	-0.77464200	-5.70067800	0.32139800
C	-1.54540800	-4.62698900	1.12846700
C	-1.89940900	0.30538000	3.16325200
C	-0.99621800	0.78259200	4.30034600
C	-0.78482300	-0.50862800	5.10521300
C	-0.68253000	-1.55469700	3.99549500
H	1.38727400	-3.24292100	1.14224900
H	0.92553800	-4.55511900	2.26351700
H	1.43416300	-5.86234400	0.25456600
H	0.75447200	-4.60370400	-0.79487900
H	-1.24039100	-5.89148200	-0.64957900
H	-0.75206300	-6.64763700	0.87036000
H	-1.86684700	-5.01391000	2.10528000
H	-2.41912800	-4.22619600	0.60885300
H	-1.75098900	0.85646600	2.23140900
H	-2.96132300	0.35025100	3.43961100
H	-1.45475900	1.58879600	4.88181300
H	-0.04430300	1.13765700	3.89205800
H	0.11048300	-0.48612200	5.73447700
H	-1.65195100	-0.71138700	5.74604800
H	-1.02471300	-2.54941700	4.29667400
H	0.33993800	-1.62988200	3.60705700
C	-1.34778800	-1.75531400	-1.81457100
H	-0.32010800	-1.87316500	-1.44753600
H	-1.78764100	-2.76345100	-1.78973600
C	-1.24484400	-1.31501600	-3.29900300
H	-2.24511600	-1.09903400	-3.70240600
H	-0.68521600	-0.36992700	-3.34724200
C	-0.55652800	-2.35329400	-4.19515600
H	0.44214500	-2.57734100	-3.78893000
H	-1.11879700	-3.30003100	-4.15439800
C	-0.41569500	-1.91907600	-5.66037500
H	-1.41155000	-1.68916500	-6.06700300
H	0.15496600	-0.98033900	-5.70480600
C	0.26329900	-2.96801500	-6.54648700
H	-0.30266500	-3.90890300	-6.55503600
H	0.34891600	-2.62381900	-7.58494100

H	1.27569600	-3.19604100	-6.18851600
H	-1.35293600	2.57873300	-1.42813900
N	-3.54764100	-0.65430400	-1.16350400
C	-4.28748300	-0.19774600	0.00458500
H	-5.32107100	0.05759500	-0.27396700
H	-4.33024000	-0.96600500	0.80896600
H	-3.83125400	0.69420000	0.44016800
C	-4.19573300	-1.86602000	-1.62960900
H	-3.78371400	-2.21302200	-2.58121300
H	-4.12416600	-2.70832400	-0.90231000
H	-5.26467400	-1.66964600	-1.78746200

12-NMe₂

E= -2786.847600 H

C	-1.41467400	5.78208200	-0.61953900
C	-1.29811100	4.46841600	-1.40568500
C	-2.47265800	3.50045900	-1.17598700
C	-2.40041700	2.15077400	-1.91461200
C	-1.55957800	1.14782400	-1.25292100
N	-0.76435500	1.48798000	-0.26224000
N	0.07675300	0.42464700	0.20281400
C	2.09718800	2.10183400	1.27972200
C	1.78548300	3.45316200	1.46077300
C	2.75317000	4.42824000	1.21791200
C	4.04391100	4.08256200	0.78891300
C	4.33423100	2.72279900	0.60418300
C	3.37235100	1.73875200	0.83822500
C	5.08351000	5.14731700	0.53192300
S	0.82053400	0.83598500	1.54870900
O	-0.01198800	1.40882900	2.64884100
O	1.62130400	-0.38190100	1.95852800
H	-2.37509500	6.26943300	-0.85290300
H	-1.44464000	5.55778700	0.45741900
H	-0.36433000	3.96572700	-1.12931200
H	-1.22558500	4.69919700	-2.47871400
H	-3.39095600	4.02502600	-1.48423200
H	-2.56516200	3.35599800	-0.08093700
H	0.79965700	3.73225700	1.81629800
H	2.50536100	5.47563900	1.37851200
H	5.33091600	2.42835300	0.28190300
H	3.61739800	0.69046200	0.70013100
H	6.08114200	4.71236800	0.41090900
H	4.85770600	5.71590900	-0.38030600
H	5.12669000	5.87113300	1.35468800
O	1.59228500	-3.51684400	2.10299000
O	1.48559700	-1.78581300	4.79819900
C	2.78700500	-3.39862500	1.28851700
C	2.44127200	-4.06874100	-0.03813600
C	1.50207000	-5.19665900	0.41404600
C	0.71388800	-4.53070900	1.54431600
C	1.13955700	-0.58068200	5.53474000

C	2.44451000	-0.09144100	6.16031300
C	3.20184200	-1.40688700	6.39494400
C	2.82295100	-2.21567200	5.15434300
H	3.02052900	-2.33563900	1.20004100
H	3.61341500	-3.91313300	1.79751500
H	3.32916300	-4.42891900	-0.56652800
H	1.91027500	-3.36497900	-0.68940800
H	0.84676000	-5.56094600	-0.38272200
H	2.08140400	-6.04539900	0.79611200
H	0.43428100	-5.22347200	2.34435200
H	-0.18952100	-4.03381600	1.17495400
H	0.69335700	0.12986500	4.83396300
H	0.40049500	-0.84683800	6.30168000
H	2.27421700	0.48110700	7.07696600
H	2.99093100	0.54386600	5.45372700
H	4.28395500	-1.27540300	6.48798900
H	2.83576000	-1.90284200	7.30172200
H	2.80134200	-3.29663200	5.32314700
H	3.49814200	-2.00334500	4.31539100
C	-0.27328500	6.77085500	-0.89313100
H	-0.26479600	7.02947700	-1.96262900
H	0.68738000	6.27509900	-0.69252500
C	-0.36318000	8.05508900	-0.06344900
H	-0.33147900	7.83614600	1.01176600
H	0.46563100	8.73862700	-0.28720800
H	-1.29900800	8.59464500	-0.26051600
C	-1.59960800	-0.28814500	-1.74909900
H	-0.60125600	-0.62210600	-2.05963100
H	-1.90855100	-0.97502200	-0.94939200
H	-2.29331300	-0.39261400	-2.58269100
Li	0.85145800	-1.84040300	2.89984700
O	-1.08763700	-2.20144100	3.11201800
C	-1.56483800	-3.09201700	4.14413200
C	-2.18355900	-1.36375100	2.63890000
C	-2.81542600	-2.41844000	4.70003700
H	-1.80489700	-4.06882600	3.70018500
H	-0.75809200	-3.22046600	4.86995000
C	-3.42181300	-1.80154500	3.43015100
H	-1.90597200	-0.32309700	2.82244200
H	-2.28905900	-1.51106600	1.56035600
H	-2.53820400	-1.63562500	5.41589300
H	-3.48411900	-3.12499200	5.20119500
H	-4.09233700	-0.96203500	3.63569200
H	-3.98654600	-2.56022600	2.87584100
Li	-1.33705500	2.18336900	-3.96402500
O	-1.86727300	3.62432800	-5.35946700
O	0.67673400	2.30620200	-4.07829700
O	-1.63230000	0.58151900	-5.22679400
C	-2.33431800	4.97187100	-5.10368800
C	-1.94974200	3.33600200	-6.77738200
C	1.59384900	1.66554500	-3.14926600
C	1.39312500	3.24654600	-4.91349400

C	-0.61530500	-0.09718400	-5.98073800
C	-2.86299700	-0.14971500	-5.42034900
C	-3.04479800	5.41309300	-6.38204200
H	-2.98264800	4.94709200	-4.22477100
H	-1.46885200	5.61152600	-4.88695500
C	-2.23962200	4.67320300	-7.45945300
H	-1.00783500	2.88021600	-7.09514100
H	-2.75984700	2.61571000	-6.94232400
C	2.89083900	2.46746800	-3.23674100
H	1.13437600	1.66747800	-2.15945900
H	1.74302300	0.62694200	-3.47304700
C	2.87574100	2.94703600	-4.69532700
H	1.06645100	3.11053700	-5.94864100
H	1.13930500	4.26576700	-4.59689200
C	-0.91607000	-1.57814600	-5.76330500
H	-0.69529700	0.17441800	-7.04518200
H	0.35092000	0.23581600	-5.59901800
C	-2.46205900	-1.60916800	-5.74472300
H	-3.44350400	-0.04286600	-4.50307000
H	-3.42213600	0.30397100	-6.24981300
H	-3.04037900	6.50025700	-6.50411200
H	-4.08666200	5.07103300	-6.37917200
H	-2.78315000	4.54755600	-8.40075600
H	-1.30539400	5.20696500	-7.67076100
H	3.76735600	1.86265000	-2.98648900
H	2.85748600	3.32188500	-2.55200100
H	3.50447000	3.82486700	-4.87275000
H	3.20798300	2.14530100	-5.36622100
H	-0.51159600	-1.89818400	-4.79741600
H	-0.48508400	-2.21253400	-6.54381200
H	-2.84503500	-2.31090700	-4.99857600
H	-2.86243400	-1.90837100	-6.71853600
N	-3.74397600	1.59055700	-2.23528100
C	-4.60631000	1.33680900	-1.07989600
H	-4.05139800	0.78464700	-0.31413400
H	-5.00298500	2.25700600	-0.60525000
H	-5.47532500	0.72903000	-1.37475600
C	-4.49274400	2.31570200	-3.24522400
H	-4.85698700	3.31161100	-2.91355100
H	-3.87651200	2.47316900	-4.13601200
H	-5.38657500	1.74453100	-3.53952100

9-OMe

E= -1830.047772 H

C	-1.45686400	5.97749200	-1.61363100
C	-2.27376900	4.73331600	-1.24145800
C	-1.40282300	3.51542300	-0.90832700
C	-2.20698800	2.26501800	-0.54120900
C	-1.35497700	0.99534100	-0.39603400
C	-1.91225800	-0.24692100	-0.83972500
N	-0.20531500	1.17965300	0.22557200

N	0.46044600	-0.07305700	0.44829200
C	3.03018900	0.84480000	0.03616100
C	3.01379700	2.22671900	-0.18765100
C	3.85878800	2.78409000	-1.14579400
C	4.73838000	1.98677700	-1.89572200
C	4.74514500	0.60665600	-1.65249000
C	3.89734900	0.03607300	-0.70078400
C	5.64763800	2.60624300	-2.93092200
S	1.86515500	0.10157900	1.21046600
O	1.88110200	1.03611000	2.37316700
O	2.37796200	-1.27372700	1.47434000
H	-0.78641800	6.23504600	-0.77991800
H	-0.80297900	5.74189500	-2.46716600
H	-2.94679500	4.48227700	-2.07630600
H	-2.91906300	4.95944900	-0.38293400
H	-0.72646700	3.74676700	-0.07792100
H	-0.76519000	3.27079100	-1.76810100
H	-2.94893400	2.08550900	-1.33650300
H	-1.20121300	-0.99962600	-1.19434100
H	2.35190200	2.85872000	0.39416200
H	3.83890400	3.85954000	-1.31253000
H	5.42406700	-0.03168200	-2.21442300
H	3.91143800	-1.03375900	-0.51787000
H	6.29699400	1.85569300	-3.39381500
H	5.07223400	3.08873700	-3.73179400
H	6.28997800	3.37985900	-2.49087700
Li	-1.05443900	-1.31870100	0.95258000
O	-0.92533900	-3.30476200	0.73948300
O	-1.70890700	-1.15604300	2.81976700
C	0.36002900	-3.91823300	0.48059100
C	0.20760200	-4.56583800	-0.89070800
C	-1.23897800	-5.08469900	-0.83043400
C	-1.95644100	-4.00649900	-0.00251300
C	-1.91949100	0.18583500	3.33624600
C	-0.94138400	0.32931100	4.49845300
C	-0.91478700	-1.09770100	5.06692700
C	-0.98721300	-1.95058800	3.79797500
H	1.11491800	-3.13123700	0.54403100
H	0.56152000	-4.67268700	1.25576900
H	0.94227700	-5.35809700	-1.06546100
H	0.31737600	-3.81019400	-1.67748100
H	-1.69396000	-5.21346800	-1.81697400
H	-1.27222100	-6.05062100	-0.31308600
H	-2.67974600	-4.42544200	0.70634600
H	-2.46960400	-3.26866500	-0.62849200
H	-1.74625300	0.89296300	2.52148000
H	-2.96261600	0.26791100	3.67232700
H	-1.26821200	1.08018000	5.22520900
H	0.04512200	0.61017200	4.11436600
H	-0.01727800	-1.31452200	5.65465500
H	-1.79179400	-1.27639100	5.70106900
H	-1.52159700	-2.89592300	3.93651300

H	0.01101400	-2.16417400	3.39843100
C	-2.31866600	7.19793800	-1.96248200
H	-2.96748200	7.43920100	-1.10801400
H	-2.99141600	6.94106800	-2.79384300
C	-1.49497700	8.43271500	-2.33939300
H	-0.86438300	8.23783900	-3.21655800
H	-2.13876000	9.28868100	-2.57750500
H	-0.83242700	8.73429700	-1.51786700
H	-2.79848000	-0.17515200	-1.47322200
O	-2.93771900	2.58157900	0.66686600
C	-4.12866000	1.83837200	0.82738700
H	-4.58256700	2.15462600	1.77330000
H	-4.84580400	2.04130900	0.01290600
H	-3.94806200	0.75448400	0.86034300

10-OMe

E= -1830.04252 H

C	-2.18112700	1.87489400	-1.39140700
C	-1.41752500	0.60409600	-1.01037300
C	-2.04551600	-0.61570200	-1.29080100
N	-0.26943900	0.93001400	-0.39338400
N	0.50925300	-0.19956600	0.05765300
C	2.98344500	0.98607300	-0.29662600
C	2.72688100	2.25279800	-0.84196300
C	3.59586800	2.78905800	-1.79061600
C	4.73945900	2.09149200	-2.21215500
C	4.98316800	0.83012400	-1.65204200
C	4.11411400	0.27732100	-0.70869700
C	5.67334400	2.68838800	-3.23873400
S	1.81242400	0.24154500	0.87200100
O	1.63267500	1.29507900	1.91556900
O	2.46819000	-1.01696600	1.34320100
H	-2.37944700	1.94214800	-2.47008400
H	-3.15156300	1.95128400	-0.88193500
H	1.85018000	2.80609400	-0.52494800
H	3.38652300	3.77206500	-2.20945200
H	5.86746500	0.27278800	-1.95560800
H	4.31090800	-0.69996700	-0.27946000
H	6.54688900	2.04862000	-3.40310400
H	5.17351900	2.82332400	-4.20717600
H	6.03580500	3.67684700	-2.92843600
Li	-0.45602600	-1.81851600	0.64592700
O	0.10686500	-3.72082400	0.98540200
O	-1.52927700	-1.47352800	2.32795800
C	1.46947000	-4.18149400	1.08962000
C	1.57361300	-5.28228100	0.03969100
C	0.20209000	-5.97310000	0.16519800
C	-0.73884400	-4.83183600	0.60665400
C	-1.86565900	-0.07410500	2.54263100
C	-1.23981600	0.28973000	3.88615100
C	-1.35907300	-1.03003700	4.66271900

C	-1.08603600	-2.06860600	3.57212500
H	2.11148200	-3.31360700	0.93094900
H	1.64623400	-4.57987100	2.10082400
H	2.41209700	-5.96158200	0.22207100
H	1.69914200	-4.83887100	-0.95479800
H	-0.12656700	-6.43816300	-0.76887900
H	0.23988700	-6.75402800	0.93250800
H	-1.36113900	-5.12058700	1.46276800
H	-1.39515000	-4.47891400	-0.19421600
H	-1.46508500	0.49912100	1.70295600
H	-2.96039400	0.01804400	2.56665700
H	-1.75474400	1.12519000	4.37185000
H	-0.19020800	0.56408100	3.73536000
H	-0.65219100	-1.11375500	5.49434900
H	-2.37360800	-1.14937900	5.06287000
H	-1.62841000	-3.00847800	3.72127900
H	-0.01597000	-2.29197500	3.48986500
C	-3.36460700	-0.81260600	-1.98645900
H	-3.76480200	0.15233000	-2.32071000
H	-3.24089600	-1.41104300	-2.91265600
C	-4.45233200	-1.51974600	-1.14281600
H	-4.04404400	-2.46997600	-0.76997500
H	-4.66463900	-0.90659800	-0.25409200
C	-5.75670800	-1.79012400	-1.90468600
H	-6.17011800	-0.83714200	-2.27065900
H	-5.53741000	-2.38808600	-2.80318400
C	-6.82429600	-2.51259600	-1.07234800
H	-6.41747000	-3.46955100	-0.71411700
H	-7.04489900	-1.92042700	-0.17231100
C	-8.12394600	-2.76961300	-1.84065900
H	-7.94499700	-3.38830800	-2.72978900
H	-8.86390800	-3.28938500	-1.21914400
H	-8.57844400	-1.82968500	-2.17985600
H	-1.58042100	2.74195200	-1.10170100
O	-1.36940900	-1.87262200	-1.08823400
C	-0.53053200	-2.23563200	-2.18456800
H	-0.19832900	-3.27006800	-2.03141200
H	-1.07951500	-2.18081200	-3.13431900
H	0.34688400	-1.57941400	-2.23400500

11-OMe

E= -1830.03475 H

C	-2.19707800	1.69651600	-1.12945000
C	-1.38693100	0.46924500	-0.74725400
C	-1.99486500	-0.86118300	-0.85774300
N	-0.20759100	0.75918600	-0.24592300
N	0.49515300	-0.38427900	0.24927200
C	3.03843100	0.56401300	-0.29002400
C	2.89010500	1.81187500	-0.90933100
C	3.76871200	2.19114700	-1.92164000
C	4.81335500	1.34804000	-2.33543200

C	4.94819800	0.10689000	-1.70029600
C	4.06875000	-0.28798800	-0.68904600
C	5.75477400	1.77263500	-3.43752500
S	1.86333000	0.04024300	0.98879800
O	1.78647800	1.21275900	1.90727700
O	2.42960800	-1.20918200	1.57426600
H	-2.53734800	1.65228500	-2.17204600
H	-3.10162400	1.79496400	-0.51483900
H	2.09070400	2.47497000	-0.59817500
H	3.64521200	3.16191500	-2.39819200
H	5.75413000	-0.56095500	-1.99784100
H	4.18185000	-1.24975100	-0.19932600
H	6.56699200	1.05037000	-3.57133900
H	5.23025500	1.86453800	-4.39789400
H	6.20581500	2.75070300	-3.22733700
Li	-0.94950200	-1.59265600	1.02170900
O	-0.60239100	-3.55243200	1.30179200
O	-1.54826900	-1.10064500	2.88034800
C	0.72534200	-4.11101400	1.24320800
C	0.63558400	-5.15891100	0.13965800
C	-0.76538400	-5.76102300	0.37562600
C	-1.55128300	-4.61199300	1.04927100
C	-1.89991900	0.29110100	3.10318500
C	-1.01201300	0.76810100	4.25182200
C	-0.82101800	-0.52055600	5.06585800
C	-0.70398100	-1.57171900	3.96283800
H	1.41441400	-3.28466600	1.05967600
H	0.97048800	-4.57471700	2.21190700
H	1.43497200	-5.90426400	0.19944000
H	0.68986900	-4.67145100	-0.83971200
H	-1.24004400	-6.09203900	-0.55253900
H	-0.70423800	-6.62491400	1.04613300
H	-2.00119200	-4.92815700	1.99937100
H	-2.33856600	-4.19628400	0.41511600
H	-1.73521700	0.83903800	2.17213400
H	-2.96558000	0.33800200	3.36429800
H	-1.47465800	1.57977200	4.82226000
H	-0.05161600	1.11476500	3.85639200
H	0.06311100	-0.50004400	5.71066900
H	-1.70040600	-0.71691900	5.69177800
H	-1.05558300	-2.56394900	4.26087100
H	0.32547100	-1.65363300	3.59389000
C	-1.29995300	-1.85060500	-1.80201100
H	-0.26925000	-2.01323300	-1.46077400
H	-1.81007200	-2.82631500	-1.73828600
C	-1.25148700	-1.44611400	-3.29420600
H	-2.27217000	-1.22359600	-3.63579900
H	-0.67682600	-0.51298900	-3.39305100
C	-0.63327400	-2.51665000	-4.20329200
H	0.38559100	-2.74666000	-3.85428400
H	-1.20549400	-3.45280700	-4.10391900
C	-0.57775000	-2.12057100	-5.68496400

H	-1.59439500	-1.88939000	-6.03554300	C	1.09809800	-1.12521900	6.19386400
H	-0.00182600	-1.18958200	-5.78786200	C	2.42187300	-1.18628800	6.95707200
C	0.03573400	-3.19894600	-6.58354100	C	2.80399400	-2.66835600	6.82612400
H	-0.53447600	-4.13557800	-6.52760300	C	2.34820700	-2.98277600	5.40296900
H	0.05461300	-2.88534900	-7.63499000	H	2.78324600	-2.18841200	1.54597500
H	1.06836900	-3.42433100	-6.28687200	H	3.09693000	-3.89354500	1.97687200
H	-1.59134800	2.59818500	-0.98774700	H	2.90011800	-4.11001600	-0.43497300
O	-3.38165200	-0.74561700	-1.31365800	H	1.68263200	-2.81776800	-0.51504700
C	-4.32081800	-0.90697500	-0.28746700	H	0.26302100	-4.82589400	-0.53185500
H	-4.22892500	-0.14427400	0.50635800	H	1.30792100	-5.63051100	0.65632600
H	-5.32487100	-0.81316500	-0.72974900	H	-0.31911300	-4.70710400	2.17672200
H	-4.24896600	-1.89590800	0.20003800	H	-0.61849500	-3.30149300	1.12472300

12-OMe

E= -2767.411117 H

C	-1.42956700	5.88006600	-0.47467200	H	0.92769300	-0.17047100	5.68991200
C	-0.81453000	4.62733600	-1.11311600	H	0.24350100	-1.34413800	6.84639200
C	-1.81410100	3.46458100	-1.27469600	H	2.31610700	-0.85395200	7.99403900
C	-1.23754100	2.19615800	-1.87392400	H	3.17317700	-0.55495200	6.46879100
C	-0.61370300	1.23604300	-1.00999100	H	3.87207100	-2.85614600	6.97048200
N	-0.27676600	1.57748000	0.22461500	H	2.24592300	-3.27484600	7.54950300
N	0.48641500	0.56969900	0.89968800	H	2.06952800	-4.02886200	5.24737200
C	2.46289400	2.23998700	2.00055900	H	3.11740800	-2.70959300	4.66880900
C	2.21593800	3.61190700	1.89578900	C	-0.45952300	7.06354400	-0.36114800
C	3.25648200	4.48336100	1.56490500	H	-0.07813400	7.31762700	-1.36110500
C	4.55477800	4.01178700	1.33259600	H	0.41621400	6.75891500	0.22957700
C	4.78414500	2.62984300	1.44483000	C	-1.08965700	8.30806300	0.27165900
C	3.75263500	1.74980800	1.76367800	H	-1.44505100	8.09982100	1.28911100
C	5.67491200	4.95223200	0.95684800	H	-0.37189000	9.13558600	0.33463200
S	1.07811900	1.10110100	2.27697500	H	-1.95046200	8.65944700	-0.31231400
O	0.16379300	1.86012700	3.17947000	C	-0.28355700	-0.13854900	-1.56965700
O	1.72497700	-0.10252900	2.93325700	H	0.79665300	-0.32733600	-1.52733900
H	-2.30836900	6.19390900	-1.06097800	H	-0.75412400	-0.93518900	-0.97809300
H	-1.80889100	5.62912100	0.52737300	H	-0.61430900	-0.23297400	-2.60678300
H	0.02772800	4.27893200	-0.50274500	Li	0.64772600	-1.62412800	3.31637900
H	-0.40091500	4.88454200	-2.09983300	O	-1.33578900	-1.63877400	3.44445600
H	-2.63651200	3.81059600	-1.92010400	C	-2.04708400	-2.54489800	4.30704200
H	-2.25771400	3.27957800	-0.27491400	C	-2.27853900	-0.67698600	2.88983500
H	1.22136400	3.99485700	2.09753100	C	-3.16952300	-1.70008900	4.89848700
H	3.05566100	5.55051700	1.49581500	H	-2.44921900	-3.38351100	3.71830300
H	5.78723200	2.24012100	1.28186100	H	-1.33213700	-2.93246600	5.03610400
H	3.94546400	0.68462500	1.84429500	C	-3.58657700	-0.84362800	3.68891000
H	6.60387300	4.70261800	1.48337900	H	-1.82425700	0.30951600	2.99507500
H	5.89369800	4.90284000	-0.11880700	H	-2.41240100	-0.88780500	1.82357400
H	5.42142600	5.99166300	1.19105800	H	-2.77723500	-1.07020800	5.70528100
O	1.13962400	-3.23368300	2.22813500	H	-3.98787500	-2.30591400	5.29978600
O	1.17324300	-2.16571900	5.18237200	H	-4.01071100	0.12152200	3.98032900
C	2.38993100	-3.20615200	1.49297600	H	-4.33757600	-1.37281400	3.09193700
C	2.04289400	-3.66470800	0.07902800	Li	-1.26477200	1.86719200	-4.60465800
C	0.90378400	-4.66162100	0.33960800	O	-2.40495700	3.04335500	-5.79459800
C	0.14812400	-3.99382500	1.49028300	O	0.60479800	2.43594100	-5.10604000
				O	-1.36495900	0.09889400	-5.59649500
				C	-2.69656900	4.43029100	-5.48112000
				C	-3.46936800	2.48703200	-6.60467300
				C	1.74173300	2.15384900	-4.24348500

C	0.92750500	3.51882000	-6.01143800
C	-0.51242700	-0.22776600	-6.71579000
C	-2.18624500	-1.04847600	-5.25900000
C	-4.13670100	4.66901100	-5.93659500
H	-2.54586600	4.58018900	-4.40849600
H	-1.98941500	5.06461200	-6.02981700
C	-4.26954500	3.68583600	-7.10905600
H	-3.01729900	1.89033300	-7.40139100
H	-4.08754900	1.83040200	-5.97888400
C	2.72336500	3.30249200	-4.46687600
H	1.36652100	2.08465700	-3.21934800
H	2.16976700	1.18855100	-4.54377100
C	2.44369500	3.68991600	-5.92637000
H	0.56929000	3.25162800	-7.01002900
H	0.40623100	4.42538700	-5.67949000
C	-0.37152500	-1.74508700	-6.66974900
H	-0.99242100	0.09944100	-7.64982300
H	0.42166600	0.32169700	-6.58579200
C	-1.77929700	-2.17115400	-6.22475000
H	-1.98611000	-1.30727800	-4.21449100
H	-3.24174900	-0.77226000	-5.35525800
H	-4.31261800	5.71078700	-6.22029000
H	-4.84013500	4.40767000	-5.13744100
H	-5.30610800	3.42398300	-7.34128900
H	-3.80787900	4.10150900	-8.01274600
H	3.75971700	3.00124700	-4.28750300
H	2.48802300	4.13814400	-3.79748800
H	2.75802600	4.70819000	-6.17506700
H	2.94745300	2.99702600	-6.61119000
H	0.37578100	-2.03240400	-5.92078400
H	-0.07694000	-2.16931100	-7.63431000
H	-1.80188800	-3.15327200	-5.74377800
H	-2.45545100	-2.20072900	-7.08684000
C	-3.32999500	1.05990800	-2.44588100
H	-3.14819200	0.22322300	-1.75767200
H	-3.94461900	1.80915900	-1.92893300
H	-3.88720300	0.69193900	-3.31547300
O	-2.10362100	1.62304700	-2.90659400

12-H

E= -2652.897666 H

C	-1.74339600	5.51574600	-0.52990600
C	-1.31413000	4.28465000	-1.33939800
C	-2.39208200	3.18656200	-1.43125700
C	-2.00900100	1.93375100	-2.21832700
C	-1.21650600	0.93359900	-1.53576200
N	-0.54381800	1.21503700	-0.43945000
N	0.22913300	0.10867000	0.05709200
C	2.32776200	1.66522300	1.13807800
C	2.11678700	3.03280500	1.34352800
C	3.13966100	3.94308600	1.07770100

C	4.38957900	3.51567400	0.60460200
C	4.57997400	2.14131400	0.39661200
C	3.56036000	1.22238900	0.65062000
C	5.49413800	4.51028900	0.33557300
S	0.96888200	0.48544500	1.40739400
O	0.16190100	1.12879800	2.49023700
O	1.68242900	-0.77492300	1.85209200
H	-2.65772600	5.94662200	-0.96939100
H	-2.01696900	5.20204600	0.48891100
H	-0.41536200	3.84818400	-0.88737900
H	-1.03204400	4.60023100	-2.35591900
H	-3.29286300	3.63574000	-1.88217100
H	-2.67095900	2.93394300	-0.38818400
H	1.16412700	3.37337600	1.73416000
H	2.96773300	5.00365900	1.25197500
H	5.54271700	1.78404400	0.03683100
H	3.72703900	0.16212200	0.48745000
H	6.41475800	4.01005100	0.01757300
H	5.21101800	5.22069100	-0.45199800
H	5.72620300	5.10311600	1.22948700
O	1.71280600	-3.72668100	2.79530500
O	1.49483500	-1.47465000	5.02860500
C	2.89344700	-3.81257500	1.95588300
C	2.55433300	-4.84169400	0.88092400
C	1.64570900	-5.81304800	1.64873900
C	0.84709800	-4.86545900	2.54529400
C	1.09164800	-0.19327100	5.58454400
C	2.36691000	0.42272500	6.15575600
C	3.14896800	-0.82039200	6.60535500
C	2.82274600	-1.82105700	5.49599400
H	3.09434600	-2.81256400	1.56626400
H	3.74058600	-4.13949900	2.57393500
H	3.44725400	-5.31812700	0.46508100
H	2.00187000	-4.36542500	0.06236000
H	0.99704300	-6.40725300	0.99836000
H	2.24748600	-6.50118600	2.25428600
H	0.57080500	-5.30657100	3.50821200
H	-0.06083500	-4.50455900	2.04949600
H	0.63855400	0.39277400	4.78119600
H	0.34747900	-0.37552800	6.37141500
H	2.15933200	1.12350500	6.97000000
H	2.91434700	0.95768300	5.37081200
H	4.22499900	-0.64671800	6.70068500
H	2.77215400	-1.18150000	7.56987700
H	2.80880200	-2.86167600	5.83411200
H	3.52412400	-1.73324500	4.65645100
C	-0.66834200	6.60736900	-0.44544200
H	-0.39317400	6.92533800	-1.46220700
H	0.24388800	6.18081300	-0.00380600
C	-1.10116100	7.83223500	0.36588600
H	-1.34210700	7.55925500	1.40145100
H	-0.31116300	8.59318200	0.39869300

H	-1.99460200	8.30192900	-0.06634300
C	-1.16543800	-0.45978900	-2.14687900
H	-0.13502900	-0.75788500	-2.37956800
H	-1.54590800	-1.21433500	-1.44591600
H	-1.75584100	-0.50845000	-3.06678500
Li	0.92370000	-1.92134500	3.16582900
O	-1.03163300	-2.24040900	3.34126900
C	-1.60242100	-2.79298700	4.54691600
C	-2.06908900	-1.56345300	2.57074200
C	-2.86539900	-1.97510700	4.79605200
H	-1.84239400	-3.85375800	4.38452400
H	-0.84905000	-2.71765200	5.33483700
C	-3.36944200	-1.74563400	3.36273900
H	-1.77582300	-0.51568400	2.47678800
H	-2.10600600	-2.01139000	1.57321900
H	-2.61099200	-1.02145100	5.27342400
H	-3.58611700	-2.49944900	5.43103500
H	-4.02723400	-0.87653800	3.27084200
H	-3.91881400	-2.62654700	3.01066000
Li	-1.14465200	2.21954100	-4.26811500
O	-1.88621500	3.73593700	-5.42363200
O	0.84224300	2.39668700	-4.43858900
O	-1.63235300	0.70869700	-5.53498600
C	-2.57111800	4.92030900	-4.94318900
C	-1.89826700	3.71487800	-6.87272900
C	1.74123500	2.02740600	-3.35878900
C	1.50547600	3.31985300	-5.33762200
C	-0.72342100	-0.23196200	-6.15814000
C	-2.99945900	0.28078500	-5.73152000
C	-3.33195400	5.47190800	-6.14682800
H	-3.21437100	4.62766900	-4.10973500
H	-1.82473900	5.63721800	-4.57764600
C	-2.40133800	5.09193600	-7.30719000
H	-0.88832300	3.48904800	-7.22694600
H	-2.57243300	2.91710200	-7.20661700
C	2.80526100	3.11891600	-3.33972200
H	1.15279800	1.95172600	-2.44226400
H	2.18117200	1.04635400	-3.58517600
C	2.94687900	3.44812800	-4.83335300
H	1.44342200	2.92489500	-6.35747200
H	0.97248900	4.27676100	-5.29868500
C	-1.58846700	-1.40008000	-6.63948800
H	-0.22440200	0.27463400	-6.99381100
H	0.03266200	-0.52692300	-5.42510200
C	-2.94848900	-0.72607200	-6.87805300
H	-3.36849300	-0.18302400	-4.80754300
H	-3.60415400	1.16741800	-5.94217100
H	-3.51108200	6.54813100	-6.06611800
H	-4.30041100	4.96822500	-6.25139400
H	-2.90504200	5.05979000	-8.27795400
H	-1.56802500	5.80135300	-7.37568300
H	3.73745800	2.77906200	-2.87980100

H	2.44364400	3.99043700	-2.78202600
H	3.36063700	4.44300300	-5.02363200
H	3.59267500	2.71099400	-5.32490200
H	-1.67434200	-2.16084300	-5.85506500
H	-1.17607400	-1.87647500	-7.53385100
H	-3.78906200	-1.42591700	-6.85350400
H	-2.95818300	-0.20850100	-7.84479400
H	-2.87961800	1.47005200	-2.70628900

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E= -1946.584794 H

C	-1.71305000	5.47488900	-2.51232100
C	-2.55288100	4.32622700	-1.93741600
C	-1.70395800	3.15887100	-1.41639600
C	-2.52095800	1.98661800	-0.81544100
C	-1.62633900	0.76886400	-0.49934800
C	-2.08651500	-0.53298100	-0.89245000
N	-0.53457000	1.04906000	0.18155200
N	0.17299100	-0.14868700	0.53539800
C	2.69304600	0.98968600	0.45186700
C	2.58844000	2.36289700	0.20036700
C	3.50857600	2.98527200	-0.64151500
C	4.55055600	2.26270500	-1.24476200
C	4.64264600	0.89070300	-0.97532400
C	3.72227300	0.25515100	-0.13925600
C	5.54133500	2.95239000	-2.15258200
S	1.44681300	0.15169700	1.46849700
O	1.22472400	1.08359700	2.61178100
O	2.03620000	-1.17474900	1.81734000
H	-1.01854100	5.83622900	-1.73883500
H	-1.08412100	5.09595700	-3.33206400
H	-3.24516200	3.96024600	-2.71148800
H	-3.18257800	4.71673600	-1.12614600
H	-0.99443200	3.52434800	-0.66512000
H	-1.09453600	2.76061600	-2.23938100
H	-3.23002300	1.66488600	-1.58893400
H	-1.30133200	-1.23131100	-1.20453100
H	1.79620800	2.93700800	0.66832300
H	3.41905100	4.05300200	-0.83290800
H	5.44542700	0.31030200	-1.42568400
H	3.80132400	-0.80765000	0.06534200
H	6.25816100	2.24123700	-2.57636800
H	5.03628800	3.45638900	-2.98649700
H	6.11189600	3.72175500	-1.61578200
Li	-1.15108500	-1.65073900	0.83855100
O	-0.68392800	-3.55274600	0.39720700
O	-1.82762600	-1.83658500	2.69803000
C	0.70776400	-3.93330600	0.30588700
C	0.89149100	-4.34147900	-1.15082700
C	-0.43127200	-5.07252400	-1.44128700
C	-1.45067900	-4.31897300	-0.56605500

C	-2.30314400	-0.62301100	3.33977800
C	-1.48185800	-0.48018700	4.62008900
C	-1.19951500	-1.94491300	4.98687200
C	-0.98034300	-2.57907500	3.61328200
H	1.30018000	-3.07386300	0.62749100
H	0.89771200	-4.78048800	0.98261000
H	1.77289000	-4.97176300	-1.30509800
H	0.98950100	-3.44816600	-1.77835000
H	-0.70779900	-5.05366200	-2.49957900
H	-0.36071300	-6.12097700	-1.13011500
H	-2.12376800	-4.99728400	-0.02849500
H	-2.05686400	-3.60914200	-1.13707800
H	-2.17109000	0.20650600	2.64147500
H	-3.37405200	-0.74328200	3.55017500
H	-2.02328000	0.06520300	5.39958500
H	-0.54793700	0.04933300	4.40436000
H	-0.33040300	-2.06921700	5.64031700
H	-2.06977600	-2.39305600	5.48203800
H	-1.26900300	-3.63355900	3.56667900
H	0.06007500	-2.47609100	3.28321800
C	-2.55246900	6.65284400	-3.02386000
H	-3.18921600	7.02418800	-2.20786800
H	-3.23782200	6.29688500	-3.80684000
C	-1.70855600	7.80666400	-3.57327600
H	-1.07732600	7.47668800	-4.40860000
H	-2.33843500	8.62749400	-3.93830000
H	-1.04467200	8.21678700	-2.80117800
H	-2.92961000	-0.54371900	-1.58741300
C	-3.35858600	2.43542000	0.37995200
C	-4.75961000	2.44686900	0.30601800
C	-2.76009900	2.87074900	1.57511000
C	-5.54178200	2.87456700	1.38316800
H	-5.24519100	2.11392600	-0.60926800
C	-3.53706200	3.30015900	2.65286600
H	-1.67805700	2.84040200	1.65714400
C	-4.93252900	3.30602700	2.56271900
H	-6.62628800	2.86956200	1.29834900
H	-3.05012200	3.63023200	3.56795100
H	-5.53628200	3.64091700	3.40291400

10-Ph

E= -1946.587866 H

C	-1.55517100	1.62138900	-2.43835500
C	-0.91070400	0.42777600	-1.73615800
C	-1.44596400	-0.92122800	-1.95415600
N	0.08335900	0.80512700	-0.96308500
N	0.63204700	-0.19319700	-0.14107900
C	3.18844500	0.87326500	-0.11646700
C	3.20776200	2.10046700	-0.78988700
C	4.29615700	2.42988200	-1.59528600
C	5.38316100	1.55382400	-1.74602000

C	5.34567000	0.33215900	-1.06113000
C	4.25788600	-0.01228600	-0.25568800
C	6.55491400	1.92631300	-2.62299200
S	1.74585900	0.40124100	0.87118300
O	1.36649100	1.64738900	1.59468900
O	2.17715100	-0.74578500	1.71621900
H	-1.71188000	1.44071500	-3.51055900
H	-2.53410300	1.88328600	-2.01307300
H	2.38004900	2.79156900	-0.67458900
H	4.30477900	3.38589200	-2.11546500
H	6.17899900	-0.36055000	-1.15766100
H	4.23802300	-0.95961200	0.27352900
H	7.32912600	1.15223000	-2.60599800
H	6.24455100	2.06593400	-3.66666700
H	7.01479300	2.86860200	-2.29881600
Li	-0.51652000	-1.70078400	0.38492000
O	-0.00415800	-3.52366000	0.90610600
O	-1.67681600	-1.20245200	1.96149000
C	1.38282700	-3.95334500	0.93316700
C	1.34420900	-5.46199000	0.69923300
C	0.00837600	-5.85389800	1.34869800
C	-0.88421700	-4.67070400	0.97304900
C	-2.23589500	0.13864800	1.97882300
C	-1.77206300	0.76993900	3.29098500
C	-1.66422200	-0.45246200	4.21461800
C	-1.11339000	-1.51343300	3.26383600
H	1.92157300	-3.39673400	0.16477000
H	1.80421400	-3.70162300	1.91305600
H	2.20686600	-5.97050800	1.14086700
H	1.32548300	-5.67805900	-0.37492800
H	-0.39123400	-6.80489000	0.98351300
H	0.11754000	-5.92168900	2.43793300
H	-1.66824800	-4.46140300	1.70785000
H	-1.34795700	-4.81336100	-0.01019600
H	-1.87814300	0.66654500	1.09217600
H	-3.32943600	0.05555600	1.93268300
H	-2.47215100	1.52917300	3.65389300
H	-0.79025000	1.23399700	3.15043000
H	-1.00683300	-0.29046000	5.07453300
H	-2.65423000	-0.74457800	4.58644200
H	-1.40586500	-2.53479000	3.52533400
H	-0.02142100	-1.45922600	3.19230400
C	-2.93709000	-1.04298900	-2.27293800
H	-3.35127700	-0.05489700	-2.51009400
H	-3.09161100	-1.64409500	-3.18613900
C	-3.83651600	-1.64345800	-1.16770600
H	-3.45027100	-2.62929100	-0.87024500
H	-3.76955300	-1.00958400	-0.27271500
C	-5.30909200	-1.78242200	-1.57849900
H	-5.70247300	-0.79313200	-1.85993500
H	-5.37902900	-2.40360900	-2.48481000
C	-6.20150900	-2.38670200	-0.48625800

H	-5.81744400	-3.38100600	-0.21499500
H	-6.12566400	-1.77360100	0.42363800
C	-7.67222700	-2.50558900	-0.89713100
H	-7.78618400	-3.13656900	-1.78818200
H	-8.27963700	-2.94811500	-0.09770200
H	-8.09992800	-1.52252700	-1.13305500
H	-0.90923100	2.49714400	-2.32022100
C	-0.59871200	-2.01720100	-2.35202300
C	-1.12883700	-3.31377200	-2.67876500
C	0.81970600	-1.89745900	-2.55774500
C	-0.33582000	-4.35678500	-3.15024500
H	-2.19239400	-3.49896800	-2.56025300
C	1.59837900	-2.94768600	-3.02803300
H	1.28853500	-0.93835500	-2.37737100
C	1.04495100	-4.20263400	-3.33199600
H	-0.81022100	-5.30988600	-3.38537600
H	2.66449400	-2.77778600	-3.17902900
H	1.66152900	-5.01756700	-3.70336900

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E= -1946.589343 H

C	-1.74407800	1.94288900	-1.74001400
C	-1.13615700	0.71267300	-1.08039300
C	-1.80531400	-0.60718800	-1.20035000
N	0.03738800	0.93154100	-0.55079400
N	0.62555800	-0.18990200	0.06833600
C	3.22282000	0.63226300	-0.44195700
C	3.23185500	1.91358300	-1.00497800
C	4.13508000	2.21434600	-2.02236900
C	5.04596400	1.25587800	-2.49549800
C	5.02580400	-0.01797900	-1.91237800
C	4.12056900	-0.33410100	-0.89694800
C	6.01782700	1.59801500	-3.59971400
S	2.00416000	0.20852400	0.82812300
O	1.93143600	1.41514300	1.69746500
O	2.49034300	-1.04116800	1.47317800
H	-1.69217700	1.85537900	-2.83571000
H	-2.80310900	2.06745800	-1.49152300
H	2.54156600	2.66706200	-0.64201400
H	4.13614000	3.21257900	-2.45577700
H	5.72779100	-0.77479600	-2.25591600
H	4.11434800	-1.32251700	-0.44882000
H	6.66792300	0.74996800	-3.83836800
H	5.49245600	1.88601300	-4.51942900
H	6.65932700	2.44447500	-3.32242600
Li	-0.86482300	-1.29676100	0.83142200
O	-0.74133100	-3.23819100	1.18879800
O	-1.55413000	-0.62645200	2.55638100
C	0.52264200	-3.89244000	1.41448000
C	0.56684000	-4.98244800	0.34513600
C	-0.91327900	-5.42638200	0.23581400

C	-1.70361300	-4.27093000	0.89603900
C	-1.40552300	0.74373800	3.00456600
C	-1.45774600	0.67025400	4.52810300
C	-2.45232700	-0.47894100	4.75324300
C	-2.09449800	-1.44560900	3.62076600
H	1.30133200	-3.13058100	1.33843100
H	0.53178300	-4.32337600	2.42780000
H	1.23798700	-5.80373100	0.61450500
H	0.91260500	-4.55548100	-0.60187900
H	-1.21139200	-5.57772400	-0.80552700
H	-1.08980800	-6.36453300	0.77135200
H	-2.17505600	-4.59596300	1.83351500
H	-2.46997000	-3.83097300	0.25426000
H	-0.46314000	1.12366700	2.60425400
H	-2.23683700	1.33950800	2.60457200
H	-1.77660100	1.61481000	4.97937300
H	-0.47103900	0.41048100	4.93033400
H	-2.36242300	-0.94717400	5.73827200
H	-3.48124400	-0.11832600	4.63794700
H	-2.95728100	-1.99780900	3.23516000
H	-1.32517700	-2.16422900	3.92764100
C	-1.06473100	-1.62801100	-2.06528100
H	0.00234600	-1.61462000	-1.80719900
H	-1.41011900	-2.64966200	-1.83775100
C	-1.17949800	-1.41679600	-3.59477500
H	-2.23917100	-1.40324800	-3.88902000
H	-0.77972600	-0.42350500	-3.84572400
C	-0.43815000	-2.47807500	-4.41922400
H	0.62194800	-2.49177100	-4.12236700
H	-0.83472500	-3.47536700	-4.17141700
C	-0.53154300	-2.26594400	-5.93610600
H	-1.58954600	-2.25353800	-6.23614300
H	-0.13267200	-1.27251600	-6.18714900
C	0.21300400	-3.33089200	-6.74734900
H	-0.18786200	-4.33402400	-6.55119100
H	0.13058100	-3.14635000	-7.82587500
H	1.28127200	-3.34771700	-6.49508300
H	-1.20863000	2.85268700	-1.44486700
C	-3.21521500	-0.74803900	-0.99029000
C	-3.99349400	-1.83501700	-1.52487200
C	-3.97329300	0.15828400	-0.16516400
C	-5.35485600	-1.98063000	-1.27004500
H	-3.51225900	-2.56193400	-2.17290400
C	-5.33335700	0.00859200	0.06609600
H	-3.44963500	0.97911700	0.31879400
C	-6.06025600	-1.06315100	-0.48052100
H	-5.88146000	-2.82529400	-1.71508600
H	-5.84042500	0.73673400	0.69955200
H	-7.12460600	-1.17820100	-0.29243600

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E= -2883.955789 H

C	-1.14250300	5.64425000	-0.74142300	H	2.95870100	0.48979900	5.71975700
C	-1.08450000	4.28007200	-1.44294600	H	4.13031400	-1.37216600	6.82327800
C	-2.31840500	3.40392000	-1.16283900	H	2.61238100	-1.97022000	7.52433600
C	-2.34893100	1.99882000	-1.78522600	H	2.68603200	-3.34088600	5.53014000
C	-1.43629800	1.02805700	-1.16927900	H	3.48147600	-2.05306700	4.59099200
N	-0.74568400	1.36865900	-0.10633900	C	0.04511200	6.56087000	-1.06422100
N	0.16956500	0.37694500	0.34002600	H	0.07615100	6.74729400	-2.14820800
C	2.13233000	2.11632100	1.39759500	H	0.98042800	6.03823100	-0.81780400
C	1.82383600	3.45428800	1.64884300	C	0.00200700	7.89991000	-0.32186100
C	2.76032200	4.45002100	1.35671400	H	0.00989300	7.75117200	0.76572900
C	4.01039800	4.13410100	0.80935000	H	0.86328100	8.53068000	-0.57607700
C	4.30139600	2.78135600	0.56389800	H	-0.90632700	8.46503800	-0.56894300
C	3.37388400	1.78080500	0.84483300	C	-1.19415500	-0.32370800	-1.82805000
C	5.01442800	5.21077000	0.47462600	H	-0.12522000	-0.43878100	-2.04941300
S	0.89035900	0.82574300	1.69430200	H	-1.45066500	-1.15951500	-1.16416600
O	0.02940400	1.38396500	2.77670200	H	-1.75585200	-0.43043900	-2.75672800
O	1.71642800	-0.36755600	2.11901900	Li	0.89635800	-1.84525100	3.01293700
H	-2.07733600	6.16056400	-1.01290000	O	-1.05230400	-2.21696500	3.14534100
H	-1.19019500	5.48771500	0.34672700	C	-1.58606900	-3.07023500	4.18091900
H	-0.18508200	3.74694100	-1.11518300	C	-2.13611600	-1.46292300	2.52501800
H	-0.98110300	4.43635200	-2.52619000	C	-2.89226300	-2.40546700	4.60115400
H	-3.20696600	3.96550600	-1.47671800	H	-1.76605600	-4.07465800	3.77100700
H	-2.40156500	3.31357600	-0.06487500	H	-0.83630500	-3.13888300	4.97275200
H	0.86740600	3.71024600	2.09187400	C	-3.41828000	-1.88491800	3.25425800
H	2.51652400	5.48851200	1.56983600	H	-1.90814400	-0.40156800	2.64763000
H	5.27141500	2.50947600	0.15236300	H	-2.15486000	-1.69554600	1.45650100
H	3.61742200	0.74027700	0.65427400	H	-2.68977900	-1.57315200	5.28559800
H	6.02808900	4.92351500	0.77812500	H	-3.57759500	-3.10146200	5.09457700
H	5.04583900	5.40133400	-0.60684900	H	-4.12016800	-1.05222300	3.35659200
H	4.76720300	6.15689000	0.96716900	H	-3.92522300	-2.69081200	2.71081000
O	1.67847200	-3.50822100	2.22932300	Li	-1.47221000	2.12560100	-4.00428800
O	1.44581100	-1.79178500	4.93554000	O	-2.09119200	3.62499300	-5.24984100
C	2.88464800	-3.38173000	1.43338600	O	0.53069600	2.31439100	-4.14600600
C	2.56742300	-4.06776200	0.10827800	O	-1.74166600	0.52521900	-5.24601600
C	1.64513600	-5.21016300	0.55944200	C	-2.28932000	5.03196500	-4.96058400
C	0.83161900	-4.55192200	1.67659100	C	-2.48081100	3.34652200	-6.61969000
C	1.07829600	-0.58688900	5.66253500	C	1.51362400	1.91725200	-3.15581600
C	2.34891100	-0.13705500	6.38090200	C	1.17274700	3.09257200	-5.18865800
C	3.05451200	-1.47396100	6.65217400	C	-0.67541100	-0.27419200	-5.78868800
C	2.74422200	-2.25887600	5.37768400	C	-2.96222900	-0.08319800	-5.71181700
H	3.10647800	-2.31653800	1.34165500	C	-3.10815700	5.58581300	-6.12578600
H	3.70941400	-3.88200500	1.95915600	H	-2.79167300	5.11946200	-3.99425500
H	3.46801300	-4.41493000	-0.40716300	H	-1.30745900	5.51775900	-4.89311700
H	2.03045600	-3.37905200	-0.55421600	C	-2.63330700	4.70910900	-7.29272900
H	1.00565500	-5.59336500	-0.24124400	H	-1.71308000	2.71436500	-7.07266400
H	2.23706500	-6.04452500	0.95352200	H	-3.43018600	2.79808300	-6.60846700
H	0.56418700	-5.24286700	2.48246400	C	2.66244600	2.90447100	-3.32401100
H	-0.08175600	-4.08317600	1.29543200	H	1.03272200	1.94008800	-2.17736100
H	0.69562300	0.14120500	4.94271400	H	1.84084400	0.89028900	-3.36939800
H	0.28278900	-0.84393900	6.37418700	C	2.66649900	3.11910600	-4.84506100
H	2.13111200	0.43165800	7.28986000	H	0.96441800	2.62659600	-6.15754000
				H	0.73417200	4.09583900	-5.18172200

C	-1.16122400	-1.72603100	-5.66950900	H	-1.55823600	5.13016700	-3.23289300
H	-0.51345500	0.00500100	-6.84076600	H	-3.33464800	4.36463400	-1.61747200
H	0.22646900	-0.04835800	-5.21915000	H	-2.44917300	5.11925100	-0.29650500
C	-2.70970900	-1.60099000	-5.67030800	H	-0.48528700	3.58583300	-0.75232100
H	-3.76933500	0.25419800	-5.06141300	H	-1.38935700	2.84223700	-2.06855600
H	-3.16082200	0.25655400	-6.73803200	H	-3.13567300	2.09075000	-0.45937000
H	-2.93251900	6.65411100	-6.28265200	H	-1.29641200	-0.91502500	-1.12350100
H	-4.17896500	5.43540200	-5.94588500	H	2.27578300	2.77819300	0.76737300
H	-3.33833400	4.67851600	-8.12874200	H	3.74618400	4.08042100	-0.74350300
H	-1.66646100	5.06331300	-7.66988700	H	5.59344100	0.43891000	-2.08271100
H	3.60745300	2.51104200	-2.93854800	H	4.10003900	-0.86339300	-0.58156600
H	2.43887300	3.84035800	-2.79909700	H	6.43944500	2.52391300	-2.90477700
H	3.13994800	4.05659400	-5.15160800	H	5.09296600	3.61437900	-3.26520600
H	3.19023600	2.29459800	-5.34289700	H	6.16946800	3.96899900	-1.91503700
H	-0.81038400	-2.16928000	-4.73300200	Li	-0.97119900	-1.40250900	1.01688600
H	-0.78555500	-2.34063700	-6.49296300	O	-0.91079500	-3.35113600	0.61520100
H	-3.13638600	-2.03844800	-4.76353800	O	-1.56080200	-1.32919500	2.90094300
H	-3.16903400	-2.09863800	-6.52953000	C	0.34241700	-3.95296400	0.21051100
C	-3.64931400	1.55853700	-2.29428900	C	0.09251700	-4.42521200	-1.21661700
C	-4.20154500	0.25669300	-2.07430200	C	-1.35776600	-4.93190200	-1.13022500
C	-4.50640900	2.43463600	-3.03587900	C	-2.00162000	-3.98198600	-0.10484400
C	-5.43987700	-0.13445600	-2.58066900	C	-1.37805300	-0.06889000	3.60639700
H	-3.66381800	-0.44530300	-1.44628700	C	-0.66712600	-0.43790500	4.90448300
C	-5.74915600	2.04511800	-3.52450800	C	-1.25554000	-1.82352300	5.20872600
H	-4.17048500	3.44705900	-3.24201200	C	-1.36663800	-2.43931900	3.81227000
C	-6.23754700	0.74661900	-3.31973900	H	1.11859300	-3.19227900	0.32124700
H	-5.80149000	-1.13913500	-2.36329700	H	0.56674700	-4.79946500	0.87672100
H	-6.34740500	2.76756800	-4.07885100	H	0.79851200	-5.19894700	-1.53409000
H	-7.20816800	0.44259300	-3.70299700	H	0.17090200	-3.57956300	-1.90966900

9-CN

E= -1807.780957 H

C	-1.69314800	5.62103600	-2.25740200	H	-0.80138200	0.59532800	2.96069600
C	-2.32368400	4.62813200	-1.27208100	H	-2.36727500	0.36851300	3.79520700
C	-1.49644300	3.34908300	-1.10106600	H	-0.84587100	0.29370100	5.69856700
C	-2.11160100	2.30791200	-0.13061800	H	0.41195900	-0.50274400	4.72664300
C	-1.31310100	0.99057200	-0.12349500	H	-0.63039800	-2.42690000	5.87429500
C	-1.94327600	-0.16519700	-0.66342500	H	-2.24747900	-1.72519800	5.66599000
N	-0.12691600	1.10471800	0.43915900	H	-2.21098800	-3.12799400	3.70410100
N	0.54517800	-0.16699500	0.46538300	H	-0.44739700	-2.96666800	3.53031900
C	3.08953400	0.87306400	0.17508000	C	-2.51900200	6.90018900	-2.44497500
C	2.99268200	2.26943800	0.13239600	H	-2.65670800	7.38780900	-1.46918800
C	3.82647700	2.99519900	-0.71659100	H	-3.52567600	6.63245000	-2.79729400
C	4.77395300	2.35431900	-1.53129600	C	-1.88521500	7.89293000	-3.42364400
C	4.86003800	0.95724400	-1.46825200	H	-1.76748500	7.44969900	-4.42096300
C	4.02434700	0.21833900	-0.62791500	H	-2.49909200	8.79558100	-3.53242800
C	5.66723800	3.15362300	-2.45037900	H	-0.89040900	8.20793300	-3.08309900
S	1.96373000	-0.08311700	1.22488600	H	-2.88411700	-0.01654300	-1.19377600
O	1.97021900	0.64698500	2.52425700	C	-2.23227000	2.86144800	1.22688000
O	2.51028600	-1.46936500	1.25136500	N	-2.36445800	3.30438300	2.29447200
H	-0.68490400	5.88799900	-1.90767100				

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E= -1807.818843 H

C	-2.17314900	1.62513100	-1.98202500
C	-1.52651300	0.45282500	-1.26310900
C	-2.08875600	-0.86058100	-1.47088300
N	-0.50479800	0.81567600	-0.52429500
N	0.13727000	-0.23094700	0.17214400
C	2.70644100	0.84750800	-0.03423000
C	2.61357000	2.09434300	-0.66573800
C	3.61125600	2.49539200	-1.55115300
C	4.71931800	1.67592100	-1.82206300
C	4.79572900	0.43542200	-1.17566500
C	3.79774700	0.01673100	-0.29266600
C	5.79202700	2.12775300	-2.78420600
S	1.37375800	0.29458300	1.05733600
O	1.12050700	1.45433200	1.95450400
O	1.87089200	-0.95919700	1.71655500
H	-2.13323200	1.51552600	-3.07471600
H	-3.23089900	1.74996000	-1.71377500
H	1.76970400	2.74330100	-0.46027200
H	3.53266800	3.46514100	-2.03863600
H	5.64876700	-0.21337900	-1.36283700
H	3.86728000	-0.94415600	0.20633200
H	6.60660800	1.39893500	-2.84753100
H	5.38843100	2.26573600	-3.79579400
H	6.22386600	3.08962500	-2.47994100
Li	0.10165800	-2.18063400	1.05429700
O	1.21421800	-3.88352600	1.30218200
O	-1.05463600	-2.17462000	2.73192900
C	2.29423900	-3.99838000	0.34570800
C	2.07948200	-5.33304100	-0.36606000
C	1.44752300	-6.18492800	0.74460400
C	0.55640800	-5.16410100	1.45592500
C	-2.23148700	-1.33421600	2.72453800
C	-1.95722700	-0.26208900	3.77336000
C	-1.20867200	-1.06665500	4.84770900
C	-0.37818400	-2.05079900	4.01118500
H	2.25644100	-3.13402000	-0.32235200
H	3.24896600	-3.97784100	0.88883800
H	3.01194600	-5.74975500	-0.75982600
H	1.37582300	-5.20730600	-1.19634900
H	0.87660800	-7.03825200	0.36575800
H	2.22159000	-6.56373700	1.42326100
H	0.43738500	-5.36206500	2.52633100
H	-0.43284600	-5.09823700	0.99125500
H	-2.35888100	-0.94716700	1.71123000
H	-3.11003400	-1.94145500	2.98770200
H	-2.87375300	0.20783000	4.14391900
H	-1.30809000	0.51259400	3.35063300
H	-0.57904900	-0.44493000	5.49151600
H	-1.92058900	-1.60474500	5.48514700

H	-0.30773000	-3.04407700	4.46889500
H	0.62969000	-1.67573500	3.81248500
C	-3.39086600	-1.07627700	-2.24326500
H	-3.48322300	-0.33153900	-3.04513300
H	-3.35531800	-2.05025300	-2.75396900
C	-4.67585800	-1.03870400	-1.38839700
H	-4.58988400	-1.78998800	-0.58967200
H	-4.74680000	-0.06429200	-0.88302600
C	-5.95874900	-1.29544300	-2.19020500
H	-6.05185400	-0.53930400	-2.98512800
H	-5.87668900	-2.26602500	-2.70330700
C	-7.23318300	-1.28630300	-1.33551700
H	-7.13555800	-2.03330200	-0.53455500
H	-7.32673000	-0.31222700	-0.83386100
C	-8.50598300	-1.56836700	-2.13911900
H	-8.46325400	-2.55527900	-2.61782400
H	-9.39817700	-1.54827700	-1.50081600
H	-8.65006200	-0.82371300	-2.93279600
H	-1.64323100	2.54325800	-1.71211500
C	-1.53532800	-2.01966600	-0.94628100
N	-1.14396700	-3.07285600	-0.55666300

11-CN

E= -1807.805832 H

C	-2.25211200	1.77306600	-1.00696100
C	-1.40454500	0.55799500	-0.68955900
C	-1.95996000	-0.79742200	-0.89385800
N	-0.21805700	0.82892100	-0.21883100
N	0.50463900	-0.30066900	0.22562500
C	3.06589000	0.59715400	-0.33510100
C	3.01584200	1.88490400	-0.88152100
C	3.88367900	2.23167300	-1.91482600
C	4.81826300	1.31337800	-2.42072900
C	4.85638400	0.03207700	-1.85522800
C	3.98671400	-0.33014000	-0.82431400
C	5.75229700	1.70390300	-3.54145300
S	1.89132300	0.11661900	0.95700800
O	1.81821400	1.30185600	1.85409200
O	2.42391700	-1.13927500	1.55202800
H	-2.51633000	1.81709600	-2.07301100
H	-3.20106400	1.74729500	-0.45406700
H	2.30892500	2.60953300	-0.49196700
H	3.83881000	3.23500900	-2.33388300
H	5.57758400	-0.69393200	-2.22456600
H	4.02665900	-1.32368700	-0.38949800
H	6.44188800	0.89036500	-3.78921900
H	5.19707500	1.96065500	-4.45300000
H	6.35252000	2.58383200	-3.27648500
Li	-0.87241800	-1.53619100	1.02993800
O	-0.64383000	-3.48015400	1.24001400
O	-1.51116400	-1.01466800	2.83795900

C	0.63456100	-4.14727200	1.16791600	N	-0.84420600	1.60891100	-0.21242900
C	0.40115700	-5.30375100	0.20370400	N	-0.02662400	0.59068600	0.34899200
C	-1.01723700	-5.75750200	0.59444100	C	1.92940800	2.39815200	1.24635200
C	-1.70270700	-4.44929200	1.03499400	C	1.58431100	3.75125800	1.31787200
C	-1.89673900	0.36232000	3.09303100	C	2.50351500	4.72274400	0.92180300
C	-1.00513400	0.83369900	4.23886600	C	3.77463400	4.36970200	0.44425300
C	-0.81220400	-0.46051200	5.04378000	C	4.09980300	3.00721000	0.37767900
C	-0.69911300	-1.50946100	3.93707600	C	3.18733900	2.02598600	0.76620900
H	1.36970400	-3.40732700	0.84645800	C	4.75549500	5.42986300	0.00373900
H	0.91237900	-4.51217800	2.16818100	S	0.70006900	1.13322400	1.66656900
H	1.14861600	-6.09619100	0.30859100	O	-0.15116300	1.77735300	2.70674000
H	0.42299400	-4.94011700	-0.82974700	O	1.52543700	-0.02672700	2.17495200
H	-1.55193300	-6.24217300	-0.22749700	H	-2.74039100	6.37500700	-1.41417600
H	-0.97208500	-6.46504400	1.42980300	H	-1.76719400	5.91747500	-0.02281400
H	-2.26582400	-4.56590200	1.96822700	H	-0.51847300	4.25357300	-1.42589400
H	-2.37522100	-4.04445200	0.27284400	H	-1.46498200	4.72386300	-2.83592400
H	-1.75804000	0.92881400	2.16925400	H	-3.55689500	3.97652400	-1.66294700
H	-2.95961300	0.37775500	3.36818700	H	-2.59453200	3.50381300	-0.26291000
H	-1.46597100	1.64088600	4.81674000	H	0.61043100	4.03669000	1.70066000
H	-0.04653300	1.18389700	3.84171700	H	2.23177400	5.77411100	0.99256500
H	0.07393700	-0.44458900	5.68568300	H	5.08270000	2.70978500	0.01844300
H	-1.68941200	-0.65815800	5.67184600	H	3.45545800	0.97583200	0.70895100
H	-1.07803100	-2.49428300	4.22605600	H	5.75276900	5.00909900	-0.16128600
H	0.33371100	-1.61330400	3.58377100	H	4.43497200	5.90162900	-0.93471400
C	-1.21983200	-1.77983200	-1.82031200	H	4.84423400	6.23027300	0.74827200
H	-0.17958000	-1.88596700	-1.49006300	O	1.28760200	-3.20958600	1.76598500
H	-1.68107300	-2.77505600	-1.73363500	O	1.68667000	-1.90838400	4.64638300
C	-1.21153800	-1.38150900	-3.31161100	C	2.49351700	-3.12142600	0.96428000
H	-2.24783700	-1.24593400	-3.65582100	C	2.07869000	-3.52749200	-0.44782600
H	-0.71882900	-0.40397100	-3.41768700	C	0.97305400	-4.55644300	-0.17000400
C	-0.50735000	-2.40255600	-4.21486000	C	0.26728800	-3.95013400	1.04355000
H	0.52308300	-2.55427400	-3.85839400	C	1.72907500	-0.75582800	5.52996200
H	-1.00966500	-3.37811900	-4.12062700	C	3.15837300	-0.69904900	6.06742000
C	-0.47272300	-1.99671400	-5.69436100	C	3.55497000	-2.18300200	6.08239100
H	-1.50051500	-1.82666900	-6.04683800	C	2.89055400	-2.69831100	4.80690900
H	0.04658100	-1.03245500	-5.79159300	H	2.86790000	-2.09727700	1.03359600
C	0.20599300	-3.03319300	-6.59467300	H	3.24147100	-3.81008100	1.37917800
H	-0.31256800	-3.99974100	-6.54826200	H	2.91480900	-3.93314400	-1.02546500
H	0.21366900	-2.71156400	-7.64369400	H	1.67133500	-2.66358000	-0.98460900
H	1.24760700	-3.20300700	-6.29254400	H	0.29055600	-4.69723700	-1.01327000
H	-1.72255500	2.69227300	-0.73521400	H	1.41027000	-5.52928100	0.08459700
C	-3.35720100	-0.92863800	-0.90398500	H	-0.15734800	-4.69773500	1.72049300
N	-4.52832100	-1.08957000	-0.87420000	H	-0.52300500	-3.25221100	0.74610400

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E= -2745.200252 H

C	-1.74317900	6.01210300	-1.11904000	H	1.43921800	0.12433600	4.95098800
C	-1.50043300	4.63033000	-1.74002700	H	1.00046400	-0.91204000	6.33593500
C	-2.57302500	3.59016500	-1.35819400	H	3.21067400	-0.22420700	7.05159500
C	-2.36237600	2.20186500	-1.94433700	H	3.80257800	-0.13826400	5.38019400
C	-1.46898900	1.25288500	-1.30428900	H	4.63702700	-2.34462300	6.07824200
				H	3.13452100	-2.68329700	6.96288300
				H	2.60319500	-3.75307000	4.85151300
				H	3.53464700	-2.54544300	3.93149000
				C	-0.69310400	7.06043500	-1.51003400

H	-0.66662900	7.15641500	-2.60541400
H	0.30269300	6.70272400	-1.21173100
C	-0.94716800	8.43685600	-0.88792500
H	-0.94630800	8.38507700	0.20862600
H	-0.17900300	9.16142300	-1.18579800
H	-1.92025500	8.83994100	-1.19749200
C	-1.29888800	-0.12823600	-1.90710000
H	-0.24188700	-0.32980600	-2.12036400
H	-1.62372900	-0.90484300	-1.20323400
H	-1.86861700	-0.24450700	-2.83320800
Li	0.78506800	-1.63366600	2.87590000
O	-1.12666300	-1.91988800	3.29785500
C	-1.53288100	-2.80405700	4.36240500
C	-2.24703200	-1.06727300	2.91809500
C	-2.65648500	-2.06027300	5.07531000
H	-1.89058800	-3.75355600	3.93755800
H	-0.65287600	-2.99854600	4.97965300
C	-3.38655500	-1.39852100	3.89483100
H	-1.90563800	-0.03237700	2.99469900
H	-2.50693400	-1.27410800	1.87515300
H	-2.23791700	-1.30163400	5.74721000
H	-3.29729400	-2.72658600	5.66099500
H	-3.94698700	-0.50482000	4.18430400
H	-4.09073900	-2.10607400	3.44233000
Li	-4.21710400	1.38117600	-5.97327500
O	-5.59551600	2.68052400	-6.54498000
O	-2.76224700	1.56434600	-7.31590700
O	-4.97976200	-0.43450400	-6.25945600
C	-5.44547900	4.07489000	-6.16803700
C	-7.00237300	2.34683400	-6.65985700
C	-1.35929100	1.37790600	-6.99018800
C	-2.89267800	2.19852100	-8.61155400
C	-4.59082700	-1.27661000	-7.37051100
C	-5.42967200	-1.25836400	-5.14871000
C	-6.84295300	4.54883800	-5.77156100
H	-4.71407400	4.13152100	-5.35709200
H	-5.06119800	4.62852700	-7.03424400
C	-7.74048500	3.68418500	-6.66933100
H	-7.14054700	1.76009800	-7.57273800
H	-7.29145100	1.73333700	-5.79732500
C	-0.58589000	2.19275100	-8.02554400
H	-1.20458600	1.70565200	-5.95944300
H	-1.12616800	0.30755400	-7.05978800
C	-1.50790700	2.11194600	-9.25174500
H	-3.67232200	1.67493000	-9.17322100
H	-3.20474600	3.24007100	-8.46498400
C	-4.36142500	-2.65865600	-6.76626400
H	-5.40350800	-1.29220400	-8.11008600
H	-3.70372600	-0.83186600	-7.82763300
C	-5.43400300	-2.69927100	-5.66733200
H	-4.72898200	-1.11960100	-4.31843800
H	-6.41770400	-0.90715900	-4.83457600

H	-6.97536500	5.62303600	-5.93029100
H	-7.03506600	4.32996900	-4.71480200
H	-8.76584700	3.59290000	-6.29924800
H	-7.77541500	4.09446000	-7.68558600
H	0.41429000	1.78810800	-8.20576300
H	-0.48186100	3.23218800	-7.69306000
H	-1.33763500	2.91226700	-9.97783200
H	-1.38177000	1.15022400	-9.76351600
H	-3.35849400	-2.71993900	-6.32742800
H	-4.46534800	-3.45884500	-7.50521300
H	-5.21541400	-3.42013100	-4.87422200
H	-6.40997500	-2.95091000	-6.09845700
C	-3.00990000	1.89519800	-3.11454300
N	-3.60101800	1.66318300	-4.12398400

9-NO₂

E= -1920.043185 H

C	-1.72546100	5.91789700	-1.20472000
C	-2.41821700	4.55915200	-1.37256600
C	-1.54804300	3.38768200	-0.89580200
C	-2.18358300	2.01419200	-1.12135300
C	-1.35665400	0.78435600	-0.72124000
C	-1.94261300	-0.50223900	-0.94456900
N	-0.20946300	1.06599200	-0.14560000
N	0.45045100	-0.13063500	0.26742200
C	3.04632100	0.75981600	-0.11680700
C	3.02119800	2.09188900	-0.54763300
C	3.93830900	2.52854700	-1.50166200
C	4.89995700	1.65843700	-2.04060500
C	4.91247900	0.33117600	-1.59204200
C	3.99332900	-0.12037600	-0.64241000
C	5.88816100	2.14727500	-3.07285900
S	1.81573000	0.16693400	1.07553000
O	1.75176300	1.24641300	2.09998800
O	2.31234400	-1.15676200	1.54749400
H	-1.45126700	6.05685900	-0.14857100
H	-0.78019300	5.91579000	-1.76766500
H	-2.68404000	4.41491600	-2.43020100
H	-3.36556400	4.57303200	-0.81480600
H	-1.29946000	3.49822900	0.16328700
H	-0.59790600	3.38481900	-1.44034300
H	-2.51513400	1.91152600	-2.15711000
H	-1.24146300	-1.29504000	-1.22254900
H	2.29768800	2.78197700	-0.12739600
H	3.91339200	3.56630600	-1.82909300
H	5.65414200	-0.35972800	-1.98763300
H	4.01417100	-1.14904800	-0.29694200
H	6.62807000	1.37721600	-3.31485100
H	5.38472300	2.43021000	-4.00676400
H	6.42876900	3.03529000	-2.72179900
Li	-1.02209700	-1.39059200	0.90449300

O	-0.78004700	-3.37029000	0.80980100	C	6.21393700	1.61098600	-1.17363500
O	-1.63885300	-1.10570700	2.76621300	S	0.41227800	0.87069200	0.68761300
C	0.52568100	-3.94613800	0.59142400	O	-0.21161400	2.21107100	0.55416400
C	0.42945900	-4.56873100	-0.79667900	O	0.49068700	0.29531300	2.05563300
C	-0.99960700	-5.14627700	-0.79161500	H	-0.75635000	-0.76036100	-4.51355300
C	-1.76966600	-4.20534800	0.16029000	H	-1.94433500	0.49961200	-4.18706600
C	-1.95598600	0.25046600	3.18376200	H	1.60226900	2.36196600	-1.52918600
C	-1.07828700	0.51976500	4.40450600	H	3.94013500	2.62969900	-2.29082000
C	-0.96445100	-0.87684300	5.03319900	H	5.28939400	0.20367500	0.98961600
C	-0.86579500	-1.77216800	3.79811500	H	2.93744600	-0.08598300	1.73548300
H	1.25405900	-3.13919500	0.69435500	H	6.91427400	1.05761500	-0.53961300
H	0.72008300	-4.71109100	1.35906300	H	6.34820600	1.26313900	-2.20577100
H	1.19625800	-5.32965700	-0.97267200	H	6.50764600	2.66846400	-1.15400100
H	0.53358900	-3.78975300	-1.56036000	Li	-0.06884900	-2.22161200	0.39573700
H	-1.44705500	-5.17442900	-1.78933000	O	1.70758100	-3.20881700	0.55008000
H	-0.99602600	-6.16820600	-0.39723100	O	-1.01049500	-2.76381100	2.08719600
H	-2.32853400	-4.75869700	0.92505400	C	2.63321000	-2.92016500	-0.53022700
H	-2.46185800	-3.53699800	-0.36002900	C	2.83670800	-4.23948300	-1.27554800
H	-1.75994300	0.92071100	2.34495500	C	2.64825900	-5.27293000	-0.15477700
H	-3.02481700	0.29065600	3.43110800	C	1.52375100	-4.64313100	0.66559800
H	-1.51928600	1.26339000	5.07589700	C	-2.35715800	-2.23635500	2.20080400
H	-0.09492300	0.87623700	4.08017900	C	-2.41646900	-1.54229300	3.56030400
H	-0.09732200	-0.98724400	5.69166900	C	-1.43957800	-2.38557100	4.39262200
H	-1.86718100	-1.11517100	5.60936400	C	-0.34335900	-2.69207000	3.37119000
H	-1.28365000	-2.77258000	3.94606400	H	2.20195700	-2.12808800	-1.14740000
H	0.17001200	-1.86556200	3.45003500	H	3.57127600	-2.55601300	-0.09265300
C	-2.58498900	7.10288800	-1.66348900	H	3.81710400	-4.29513600	-1.75873200
H	-3.52735900	7.10786600	-1.09694200	H	2.06451400	-4.36551900	-2.04223000
H	-2.86350900	6.96220800	-2.71795000	H	2.38250600	-6.26879200	-0.52248400
C	-1.88663000	8.45563100	-1.49866500	H	3.56222400	-5.35990900	0.44570200
H	-0.95741400	8.49845000	-2.08132100	H	1.55548700	-4.90654200	1.72728400
H	-2.52656000	9.28100400	-1.83445300	H	0.53829000	-4.90034600	0.26087700
H	-1.62661700	8.64396000	-0.44904900	H	-2.53026800	-1.56069900	1.36014400
H	-2.85001200	-0.51730200	-1.55005600	H	-3.06411800	-3.07301400	2.13617100
N	-3.50257900	1.95316900	-0.34844600	H	-3.43107200	-1.51677000	3.97002100
O	-4.52244000	1.64934500	-0.97013800	H	-2.04653800	-0.51549800	3.47120500
O	-3.48762600	2.22249300	0.85347100	H	-1.05074100	-1.86014000	5.27042500

10- NO₂

E= -1920.099157 H

C	-1.00970900	0.05493200	-3.82105700	C	-3.60990800	-1.22328600	-2.55592200
C	-1.12515200	-0.44932400	-2.39301600	H	-3.63670100	-0.43833900	-3.32141000
C	-2.18166600	-1.44510200	-2.11726700	H	-3.99136400	-2.14432600	-3.01888800
N	-0.29653700	0.10351400	-1.56095600	C	-4.57259100	-0.82826500	-1.41633900
N	-0.30609000	-0.28530300	-0.22943600	H	-4.53032300	-1.61280100	-0.65200400
C	2.12345900	1.10271800	0.14170200	H	-4.21796200	0.10042300	-0.94703800
C	2.40730300	1.87614100	-0.99020400	C	-6.01996800	-0.64298000	-1.88909600
C	3.72736500	2.02823500	-1.40923900	H	-6.05772700	0.14624900	-2.65616700
C	4.78801900	1.42724700	-0.71209300	H	-6.36088800	-1.56500500	-2.38464200
C	4.48353700	0.66750400	0.42482100	C	-6.99598100	-0.29271000	-0.75823000
C	3.16330300	0.49858500	0.84967000	H	-6.96385500	-1.08499900	0.00346100
				H	-6.65675300	0.62559000	-0.25774400

C	-8.43843200	-0.10658600	-1.23769900
H	-8.81960900	-1.01853900	-1.71561500
H	-9.11086000	0.13748800	-0.40576700
H	-8.51171600	0.70566600	-1.97251800
H	-0.22709300	0.81746400	-3.88124900
N	-1.91569300	-2.60886200	-1.51690600
O	-0.67544200	-2.94222400	-1.23021800
O	-2.84318500	-3.45204600	-1.25948700

11- NO₂

E= -1920.083686H

C	-1.91491100	1.41178400	-1.44270100
C	-1.11288800	0.31976800	-0.77130900
C	-1.35094000	-1.09924700	-1.13768100
N	-0.18227100	0.70323800	0.04803400
N	0.50541900	-0.33109100	0.68701000
C	2.98879400	0.89560400	0.83591000
C	2.91251600	2.18070800	0.28777600
C	3.97107200	2.66755600	-0.47649700
C	5.11967000	1.89351600	-0.70728000
C	5.17846900	0.61314900	-0.14058300
C	4.12261600	0.11063900	0.62217100
C	6.24969500	2.42431200	-1.55658500
S	1.58866100	0.23294200	1.76919700
O	1.10999100	1.36413400	2.60411700
O	2.08727400	-0.97293300	2.48043100
H	-1.68213100	1.47170600	-2.51626600
H	-2.98366300	1.19488400	-1.35091100
H	2.03598000	2.79417700	0.46636300
H	3.90728800	3.66853500	-0.89806900
H	6.06366800	0.00008200	-0.29542200
H	4.17926400	-0.87964800	1.06217600
H	7.16226600	1.83377400	-1.42417800
H	5.99082600	2.39642600	-2.62378700
H	6.48101700	3.46760200	-1.31155000
Li	-0.64205700	-1.90354700	1.11837400
O	-0.22838500	-3.80298200	1.07413400
O	-1.84568000	-1.75294600	2.67116400
C	1.02553200	-4.44044200	0.73418300
C	0.64869000	-5.65278200	-0.11455600
C	-0.69864200	-6.06555300	0.49793400
C	-1.33896400	-4.71648600	0.83318100
C	-2.89029900	-0.74881000	2.69017400
C	-2.36307600	0.31916300	3.63855200
C	-1.70265800	-0.53478100	4.73662100
C	-1.18335600	-1.76449500	3.96662500
H	1.64883000	-3.70833400	0.21450700
H	1.53158100	-4.74000700	1.66154400
H	1.40619900	-6.44132900	-0.06772800
H	0.51969800	-5.35928300	-1.16274300
H	-1.31934900	-6.65480800	-0.18367400

H	-0.53799000	-6.65387900	1.40929800
H	-1.95844900	-4.74365300	1.73463900
H	-1.92889100	-4.31230200	0.00248100
H	-3.05384500	-0.43780600	1.65592900
H	-3.81563300	-1.20387100	3.07501600
H	-3.15522500	0.97074200	4.02114100
H	-1.61238600	0.93265700	3.12940900
H	-0.89459400	-0.00928300	5.25388000
H	-2.44466100	-0.83615900	5.48488900
H	-1.41804400	-2.70708400	4.47514100
H	-0.10603400	-1.71878600	3.78216200
C	-0.31611300	-1.86210300	-1.93466100
H	0.67607700	-1.49242900	-1.64826900
H	-0.35468600	-2.92538100	-1.66617900
C	-0.47827500	-1.74483200	-3.46582300
H	-1.48795700	-2.08289200	-3.73050100
H	-0.40637100	-0.68726900	-3.75869700
C	0.56206800	-2.55660500	-4.24802700
H	1.57308600	-2.23599100	-3.95239400
H	0.48424500	-3.61740500	-3.96312400
C	0.42219600	-2.43489600	-5.77121400
H	-0.58629600	-2.75642500	-6.06883400
H	0.50102700	-1.37618700	-6.05789900
C	1.46423300	-3.24832500	-6.54473400
H	1.38805000	-4.31829600	-6.31119800
H	1.33847600	-3.13633700	-7.62890800
H	2.48432200	-2.92894700	-6.29446500
H	-1.69967300	2.38509000	-0.98856300
N	-2.61002100	-1.60137300	-1.08607400
O	-2.86784500	-2.74893400	-1.60238300
O	-3.55310800	-0.95836600	-0.49102300

12- NO₂

E= -2857.491284 H

C	-2.03575900	5.82320300	-1.14557100
C	-1.79255000	4.40152400	-1.66540000
C	-2.73895100	3.35559800	-1.04347600
C	-2.54037600	1.96102100	-1.58834000
C	-1.76809500	0.96489300	-0.83546400
N	-0.97026600	1.45086700	0.07407400
N	-0.24902100	0.52636700	0.81463200
C	1.80194800	2.40117500	1.22591900
C	1.54326200	3.77075900	1.13411900
C	2.46400700	4.60586100	0.50130400
C	3.64779200	4.09568200	-0.05177000
C	3.88761200	2.71768900	0.05437600
C	2.97366900	1.87099600	0.68086000
C	4.62382600	5.00477500	-0.75869300
S	0.57595000	1.30791000	1.98112000
O	-0.22036800	2.16915900	2.88913200
O	1.38409800	0.23758800	2.66601200
H	-3.07699300	6.11447600	-1.35313200

H	-1.92845900	5.83545500	-0.05016500	Li	0.93757600	-1.54339600	3.17679300
H	-0.75554300	4.10641700	-1.45681200	O	-0.88272900	-2.02891800	3.75781600
H	-1.92055800	4.38263600	-2.75534300	C	-1.15604100	-3.28537600	4.42742700
H	-3.77508200	3.66595600	-1.22302300	C	-2.05702700	-1.17546100	3.80072700
H	-2.57629300	3.32480700	0.03777900	C	-2.50246800	-3.09910300	5.12721300
H	0.63722500	4.17660000	1.57060400	H	-1.20232600	-4.07917100	3.67108600
H	2.26089200	5.67289600	0.44161400	H	-0.32779000	-3.49727400	5.10941300
H	4.80333800	2.30107300	-0.35907100	C	-3.20743200	-2.09448400	4.20358100
H	3.17646800	0.80713300	0.75229600	H	-1.89177400	-0.38655900	4.54508400
H	5.60403500	4.53045100	-0.87265200	H	-2.17275100	-0.71243700	2.81848000
H	4.26437700	5.26382900	-1.76378400	H	-2.36065700	-2.66596300	6.12434100
H	4.76085600	5.94691300	-0.21546600	H	-3.04327000	-4.04377900	5.23757800
O	1.57653700	-2.90844900	1.87463600	H	-4.01947100	-1.54925400	4.69356900
O	2.01449200	-1.90346400	4.81910600	H	-3.61549000	-2.60404000	3.32259600
C	2.69907700	-2.54507100	1.03474100	Li	-3.89315700	1.50824600	-5.07830200
C	2.16985700	-2.63264700	-0.39164700	O	-5.08437300	2.93069100	-6.15356600
C	1.23173000	-3.84603700	-0.30012700	O	-2.38119900	1.41222600	-6.47431400
C	0.63123100	-3.70247100	1.10394300	O	-5.15506600	-0.06529600	-5.53632100
C	1.87670000	-0.96638400	5.91955900	C	-4.84236100	4.32459900	-5.84515300
C	3.29141400	-0.73856100	6.45179600	C	-6.50526700	2.70367200	-6.30504400
C	3.96982700	-2.08287700	6.14764200	C	-1.16445900	0.68676200	-6.16152400
C	3.35797600	-2.44469700	4.79578200	C	-2.12082200	2.38679300	-7.51235300
H	3.02107500	-1.54348900	1.32957700	C	-4.84937400	-0.92091600	-6.65602500
H	3.52165000	-3.25325200	1.20674200	C	-5.65595900	-0.86593400	-4.43332200
H	2.96895300	-2.75801400	-1.12859300	C	-6.20344100	4.91334400	-5.47573700
H	1.60475400	-1.72610300	-0.63376900	H	-4.11038900	4.36397600	-5.03579100
H	0.45982600	-3.85204800	-1.07502700	H	-4.42673000	4.81621200	-6.73618900
H	1.80429200	-4.77746200	-0.38029800	C	-7.15089300	4.08924500	-6.35958600
H	0.49182700	-4.66384300	1.60936800	H	-6.66689200	2.10982000	-7.21032100
H	-0.32250000	-3.16621700	1.09099000	H	-6.86410400	2.12682400	-5.44435000
H	1.40079000	-0.05903400	5.53788300	C	-0.03180900	1.50317000	-6.77869000
H	1.22606200	-1.41887300	6.67859500	H	-1.12117800	0.58356000	-5.07580000
H	3.29608800	-0.47939900	7.51460100	H	-1.22448200	-0.31323500	-6.61457700
H	3.78215800	0.07026600	5.89801000	C	-0.71107300	2.08659800	-8.02685900
H	5.06116100	-2.01925100	6.10406100	H	-2.89534100	2.29619000	-8.27981200
H	3.69735500	-2.82960400	6.90292500	H	-2.18024700	3.39026300	-7.07371200
H	3.28898500	-3.52130500	4.61577800	C	-4.61892800	-2.30262200	-6.05107700
H	3.91306200	-1.98316300	3.96887800	H	-5.69892900	-0.92908500	-7.35522900
C	-1.08991800	6.86614500	-1.75554300	H	-3.97828600	-0.49886000	-7.16273700
H	-1.19486900	6.85329100	-2.85023300	C	-5.66064000	-2.32179500	-4.92150500
H	-0.05006500	6.57616300	-1.54621800	H	-4.97782200	-0.70765800	-3.58963500
C	-1.33544800	8.28660600	-1.23863600	H	-6.65535900	-0.50624800	-4.16262300
H	-1.20395300	8.34258900	-0.15031900	H	-6.25660700	5.99016500	-5.66367300
H	-0.64210600	9.00535600	-1.69299400	H	-6.42010800	4.73674300	-4.41560100
H	-2.35581300	8.62229900	-1.46490200	H	-8.18461800	4.07854100	-6.00042800
N	-3.04592000	1.70860800	-2.79225700	H	-7.14859000	4.47589600	-7.38601700
O	-2.85149300	0.59901500	-3.45662800	H	0.84587400	0.89066800	-7.00707100
O	-3.78041500	2.60202400	-3.41869600	H	0.27721400	2.30615800	-6.09859700
C	-1.95645800	-0.52339200	-1.01993200	H	-0.21488600	2.98035300	-8.41728400
H	-1.09467200	-0.98043300	-1.52493800	H	-0.74540300	1.33678800	-8.82643700
H	-2.03357200	-0.99941900	-0.03509100	H	-3.60430000	-2.37023500	-5.64134100
H	-2.84128500	-0.74377700	-1.61389500	H	-4.75345900	-3.10830300	-6.77953300

H	-5.41485200	-3.02375400	-4.11910900
H	-6.64526200	-2.59348700	-5.31978000