

Theoretical Study on the Mechanism of Hydrogen Donation and Transfer for Hydrogen-Donor Solvents during Direct Coal Liquefaction

Haigang Hao ^{1,†}, Tong Chang ^{2,†}, Linxia Cui ¹, Ruiqing Sun ¹ and Rui Gao ^{1,*}

¹ College of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot 010021, China; haohaigang@imu.edu.cn (H.H.); imucuilinxia@163.com (L.C.); imusunruiqin@163.com (R.S.)

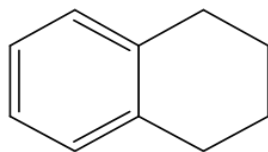
² Department of Applied chemistry, Yuncheng University, Yuncheng 044000, China; changtongct@163.com

* Correspondence: gaorui@imu.edu.cn; Tel.: +86-0471-4995400

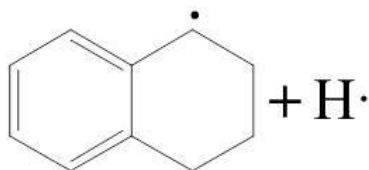
† These authors contributed equally to this work.

Appendix S1. The Cartesian coordinates of intervening species (reactants, transition states and products) in the energy profiles.....1.

Appendix S1. The Cartesian coordinates of intervening species (reactants, transition states and products) in the energy profiles.

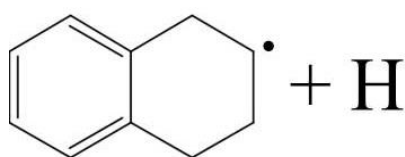


C	-2.58004500	-0.69913500	-0.02180100
C	-1.36682500	-1.38570900	-0.04459600
C	-0.13769800	-0.70455000	-0.02407300
C	-0.13768400	0.70455200	0.02394300
C	-1.36680400	1.38572300	0.04461000
C	-2.58003600	0.69916400	0.02196500
H	1.31057600	-1.85294100	-1.11069000
H	-3.51402400	-1.24564400	-0.03710400
H	-1.36437100	-2.46911000	-0.07828100
C	1.15982600	-1.49875500	-0.08329300
C	1.15988600	1.49876400	0.08297500
H	-1.36433400	2.46912400	0.07829100
H	-3.51400900	1.24568200	0.03736600
C	2.39343600	0.68680900	-0.34445000
C	2.39333400	-0.68687000	0.34474700
H	1.06625200	2.39646800	-0.53420000
H	2.38647400	0.54557400	-1.43078000
H	2.38598900	-0.54577700	1.43108300
H	1.31039000	1.85344600	1.11023900
H	3.30337500	1.24157700	-0.10329300
H	3.30327100	-1.24164100	0.10372000
H	1.06608100	-2.39670500	0.53349000

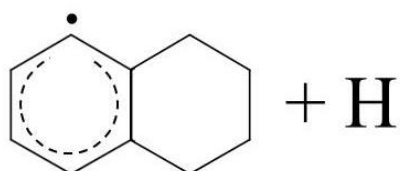


C	2.51969900	0.80042600	-0.04608800
C	1.27742000	1.38944600	-0.22753800
C	0.07828900	0.61378500	-0.20707200
C	0.19394900	-0.80437300	0.00096600
C	1.45404800	-1.36748300	0.18891300
C	2.61775200	-0.58459400	0.16695800
H	-1.23908000	2.27905300	-0.58505300
H	3.41447900	1.40899400	-0.06510100
H	1.20006300	2.45838800	-0.38588600

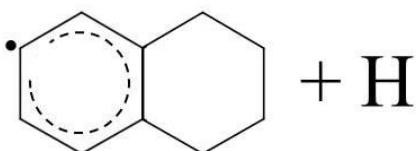
C	-1.18946200	1.21515100	-0.38218200
C	-1.06277000	-1.65269500	-0.01706100
H	1.53334900	-2.43586200	0.35289800
H	3.58471300	-1.04640700	0.31533900
C	-2.29053300	-0.87460900	0.49171000
C	-2.47029400	0.43632200	-0.30025700
H	-1.26020700	-1.98809200	-1.04387600
H	-3.18827600	-1.49108300	0.41134600
H	-3.25614600	1.04895300	0.15204600
H	-0.91012700	-2.55704900	0.57662300
H	-2.15381400	-0.63922600	1.55138200
H	-2.83256400	0.19661100	-1.31238000
H	-1.66098300	7.73746300	2.02256100



C	2.45689100	-0.85441800	-0.19557900
C	1.24037200	-1.44292800	0.15814800
C	0.06206500	-0.68576000	0.21816500
C	0.10907000	0.68845500	-0.09368300
C	1.33211300	1.26865100	-0.45656900
C	2.50282800	0.50804200	-0.50431800
H	-1.49660800	-1.07965500	1.64639900
H	3.35711800	-1.45356700	-0.23673600
H	1.20071800	-2.50083000	0.38888300
C	-1.26655600	-1.30654600	0.59857200
C	-1.16094600	1.52071600	-0.02106300
H	1.36540100	2.32287500	-0.70506600
H	3.43887400	0.97219600	-0.78622500
C	-2.41124900	0.73873200	-0.31273200
C	-2.41186500	-0.75876200	-0.28510100
H	-1.22888100	1.97141400	0.98555700
H	1.91810900	2.75887800	6.04633500
H	-2.28885500	-1.16972400	-1.30083400
H	-1.07753600	2.37755000	-0.69921500
H	-3.31814100	1.27618900	-0.56268900
H	-3.37508100	-1.13849300	0.07048800
H	-1.21147100	-2.39392400	0.51806500



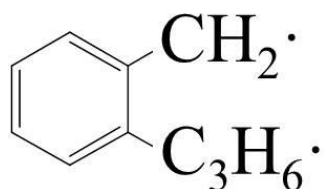
C	-2.60193200	-0.77224200	0.06483900
C	-1.38604200	-1.44695400	0.18590000
C	-0.15000000	-0.78287200	0.07952700
C	-0.13570200	0.61601200	-0.15486000
C	-1.37677300	1.22284500	-0.26329100
C	-2.60909000	0.61604600	-0.16992300
H	1.30807400	-2.11638200	-0.74909200
H	-3.53732900	-1.30996800	0.15248700
H	-1.38805400	-2.51491900	0.36791200
C	1.14812600	-1.56981000	0.18841200
C	1.15835900	1.41056200	-0.25292500
H	-3.53676700	1.16340400	-0.26850000
C	2.39024600	0.52172200	-0.49069400
C	2.37590800	-0.68450900	0.46131200
H	2.39553300	0.16434300	-1.52600700
H	2.35265400	-0.32794300	1.49669500
H	1.06598800	2.15748600	-1.04451500
H	3.29998000	1.11075600	-0.35397400
H	3.28786500	-1.27537100	0.34977500
H	1.04785600	-2.32938100	0.96834300
H	1.29640000	1.97183200	0.67867200
H	-0.47080100	8.52134800	2.03843000



C	2.44375700	-0.98875900	-0.07247600
C	1.15703100	-1.53836600	0.02634300
C	0.00667000	-0.72911200	0.02939700
C	0.13796100	0.67260900	-0.07117100
C	1.43157900	1.23643000	-0.17031000
C	2.51456900	0.38765600	-0.16677000
H	-1.50542500	-1.68063700	1.21718000
H	3.32123200	-1.62077100	-0.07511100
H	1.04582200	-2.61415900	0.10125300
C	-1.36100300	-1.38560900	0.17063000
C	-1.07508000	1.59112500	-0.10691900
H	8.44027200	2.26637100	1.05411700
C	-2.36535600	0.91761300	0.38957600

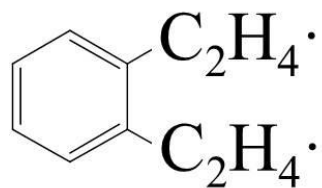
C	-2.52328400	-0.47079700	-0.24858800
H	-2.33333200	0.81281100	1.47931700
H	-2.54019400	-0.36788500	-1.33894200
H	-0.86815600	2.49054800	0.47891300
H	-3.22410500	1.55154000	0.15684300
H	-3.47351300	-0.92440100	0.04237100
H	-1.38221200	-2.31178400	-0.40960900
H	-1.22727600	1.93069200	-1.13875400
H	1.54582900	2.31094000	-0.24584200

The final state of cracking $C_1=C_2$:



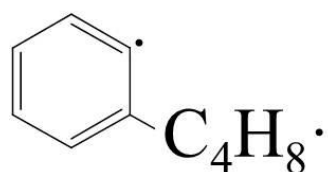
C	2.12997500	-1.48051600	-0.09108100
C	0.76729400	-1.45530800	0.23529100
C	0.05216100	-0.26159100	0.34236200
C	0.73950000	0.98676800	0.11379700
C	2.13230600	0.92970200	-0.21514100
C	2.81045200	-0.27380700	-0.31701100
H	-1.69512100	0.49855100	1.35720700
H	2.65227200	-2.42489400	-0.16435900
H	0.24913800	-2.38983600	0.41429300
C	-1.42669000	-0.30260300	0.66477200
C	0.09988100	2.23894500	0.20605500
H	2.65655900	1.86203000	-0.38480300
H	3.86295100	-0.28265900	-0.56794200
C	-3.79302000	-0.26500500	-0.27165700
C	-2.33587500	-0.20467600	-0.59162900
H	0.65569200	3.14975400	0.02845300
H	-4.15295500	-0.86331600	0.55708500
H	-2.10509000	0.71149900	-1.14362200
H	-0.94356100	2.34288300	0.46105300
H	-4.52869300	0.19198400	-0.92080900
H	-2.05472000	-1.02674500	-1.27030400
H	-1.65237200	-1.24071100	1.17920200

The final state of cracking $C_2=C_3$:



C	2.45412900	-0.66240700	0.21874200
C	1.23820700	-1.31610500	0.43461000
C	0.01071400	-0.67134800	0.22201300
C	0.01068600	0.67136100	-0.22195900
C	1.23815400	1.31615300	-0.43459900
C	2.45410200	0.66249900	-0.21874900
H	-1.98623500	-0.82264900	1.02665000
H	3.38711700	-1.18262300	0.39142000
H	1.23732300	-2.34435000	0.77582700
C	-1.28729100	-1.43542500	0.45025800
C	-1.28735100	1.43536800	-0.45025300
H	1.23722900	2.34439300	-0.77582900
H	3.38707000	1.18274200	-0.39145400
C	-1.94937400	1.90575400	0.81148800
C	-1.94922900	-1.90582900	-0.81152400
H	-1.06100600	2.29934100	-1.09481400
H	-1.35445900	2.22273900	1.65846000
H	-1.35425200	-2.22280600	-1.65845600
H	-1.98623900	0.82255500	-1.02667900
H	-3.02113000	2.05303700	0.85297600
H	-3.02098000	-2.05312100	-0.85308700
H	-1.06092800	-2.29938900	1.09482500

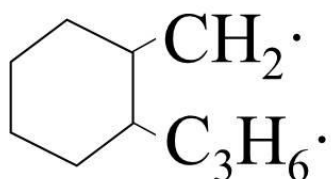
The final state of cracking $C_1=C_9$:



C	2.23906300	0.51597800	1.00672700
C	0.97722500	-0.02924300	1.27191200
C	0.23056800	-0.67372600	0.26212600
C	0.84984600	-0.72183800	-0.97940300

C	2.08488000	-0.20362700	-1.30355400
C	2.79898400	0.43615300	-0.27214000
H	-1.37535600	-1.16516000	1.58781500
H	2.78540500	1.00605700	1.80175000
H	0.55623100	0.04180400	2.26776800
C	-1.12485000	-1.29728800	0.53130200
C	-1.77809500	1.75676300	-0.37665700
H	2.49927400	-0.28115100	-2.30002300
H	3.77426700	0.85967500	-0.47380600
C	-2.73930000	0.68001500	0.00712100
C	-2.28562700	-0.75915900	-0.33653000
H	-1.61296700	2.62035400	0.25375000
H	-2.96794400	0.73921300	1.07678100
H	-2.00231400	-0.81123100	-1.39264700
H	-1.27788900	1.72883100	-1.33628100
H	-3.70349300	0.84264900	-0.50458000
H	-3.14153000	-1.42871200	-0.20924200
H	-1.04985000	-2.37650700	0.36329700

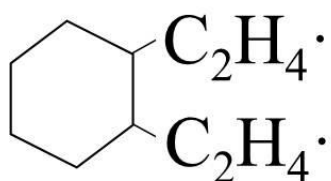
The final state of cracking $C_7=C_8$:



C	2.66933300	-0.66881000	-0.31210100
C	1.36776400	-1.23264500	0.07329700
C	0.20317800	-0.60561500	0.34251300
C	-0.00965400	0.87524900	0.32979600
C	0.61792300	1.71271600	1.13312200
C	3.00405400	0.58556400	-0.56898000
H	-1.40782100	-1.18126700	1.64032600
H	3.45296100	-1.42733200	-0.41956100
H	1.35497900	-2.31774700	0.11611500
C	-1.07272900	-1.38464400	0.61582400
C	-1.12757500	1.32477700	-0.62474700
H	0.61384000	2.77340600	1.33918400
H	3.91057300	1.10438300	-0.84498000
C	-2.43278800	0.54845100	-0.34077900
C	-2.20078100	-0.97277800	-0.36058100
H	-1.29100600	2.39960700	-0.53510600

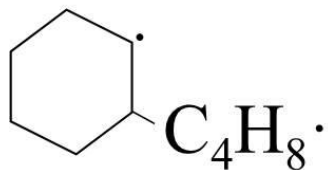
H	-2.81879600	0.84687500	0.63935400
H	-1.92856400	-1.28777200	-1.37324400
H	-0.80352800	1.12679200	-1.65258200
H	-3.19001300	0.82539200	-1.07911700
H	-3.12264000	-1.49863200	-0.09958800
H	-0.88232900	-2.45729000	0.54501800

The final state of cracking $C_6=C_7$:

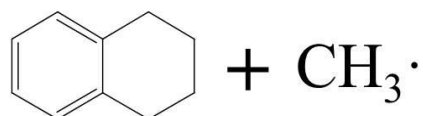


C	-2.49773000	-1.71112200	0.29588900
C	-1.27691000	-1.77754000	-0.20424100
C	-0.15852800	-0.81383200	-0.09240200
C	-0.29629400	0.54078600	-0.04135600
C	-1.60530600	1.20547500	-0.12010000
C	-1.83904600	2.48957400	0.10757100
H	1.42501400	-1.86595200	-1.08570400
H	-3.38297200	-2.32926200	0.31072900
H	-1.00870000	-2.69403800	-0.74468300
C	1.20870500	-1.49055700	-0.07591700
C	0.91002400	1.46279200	0.08592000
H	-2.44755400	0.57191000	-0.40292200
H	-2.68694800	3.15745300	0.08927000
C	2.24346700	0.79662800	-0.27968600
C	2.35229300	-0.57865400	0.39015400
H	0.74446400	2.34401700	-0.53873100
H	2.30858400	0.67666300	-1.36641800
H	2.30204300	-0.45517800	1.47700800
H	0.95579800	1.83720700	1.11639200
H	3.07405000	1.44080900	0.01856500
H	3.31382500	-1.04778500	0.16832600
H	1.15834300	-2.37714300	0.56317000

The final state of cracking C₈=C₉:

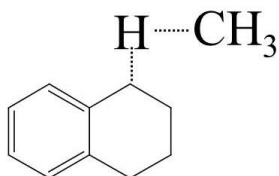


C	2.51021100	-0.86386000	-0.20202800
C	1.24122300	-1.29682100	-0.38307100
C	-0.03191400	-0.57979900	-0.23331500
C	-0.29693100	0.64948300	-0.66702700
C	2.38350400	1.57117700	0.48533100
C	3.01927700	0.43093300	0.26284000
H	-0.97496500	-1.40400600	1.52858900
H	3.29085500	-1.59975500	-0.36635600
H	1.12919200	-2.35006700	-0.63180800
C	-1.17695300	-1.35879000	0.45234400
C	-1.52916200	1.46920400	-0.59660300
H	2.66149000	2.55824900	0.82606700
H	4.09495900	0.41616900	0.47398200
C	-2.53260600	0.80178300	0.39331500
C	-2.55731700	-0.72496200	0.19513700
H	-1.30544800	2.48893100	-0.26982600
H	-2.22490100	1.03096100	1.41750500
H	-2.87077500	-0.94692200	-0.83032700
H	-1.98515000	1.55698700	-1.58908600
H	-3.52708500	1.22990300	0.24842300
H	-3.29921000	-1.17762800	0.85777200
H	-1.16495100	-2.39291000	0.09352400



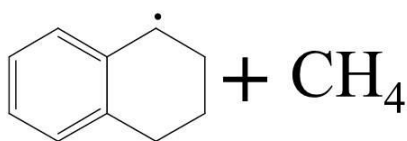
C	-0.59125200	2.74833800	-0.23631000
C	-1.42262000	1.68973300	-0.59958900
C	-1.11477700	0.36276700	-0.25411900
C	0.06100100	0.10181700	0.47894900
C	0.89175800	1.17710000	0.83877300
C	0.57668300	2.48962500	0.48879700
H	-1.87482400	-0.95031800	-1.76954000
H	-0.84993200	3.76207700	-0.51303300
H	-2.32864400	1.88778800	-1.16062900
C	-2.03871300	-0.76171900	-0.70114800

C	0.43283400	-1.30939800	0.91252600
H	1.79542800	0.97484600	1.40197500
H	1.23244100	3.30091000	0.77688400
C	-0.32124100	-2.40490300	0.14093200
C	-1.82012600	-2.07352500	0.07020000
H	1.51222300	-1.44964400	0.80832900
H	0.07865800	-2.48401800	-0.87587300
H	-2.21698800	-1.97664900	1.08661000
H	0.21538500	-1.41872600	1.98232200
H	-0.16001400	-3.37301800	0.62102600
H	-2.37405300	-2.88296100	-0.41117400
H	-3.07880400	-0.43734400	-0.60894900
C	4.45777700	-0.78634500	-0.90692900
H	4.44334000	-1.67703800	-1.51725200
H	3.68308400	-0.04253300	-1.01891900
H	5.25475200	-0.63430600	-0.19427000

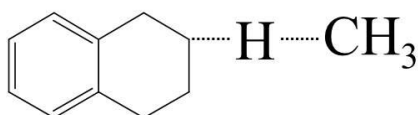


C	2.89750500	0.10641700	0.23085800
C	2.02131500	-0.94047400	0.51979600
C	0.64898700	-0.84278000	0.24518000
C	0.14520200	0.34095800	-0.34325700
C	1.04513500	1.38300300	-0.64576000
C	2.40425300	1.27508100	-0.36100000
H	-0.64142600	-1.95178400	1.56871600
H	3.95220300	0.00913700	0.45246100
H	2.40407200	-1.85500900	0.95764500
C	-0.27930900	-2.00930300	0.53435800
C	-1.31043000	0.51640400	-0.63753100
H	0.66364200	2.28608100	-1.10756800
H	3.07485900	2.09017100	-0.60005600
C	-2.23050800	-0.67226000	-0.32622000
C	-1.49105800	-2.01980700	-0.41149600
H	-1.72321300	1.46390800	0.07819200
H	-2.63218600	-0.57048100	0.68888000
H	-1.15349600	-2.19710800	-1.43745300
H	-1.47058700	0.92896500	-1.63620400
H	-3.09009900	-0.66221200	-0.99968500
H	-2.16784100	-2.83656800	-0.14870500
H	0.27671600	-2.94679200	0.45648700
C	-2.26055400	2.54335300	0.94110600

H	-3.33028600	2.50010000	0.76419900
H	-1.94131100	2.22950200	1.92949600
H	-1.76427900	3.42852900	0.55738700

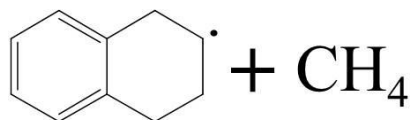


C	2.57620400	-1.40775300	-0.50797000
C	2.13638600	-0.16192500	-0.97945100
C	1.00462200	0.45707600	-0.45403900
C	0.27543600	-0.18654400	0.60510900
C	0.74101900	-1.45552400	1.06645100
C	1.86684100	-2.05218600	0.51887500
H	-0.20776700	1.60482900	-1.80330400
H	3.45833700	-1.86765000	-0.93295700
H	2.68590400	0.33199600	-1.77234800
C	0.50303000	1.78512700	-0.98604500
C	-0.86567500	0.42859800	1.17126500
H	0.19670100	-1.94869600	1.86281000
H	2.20114300	-3.01399400	0.88562300
C	-1.33382500	1.79464800	0.75912900
C	-0.20130300	2.61186900	0.10563800
H	-3.48426900	-1.51461300	-0.51598000
H	-2.17051300	1.70987800	0.04806400
H	0.52812800	2.89282000	0.87108700
H	-1.42048300	-0.10337600	1.93588800
H	-1.73958100	2.33050100	1.62267000
H	-0.59814600	3.53695600	-0.31763700
H	1.33173200	2.35013500	-1.41919700
C	-4.44815400	-1.87020600	-0.87731900
H	-4.33456700	-2.26005400	-1.88787000
H	-4.81262100	-2.66070500	-0.22269900
H	-5.16148100	-1.04711500	-0.88399900



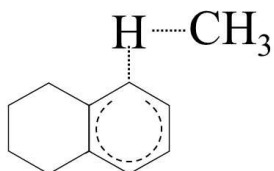
C	-2.52745200	-1.25171200	-0.03544200
C	-1.29422000	-1.40438900	0.60632200
C	-0.37565300	-0.34903700	0.64763900
C	-0.69684100	0.87631100	0.02713300
C	-1.92942600	1.01842300	-0.62084700
C	-2.84591700	-0.03757900	-0.64993900

H	1.19109700	-1.49433000	1.58436900
H	-3.23012400	-2.07440700	-0.05943900
H	-1.04355300	-2.34755300	1.07697200
C	0.96419600	-0.45300700	1.34238700
C	0.33740200	1.97797300	0.08512500
H	-2.17189600	1.95754000	-1.10377600
H	-3.79661200	0.08497600	-1.15227300
C	1.74565800	1.43341100	-0.27133000
C	2.10265400	0.15844700	0.51207900
H	0.06811400	2.79389300	-0.58851500
H	1.76466300	1.22729500	-1.34697800
H	3.02189000	0.24822900	1.09287700
H	0.36885200	2.40288500	1.09584900
H	2.49276100	2.21091900	-0.09509000
H	2.42303500	-0.74209700	-0.35626900
H	0.90977900	0.07457200	2.30607900
C	2.76909400	-1.73328500	-1.30871600
H	1.82626300	-1.99006400	-1.78207300
H	3.47621300	-1.23280400	-1.96385700
H	3.20255200	-2.53239500	-0.71434300

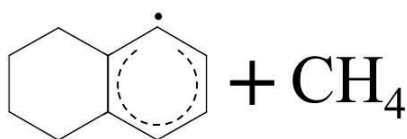


C	-2.45914400	-1.78124800	-0.11638200
C	-1.29117300	-1.58952500	0.62609500
C	-0.63567500	-0.35127900	0.63084600
C	-1.15969900	0.71116300	-0.13376700
C	-2.32675600	0.50685200	-0.88248000
C	-2.97965200	-0.72826100	-0.87376600
H	1.12812700	-1.08620100	1.62215300
H	-2.95321200	-2.74399700	-0.10899700
H	-0.88228400	-2.40820100	1.20638500
C	0.62290300	-0.12917500	1.45358900
C	-0.43224200	2.03998900	-0.13108300
H	-2.72287000	1.32143900	-1.47707700
H	-3.87991500	-0.86922500	-1.45745500
C	1.09991400	1.83673300	-0.19896100
C	1.56903500	0.86628100	0.84130900
H	-0.77056300	2.65739100	-0.96534800
H	1.35485500	1.48021600	-1.21020800
H	2.60062600	0.88172700	1.17193500
H	-0.66969400	2.59202600	0.78615500

H	1.61133000	2.79869400	-0.08963400
H	4.35024600	-0.85489800	-0.59070700
H	0.32669100	0.20999000	2.46300500
C	5.28119000	-1.31223700	-0.92321300
H	5.11054900	-2.36589800	-1.13948400
H	5.63126400	-0.80934600	-1.82359300
H	6.03265000	-1.21947500	-0.14024600

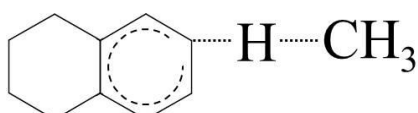


C	-1.26991100	2.36143700	0.01950400
C	0.11526100	2.19915900	0.02955200
C	0.71086500	0.92544400	0.02136900
C	-0.11698700	-0.22175200	-0.00139500
C	-1.49964100	-0.02108800	-0.01049600
C	-2.09800000	1.22918500	0.00034100
H	2.56873000	1.00603100	1.08795600
H	-1.70296900	3.35370300	0.02470300
H	0.75497700	3.07381100	0.04316900
C	2.22790800	0.80525600	0.06466400
C	0.46697600	-1.62772400	-0.04756200
H	-2.33967300	-1.11448800	-0.02673700
H	-3.17574900	1.33369100	-0.00591200
C	1.95108900	-1.68483800	0.35065100
C	2.74223300	-0.57846000	-0.36423600
H	-0.12144700	-2.28799500	0.59368800
H	2.04948900	-1.55545900	1.43393700
H	2.63075600	-0.69614100	-1.44759100
H	0.35818700	-2.02010500	-1.06601800
H	2.35887500	-2.66962000	0.11073800
H	3.80916400	-0.66106900	-0.14406200
H	2.67253700	1.58476300	-0.55991000
C	-3.18593800	-2.11215400	-0.04489800
H	-3.06937400	-2.61452200	0.91184800
H	-4.16293100	-1.65196700	-0.16902900
H	-2.89370100	-2.72742600	-0.89174400



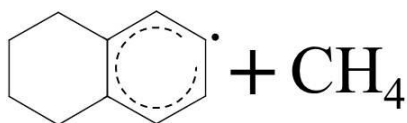
C	-0.09561300	2.76971300	-0.01177000
---	-------------	------------	-------------

C	-1.26389900	2.00618600	0.00535600
C	-1.23682900	0.59940300	-0.00493400
C	0.01517100	-0.06679700	-0.03004600
C	1.13339900	0.75107200	-0.04518300
C	1.15702100	2.12740900	-0.03942700
H	-2.96638100	-0.14716800	-1.02576200
H	-0.14788500	3.85088800	-0.00193300
H	-2.22423500	2.50712800	0.02805300
C	-2.53954800	-0.18731500	-0.01612500
C	0.12902200	-1.58404400	-0.01077900
H	4.06913100	-0.62450600	0.04829900
H	2.07805400	2.69413200	-0.05373200
C	-1.18814900	-2.29026500	-0.37201800
C	-2.36481400	-1.66011700	0.38977600
H	0.92798300	-1.89603300	-0.68698700
H	-1.37003300	-2.20774800	-1.44893400
H	-2.17682500	-1.72790100	1.46671800
H	0.44128300	-1.89831600	0.99201600
H	-1.10708700	-3.35578000	-0.14520300
H	-3.28943700	-2.20794600	0.19417200
H	-3.26477700	0.30273700	0.63893100
C	5.06238500	-1.07049200	0.08534800
H	4.99122700	-2.13569900	-0.13092900
H	5.70325200	-0.59256300	-0.65441400
H	5.48684600	-0.92975100	1.07851500

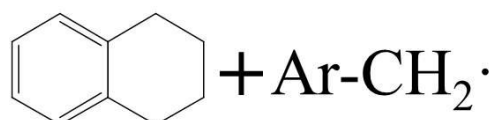


C	1.74848300	1.39894500	-0.03366400
C	0.40018400	1.76938900	-0.04656700
C	-0.62652700	0.80911600	-0.02447300
C	-0.29070300	-0.56050100	0.01465200
C	1.06966400	-0.93066100	0.02470300
C	2.05508400	0.04292600	0.00079700
H	-2.31545800	1.57735700	-1.09995400
H	2.52501400	2.15320800	-0.04927500
H	0.13576400	2.82067000	-0.07401400
C	-2.07783800	1.26826000	-0.07446400
C	-1.35933600	-1.64289400	0.07768200
H	1.33124900	-1.98283700	0.05141000
H	3.38103900	-0.34800500	0.01245800
C	-2.75446000	-1.14812800	-0.33831000
C	-3.07773600	0.18305300	0.35763000

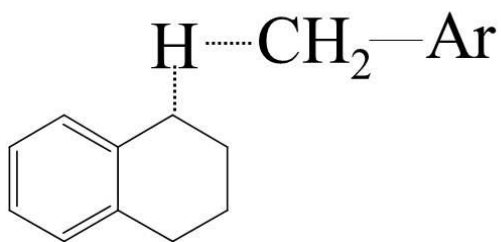
H	-1.05709500	-2.48988900	-0.54409500
H	-2.78921000	-1.00602400	-1.42385000
H	-3.02829100	0.04413700	1.44306400
H	-1.41222500	-2.02589600	1.10437000
H	-3.50305400	-1.90532000	-0.09337800
H	-4.09560900	0.50467700	0.12491900
H	-2.19954800	2.16111900	0.54462400
C	4.62976100	-0.71136700	0.02715000
H	4.78933300	-1.25052600	-0.90289800
H	5.19694700	0.21410800	0.08600300
H	4.74169300	-1.33560800	0.90980300



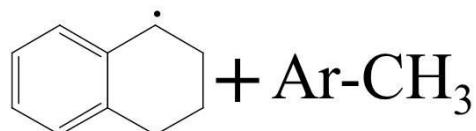
C	1.49540700	1.49913900	-0.06099600
C	0.12637700	1.80405800	-0.05177900
C	-0.85414000	0.79591700	-0.02461100
C	-0.46258800	-0.55997100	-0.00271800
C	0.91587800	-0.87761100	-0.01392600
C	1.82206700	0.15719300	-0.04215100
H	-2.59120200	1.49630700	-1.06970600
H	2.24135700	2.28171400	-0.08054700
H	-0.18452100	2.84251500	-0.06566100
C	-2.32515300	1.19194500	-0.05000800
C	-1.48175700	-1.68803800	0.06498100
H	1.22980000	-1.91420000	-0.00026300
H	4.94995900	-0.38722200	-0.00693500
C	-2.90341700	-1.24892000	-0.32224000
C	-3.27029200	0.06190400	0.39026000
H	-1.15380700	-2.51379100	-0.57182800
H	-2.96415600	-1.10093600	-1.40577700
H	-3.19635900	-0.08270000	1.47351700
H	-1.49930400	-2.08351100	1.08789400
H	-3.61399300	-2.03943100	-0.06993800
H	-4.30449400	0.34210100	0.17735500
H	-2.47583400	2.07459700	0.57703500
C	6.01373400	-0.61158300	0.06271700
H	6.21745300	-1.56218600	-0.42849300
H	6.58478500	0.17769600	-0.42453200
H	6.30361700	-0.67515100	1.11070800



C	2.37070500	2.77746800	0.25138600
C	3.42821900	1.88364800	0.41399100
C	3.28632100	0.51712400	0.11766300
C	2.04543600	0.04550100	-0.35739900
C	0.98565000	0.95529300	-0.51502900
C	1.13838200	2.30888100	-0.21647300
H	4.55950900	-0.61724600	1.41740300
H	2.50460500	3.82579100	0.48444700
H	4.38425300	2.24446500	0.77559300
C	4.46170300	-0.42408500	0.34178200
C	1.83953000	-1.41569400	-0.73197600
H	0.03150600	0.59120100	-0.87764400
H	0.30796200	2.99040600	-0.34761000
C	2.91301300	-2.35255900	-0.15403300
C	4.31485700	-1.76835500	-0.38956300
H	0.84457700	-1.73735100	-0.41254900
H	2.75258600	-2.48178400	0.92193000
H	4.47016600	-1.62457500	-1.46432700
H	1.84725100	-1.50335000	-1.82555300
H	2.82411100	-3.34202900	-0.60877800
H	5.08644900	-2.46218800	-0.04750600
H	5.38836100	0.07139900	0.03978600
C	-2.49055100	-1.70731100	1.34913300
H	-2.64534300	-2.77776900	1.34487300
H	-1.64046800	-1.32468100	1.89744100
C	-3.37086000	-0.84063400	0.67061600
C	-4.49953600	-1.34023800	-0.05175100
C	-3.17279600	0.57609500	0.67655400
C	-5.36274900	-0.48078500	-0.71697700
H	-4.67361300	-2.40868200	-0.07311700
C	-4.04411700	1.42447400	0.00736700
H	-2.32565300	0.98130900	1.21521700
C	-5.14503200	0.90665000	-0.69461800
H	-6.21028500	-0.88271700	-1.25663400
H	-3.87414600	2.49302900	0.02736400
H	-5.82087700	1.57193100	-1.21436700



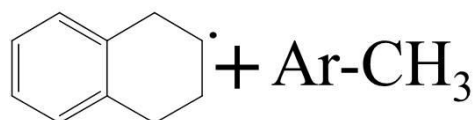
C	-3.54087000	-2.15434900	0.02372600
C	-2.29247600	-1.71533500	0.45580400
C	-1.94685600	-0.34588700	0.44013400
C	-2.90485100	0.59241900	-0.02389700
C	-4.15501800	0.13259700	-0.45871000
C	-4.48009100	-1.22563800	-0.44101600
H	0.24061600	-0.22890700	-0.14425600
H	-3.78292700	-3.20884800	0.04772200
H	-1.56467000	-2.43286100	0.81624300
C	-0.59548400	0.08194200	0.85723100
C	-2.60399100	2.08286100	-0.00444900
H	-4.88409500	0.85243700	-0.81232400
H	-5.45196000	-1.55580500	-0.78341500
C	-1.09823400	2.39542300	-0.00232900
C	-0.37546600	1.57171500	1.07729100
H	-0.67390100	2.15855400	-0.98306000
H	-0.75412800	1.86092000	2.06690300
H	-3.08977900	2.56712200	-0.85555600
H	-0.94009000	3.46361400	0.16253700
H	0.69457400	1.79464400	1.08072300
H	-0.15205600	-0.55195800	1.62625400
C	1.13400500	-0.58035400	-1.14556900
H	0.79447100	-1.59865000	-1.32018700
H	0.82889200	0.10395900	-1.93328700
C	2.50263300	-0.42973900	-0.65150800
C	3.14246700	-1.47334900	0.05812500
C	3.21651400	0.77955900	-0.82621900
C	4.43140800	-1.31516500	0.56473100
H	2.61905000	-2.41075100	0.20151700
C	4.50556000	0.93460800	-0.31920900
H	2.75034100	1.59178000	-1.37032200
C	5.12152400	-0.11069700	0.38026200
H	4.90123200	-2.13008200	1.10019600
H	5.03337700	1.86728600	-0.47107000
H	6.12259600	0.01020600	0.77178200
H	-3.05618500	2.52367100	0.89321000



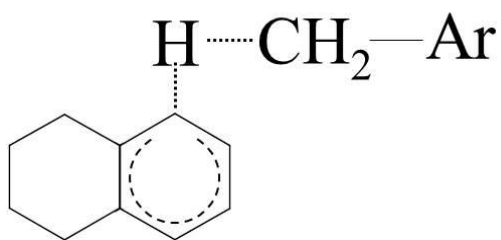
C	-4.05561600	-1.87021000	0.05429300
C	-2.93491500	-1.51209400	0.78854100
C	-2.36407300	-0.20716400	0.68229200
C	-2.99108600	0.73510900	-0.20489600
C	-4.11035600	0.34480000	-0.93627900
C	-4.65107000	-0.94416600	-0.81790900
H	-4.46998200	-2.86534700	0.15115800
H	-2.47133000	-2.22715100	1.45749900
C	-1.21414400	0.15515300	1.42171000
C	-2.42888800	2.14019500	-0.29749100
H	-4.57364300	1.05719400	-1.60891300
H	-5.52166700	-1.22203900	-1.39682300
C	-0.90775500	2.16937000	-0.05892500
C	-0.55310000	1.49567700	1.28164700
H	1.04869800	-1.96322600	-0.30601400
H	-0.86091800	2.15606600	2.10779900
H	-2.67233500	2.57546300	-1.26957400
H	-0.40397800	1.63824900	-0.87187700
H	0.53152400	1.39268700	1.37884500
C	2.04115600	-2.24590500	-0.66922200
H	1.94330400	-2.47315600	-1.73200200
H	2.32924100	-3.16324200	-0.15416500
H	-0.54320100	3.19858300	-0.07220300
H	-0.79564900	-0.56062400	2.12036600
C	3.04527500	-1.14024400	-0.43054800
C	3.85632900	-1.13427200	0.71537400
C	3.17704400	-0.07929200	-1.34198200
C	4.76693900	-0.09917600	0.94829300
H	3.77563200	-1.94674400	1.42725600
C	4.08635600	0.95702100	-1.11361000
H	2.56569200	-0.06854700	-2.23615400
C	4.88528800	0.95142200	0.03403400
H	5.38380800	-0.11622900	1.83749300
H	4.17344800	1.76332300	-1.83040800
H	5.59154800	1.75172200	0.21079700
H	-2.91450000	2.77567500	0.45499400



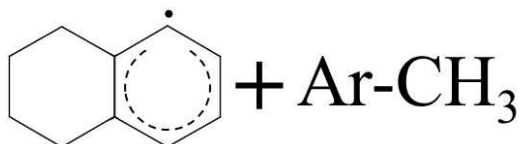
C	4.37400900	1.37756800	-0.58954800
C	3.21084900	1.64428000	0.13050400
C	2.29486700	0.62646300	0.44928800
C	2.56830300	-0.69178300	0.03381500
C	3.74448900	-0.94941000	-0.69117700
C	4.64280400	0.06884700	-1.00524300
H	0.30389100	1.41944300	0.50674300
H	5.06434900	2.17772100	-0.82241400
H	3.00168300	2.65673000	0.45582600
C	1.02228000	0.97529300	1.20477000
C	1.63724000	-1.84872000	0.37054200
H	3.95175500	-1.96444300	-1.01010700
H	5.54137900	-0.15308100	-1.56590500
C	0.29997000	-1.42559400	0.94833000
C	0.36194500	-0.23672200	1.88640700
H	-0.49872600	-1.02888200	-0.14360200
H	0.94365000	-0.50949200	2.77996600
H	1.48568600	-2.46729100	-0.52049400
H	-0.30263600	-2.25920400	1.31012600
H	-0.63659900	0.03086500	2.23847100
H	1.23844000	1.74823300	1.94667500
C	-1.23836800	-0.75940500	-1.20189600
H	-0.61557400	-0.05788300	-1.75307300
H	-1.27047400	-1.73410000	-1.68629300
C	-2.54606700	-0.23407500	-0.77159700
C	-3.60572700	-1.10517600	-0.43416400
C	-2.76953700	1.15435900	-0.63835100
C	-4.83017800	-0.61085400	0.01510300
H	-3.46140800	-2.17424800	-0.53281600
C	-3.99476500	1.64775000	-0.18931700
H	-1.97624400	1.84385300	-0.90027100
C	-5.03232800	0.76861200	0.14165800
H	-5.62817900	-1.29886100	0.26318800
H	-4.14311900	2.71638300	-0.10154300
H	-5.98284300	1.15160900	0.48817100
H	2.14625900	-2.50594500	1.09261100



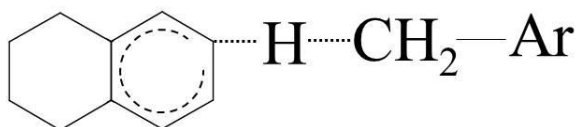
C	-5.66485900	0.52267900	-0.05722400
C	-4.52365300	1.28760300	0.19536100
C	-3.24787700	0.70682200	0.18481000
C	-3.11901400	-0.66898300	-0.09539300
C	-4.26830300	-1.42662800	-0.35801900
C	-5.53640700	-0.84097100	-0.33566500
H	-1.66710100	1.36043000	1.48804200
H	-6.64220400	0.98709100	-0.04447000
H	-4.62007600	2.34700300	0.40115700
C	-1.99846400	1.52008100	0.45497000
C	-1.74093400	-1.31045000	-0.09346300
H	-4.16744700	-2.48184800	-0.58289600
H	-6.41347300	-1.44092000	-0.54030000
C	-0.63791100	-0.37007300	-0.49350000
C	-0.85042600	1.11228000	-0.49777400
H	1.90062400	-0.95688300	1.58956100
H	-1.10094400	1.46832100	-1.51078700
H	-1.54273000	-1.71085100	0.91718500
H	0.30867600	-0.78102800	-0.82319200
H	0.07137300	1.63484800	-0.22339100
H	-2.21380300	2.58577300	0.35611600
C	2.95273200	-1.03758400	1.87975100
H	3.06831200	-0.51415000	2.83025000
H	3.16470200	-2.09401400	2.04950700
C	3.85624900	-0.45667600	0.81473500
C	4.42070300	-1.27295100	-0.17842400
C	4.13486400	0.91975300	0.78022800
C	5.23278000	-0.73154900	-1.17947400
H	4.22444400	-2.33812600	-0.16538800
C	4.94615000	1.46507000	-0.21841300
H	3.71521100	1.56543600	1.54209600
C	5.49814700	0.64050700	-1.20358700
H	5.65917300	-1.37934200	-1.93443000
H	5.14969100	2.52805600	-0.22497700
H	6.12843400	1.06060800	-1.97606000
H	-1.74552400	-2.19398300	-0.74153700



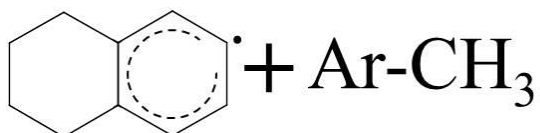
C	-1.10806200	2.58388700	-0.03304300
C	-2.45696700	2.22883900	-0.03460600
C	-2.86979800	0.88443400	-0.02098600
C	-1.88985600	-0.13745100	-0.00173300
C	-0.55385200	0.26268500	-0.00086000
C	-0.12716800	1.57881800	-0.01712600
H	-4.72675700	0.70449100	-1.07632700
H	-0.81757900	3.62683600	-0.04234700
H	-3.21266800	3.00546100	-0.04577500
C	-4.35531400	0.55334100	-0.05518600
C	-2.27059200	-1.61127400	0.04917400
H	0.55268300	-0.77199200	0.01023100
H	0.92552600	1.83076000	-0.01721900
C	-3.73417100	-1.87464700	-0.34183000
C	-4.66867100	-0.88861700	0.37629000
H	-1.59887400	-2.18340400	-0.59505100
H	-3.85454200	-1.76153200	-1.42468700
H	-4.53680900	-0.98847200	1.45911400
H	-2.10279100	-1.98235800	1.06748800
H	-3.99998800	-2.90633700	-0.09952900
H	-5.71453400	-1.11985100	0.16115300
H	-4.90033700	1.26331800	0.57273100
C	1.47492100	-1.59313700	0.01769100
H	1.28793100	-2.17565400	0.91906100
H	1.29098600	-2.19018700	-0.87482700
C	2.78120400	-0.88745300	0.01343100
C	3.40907600	-0.51564700	1.21943900
C	3.41206900	-0.53622900	-1.19718100
C	4.62214200	0.17466300	1.21535300
H	2.94083100	-0.77494300	2.16089500
C	4.62516900	0.15399900	-1.20185500
H	2.94615000	-0.81152500	-2.13524300
C	5.23649900	0.51277700	0.00453400
H	5.08893900	0.44610100	2.15327400
H	5.09432400	0.40933900	-2.14311700
H	6.17773900	1.04602500	0.00113300



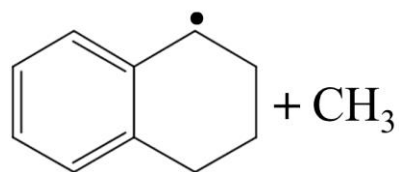
C	2.80327300	2.76513700	-0.33538000
C	3.80040000	1.80532900	-0.51480400
C	3.57445900	0.43872600	-0.26772500
C	2.29370300	0.01953800	0.17532400
C	1.35165500	1.02330100	0.33185000
C	1.52592900	2.36995500	0.10583700
H	5.38997100	-0.48296600	0.40053900
H	3.00590700	3.80940900	-0.53576400
H	4.78041400	2.11618800	-0.85627800
C	4.70367900	-0.56467500	-0.45131900
C	1.96142600	-1.44269800	0.43308000
H	-1.53512000	0.35994500	1.18516400
H	0.73504700	3.09284700	0.25230800
C	3.21095700	-2.32863000	0.56601600
C	4.21472300	-2.01888800	-0.55595500
H	1.34111000	-1.52078500	1.32874400
H	3.68893500	-2.15259700	1.53566900
H	3.73345100	-2.17851600	-1.52674100
H	1.34582500	-1.81222500	-0.39530100
H	2.91851800	-3.38090700	0.54320600
H	5.06838000	-2.69881200	-0.50902600
H	5.28668300	-0.29680800	-1.33650200
C	-2.48582900	0.16762800	1.69278800
H	-2.34650100	-0.71930100	2.31372700
H	-2.67943700	1.01323000	2.35388300
C	-3.61026500	-0.02435400	0.69974100
C	-3.79419000	-1.25715400	0.05138900
C	-4.48570200	1.02688300	0.38552300
C	-4.81629500	-1.43249100	-0.88476100
H	-3.13259400	-2.08296000	0.28365000
C	-5.51016600	0.85601000	-0.55061100
H	-4.36418200	1.98370000	0.87838800
C	-5.67909900	-0.37499900	-1.19010100
H	-4.94100100	-2.39115300	-1.37154900
H	-6.17468900	1.67997000	-0.77643200
H	-6.47265900	-0.50996600	-1.91303200



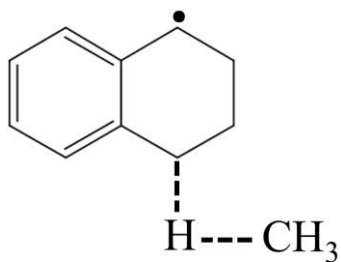
C	0.21167700	-0.91460700	-0.03510400
C	1.45549700	-1.55672400	-0.04518300
C	2.65934700	-0.83040800	-0.02013000
C	2.61742600	0.57920000	0.02003700
C	1.36356100	1.22695600	0.02755700
C	0.20434100	0.47316500	0.00045200
H	4.15062000	-1.93611100	-1.09411400
H	-0.70573300	-1.48839400	-0.05377900
H	1.49504300	-2.64000900	-0.07306100
C	3.98342800	-1.58219700	-0.06928500
C	3.88792400	1.41505900	0.08387500
H	1.32724200	2.31044700	0.05349700
H	-1.14310700	1.18599300	-0.00627600
C	5.14831500	0.64066800	-0.33490700
C	5.18838100	-0.72911900	0.36037600
H	3.76869300	2.30721000	-0.53663300
H	5.15075600	0.49527300	-1.42057800
H	5.17213500	-0.58371800	1.44599300
H	4.02067600	1.77668800	1.11104300
H	6.03869900	1.22518200	-0.09125100
H	6.11622000	-1.25596800	0.12526100
H	3.91657000	-2.47945800	0.55177800
C	-2.21074200	1.79044700	-0.02129500
H	-2.15896200	2.42338800	0.86393500
H	-2.15172900	2.39009500	-0.92895400
C	-3.34010800	0.82530000	-0.00787100
C	-3.88649700	0.36500900	1.20692600
C	-3.87074200	0.31316200	-1.20888300
C	-4.92386200	-0.56868400	1.22060100
H	-3.49391700	0.74670600	2.14131100
C	-4.90803600	-0.62064400	-1.19596700
H	-3.46602800	0.65453000	-2.15365000
C	-5.43952100	-1.06661600	0.01904100
H	-5.33142100	-0.90513900	2.16506300
H	-5.30321300	-0.99766500	-2.13032300
H	-6.24487800	-1.78884900	0.02928500



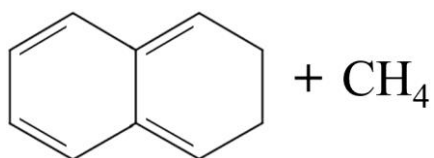
C	0.37751500	-0.45976500	-0.06896500
C	1.52157300	-1.27095100	-0.09844300
C	2.81669600	-0.72296000	-0.07257900
C	2.98189600	0.67751300	-0.01311700
C	1.83462300	1.50463600	0.01492200
C	0.59783600	0.90269100	-0.01367800
H	4.13028200	-2.01536600	-1.17043300
H	-0.61381000	-0.89094000	-0.08787900
H	1.40439900	-2.34780400	-0.14177800
C	4.01843900	-1.65744900	-0.13962200
C	4.35984100	1.32005800	0.05313700
H	1.94848700	2.58097200	0.05711800
H	-2.10581300	2.03627000	0.21741100
C	5.49332100	0.37561500	-0.37971300
C	5.33457000	-0.99386200	0.29809900
H	4.36866700	2.22711500	-0.55686500
H	5.47311400	0.24547500	-1.46698100
H	5.33965900	-0.86171700	1.38543600
H	4.54560700	1.64644000	1.08372300
H	6.45912700	0.82161400	-0.13121400
H	6.17578700	-1.64656300	0.05371600
H	3.82417000	-2.54509400	0.46806500
C	-3.17781100	2.17854000	0.38720700
H	-3.29593000	2.55683100	1.40447900
H	-3.51949200	2.95215700	-0.30133300
C	-3.93796100	0.88671200	0.18603900
C	-3.92997700	-0.11211800	1.17487300
C	-4.65286500	0.64256100	-0.99689300
C	-4.61053200	-1.31753100	0.98534600
H	-3.38832400	0.05883000	2.09728800
C	-5.33553000	-0.56246300	-1.19070400
H	-4.67498100	1.40147700	-1.76927900
C	-5.31660400	-1.54773900	-0.20007000
H	-4.59319100	-2.07245400	1.76079700
H	-5.88173600	-0.72850700	-2.11024700
H	-5.84620300	-2.47966900	-0.34704300



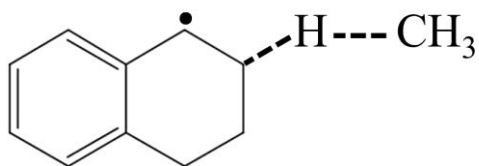
C	2.88472100	-0.32667400	-0.90829700
C	1.81938200	0.52324500	-1.24049100
C	0.65401200	0.56240300	-0.47869300
C	0.54260200	-0.27648600	0.68409000
C	1.63930500	-1.13487300	1.00058200
C	2.78416000	-1.15929800	0.21841700
H	-1.19193400	0.89295900	-1.52250300
H	3.77893300	-0.33861000	-1.51700300
H	1.90027000	1.16317600	-2.11142800
C	-0.51684800	1.44799700	-0.85779500
C	-0.62042200	-0.24246100	1.48767600
H	1.56332000	-1.77150200	1.87387300
H	3.60256400	-1.81790400	0.47883300
C	-1.75997000	0.69763400	1.21920800
C	-1.31293700	1.90933200	0.37717400
H	-2.56708100	0.16975500	0.68744700
H	-0.68219600	2.56097400	0.98929500
H	-0.69223100	-0.91994800	2.33117700
H	-2.20248000	1.03280900	2.16233500
H	-2.18062800	2.49639200	0.06900500
H	-0.16305900	2.30943700	-1.42907400
C	-4.20482500	-1.97416400	-1.22409800
H	-3.30811300	-2.46583500	-0.87785200
H	-5.06118700	-1.88990200	-0.57175100
H	-4.25124400	-1.58172600	-2.22898600



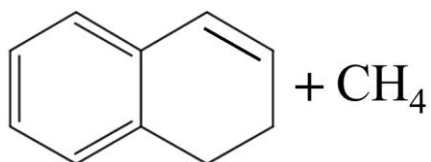
C	-2.60399900	1.05690000	-0.24150600
C	-1.27845900	1.34340100	-0.61001100
C	-0.25161800	0.42222200	-0.41114400
C	-0.55599300	-0.85321600	0.18387100
C	-1.90557400	-1.12149500	0.54298800
C	-2.91091700	-0.18110500	0.33595000
H	1.70690000	1.28505700	0.24850200
H	-3.38163800	1.79049100	-0.40692600
H	-1.04576900	2.30053700	-1.06176800
C	1.16350700	0.73108000	-0.77067300
C	0.47156400	-1.80863300	0.39742500
H	-2.14414800	-2.08107900	0.98558000
H	-3.92975700	-0.40932100	0.62055700
C	1.89871700	-1.56240900	0.00941700
C	2.02377200	-0.48800300	-1.09146000
H	2.47563000	-1.23613900	0.88903400
H	1.70150300	-0.91702300	-2.04781800
H	0.21755200	-2.74699700	0.87745000
H	2.36965100	-2.49474900	-0.31638600
H	3.06838500	-0.19299000	-1.21474900
H	1.24499800	1.52329200	-1.51654500
C	2.34331500	1.95402400	1.36547400
H	1.95373500	2.96434400	1.29010000
H	1.99130300	1.39749500	2.22800400
H	3.40575500	1.86048300	1.16298900



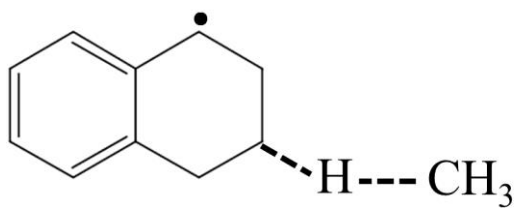
C	-1.97569100	-1.99794200	0.29182700
C	-0.79540700	-1.57733800	0.80978700
C	-0.30401400	-0.22409300	0.58038100
C	-1.09026800	0.64858200	-0.33901400
C	-2.37025400	0.14269000	-0.81959400
C	-2.78868800	-1.11319500	-0.52674000
H	-2.33480800	-2.99935600	0.48970400
H	-0.20018600	-2.23185100	1.43515800
C	0.78908600	0.27660100	1.21466300
C	-0.57499200	1.83910500	-0.74359400
H	-2.96781200	0.79399400	-1.44615300
H	-3.73273400	-1.47921100	-0.90852600
C	0.81121000	2.26952200	-0.33197500
C	1.18646300	1.72399300	1.05841900
H	3.66244500	-1.38504500	-0.56070300
H	0.67318000	2.31547700	1.83371500
H	-1.12459100	2.45603100	-1.44580100
H	1.53166500	1.89573600	-1.07747400
H	2.25527300	1.85590600	1.23622700
C	4.63386700	-1.75503600	-0.88556100
H	5.32426400	-1.75543700	-0.04310100
H	4.52617100	-2.76944100	-1.26695100
H	5.02279900	-1.11111900	-1.67316200
H	0.90129400	3.35730600	-0.34416300
H	1.33517000	-0.34031800	1.91963700



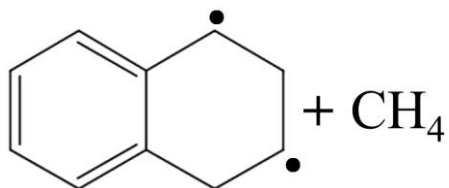
C	-2.96881700	0.44573400	0.45561400
C	-1.82565300	1.25895500	0.39956400
C	-0.58076300	0.74541700	0.05141800
C	-0.46121700	-0.65753500	-0.28486400
C	-1.64582300	-1.46758300	-0.21228200
C	-2.86414500	-0.92688800	0.15233500
H	1.12228500	1.57286100	1.05211900
H	-3.92426700	0.87127800	0.73113700
H	-1.91071600	2.31232900	0.64018800
C	0.66367400	1.60822600	0.05541000
C	0.77212200	-1.19569600	-0.66989900
H	-1.56576100	-2.52003100	-0.45606500
H	-3.74298300	-1.55682700	0.19954800
C	2.00126600	-0.34355700	-0.82834600
C	1.71084600	1.14183200	-0.97672700
H	2.68912200	-0.50429700	0.31866000
H	1.32665600	1.33971100	-1.98639600
H	0.84374500	-2.25480700	-0.88751600
H	2.70750700	-0.73150700	-1.56412900
H	2.62987300	1.72457000	-0.87443800
H	0.39506000	2.65225800	-0.12116300
C	3.35571700	-0.71395200	1.48735800
H	2.59848000	-0.68489200	2.26505600
H	3.81460700	-1.69101900	1.36397900
H	4.07314100	0.10066600	1.54152800



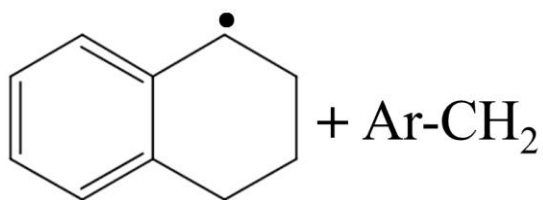
C	3.08983200	-0.37206600	-0.80401300
C	2.16891400	0.66851900	-0.97640900
C	0.92328500	0.63739300	-0.34518200
C	0.59444000	-0.46240100	0.48488300
C	1.52148200	-1.50501800	0.64451400
C	2.76274500	-1.46288800	0.00543500
H	-0.76808500	1.39059200	-1.40964900
H	4.05094600	-0.33040400	-1.29930400
H	2.42115100	1.50959300	-1.61105600
C	-0.12729500	1.70881700	-0.57684900
C	-0.70318500	-0.47277100	1.17584000
H	1.26753500	-2.34649200	1.27777000
H	3.46822400	-2.27214500	0.13999700
C	-1.46350100	0.63141500	1.27022400
C	-1.01747000	1.94159000	0.65989000
H	-4.19040500	-0.99787100	-0.64450100
H	-0.46628900	2.52123200	1.41333700
H	-1.01112300	-1.39725300	1.65077600
H	-2.39107600	0.61350500	1.83005600
H	-1.88139500	2.54920000	0.38286800
H	0.34457800	2.64314500	-0.88671700
C	-5.15295200	-1.27556300	-1.07165700
H	-5.31345300	-0.72176100	-1.99564800
H	-5.16118600	-2.34385300	-1.28334600
H	-5.94719600	-1.03964800	-0.36463300



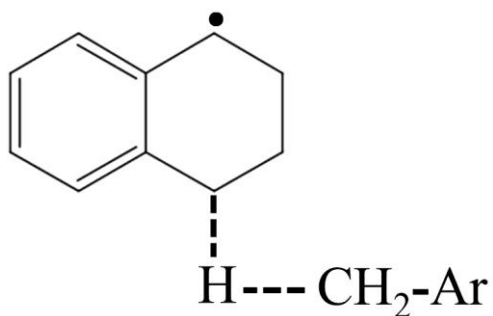
C	2.89338500	-1.17413400	-0.03606100
C	1.54527700	-1.55892100	0.00686200
C	0.52240500	-0.61558600	0.06216600
C	0.84823500	0.78498100	0.05607500
C	2.22820000	1.15102200	0.01851700
C	3.22732800	0.19024300	-0.02534800
H	-1.21096600	-1.12115400	1.22237400
H	3.67055100	-1.92548900	-0.07682300
H	1.29057700	-2.61226400	0.00289200
C	-0.93867200	-1.02749900	0.16200700
C	-0.17192200	1.76378800	0.07819200
H	2.48540800	2.20334600	0.01837800
H	4.26604700	0.49252300	-0.05576400
C	-1.63594800	1.40892800	0.04270800
C	-1.85640900	-0.00237200	-0.49494600
H	-2.05855600	1.48191800	1.05833500
H	-1.82453700	-0.04762100	-1.58542500
H	0.10529800	2.81123200	0.12008000
H	-2.18591600	2.14120300	-0.55551800
H	-3.09190000	-0.34533200	-0.22031900
H	-1.07792900	-2.01582200	-0.28127400
C	-4.39688800	-0.70796700	0.10501400
H	-5.01369300	0.05592100	-0.35992300
H	-4.51853500	-1.69631200	-0.32915900
H	-4.42579000	-0.69705000	1.19104300



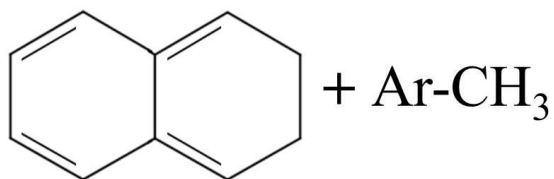
C	-3.21167800	-1.05446500	-0.25180400
C	-1.91788200	-1.53001200	0.00128700
C	-0.83116100	-0.66447700	0.11001900
C	-1.03684500	0.74915400	-0.02905000
C	-2.36455300	1.20941200	-0.29279400
C	-3.42660200	0.32615800	-0.40189400
H	0.93969000	-1.61666600	-0.61889900
H	-4.03859400	-1.74740500	-0.33023800
H	-1.75460300	-2.59572700	0.11267400
C	0.57091300	-1.20485900	0.34066100
C	0.03490700	1.66078500	0.09239800
H	-2.52951900	2.27443800	-0.40223200
H	-4.42270000	0.70010100	-0.59976000
C	1.43556200	1.24589700	0.43643200
C	1.53513800	-0.18591000	0.86120200
H	2.09723400	1.44139700	-0.43413600
H	2.41338100	-0.51685400	1.40179800
H	-0.15899200	2.71673200	-0.05749600
H	1.84032100	1.90246700	1.21835200
H	5.00625400	-0.48969800	-0.31174100
H	0.52911800	-2.06638600	1.01390700
C	6.03577100	-0.38019800	-0.65021700
H	6.05823300	0.22806800	-1.55331900
H	6.62480000	0.10335300	0.12781500
H	6.45395200	-1.36273700	-0.86416400



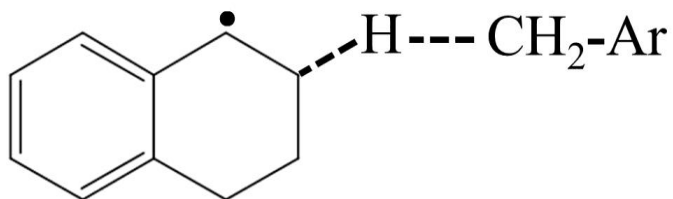
C	4.79625000	-1.06428500	-1.03198000
C	4.21638500	0.21186800	-1.08609300
C	3.12281700	0.54909600	-0.29218200
C	2.58107300	-0.42656400	0.61511900
C	3.18699500	-1.71945500	0.65037300
C	4.27024000	-2.02990800	-0.15799500
H	1.67330000	1.88940400	-1.13468100
H	5.64511100	-1.30107000	-1.65938500
H	4.62433300	0.95447200	-1.76197300
C	2.46739400	1.91368900	-0.37660900
C	1.48317700	-0.10520000	1.44645500
H	2.78484600	-2.46151200	1.32956700
H	4.71326200	-3.01633600	-0.11267800
C	0.87108300	1.26518500	1.48161200
C	1.85013400	2.33982800	0.96840800
H	-0.04175400	1.28656100	0.86610600
H	2.64899700	2.48056100	1.70269900
H	1.06700500	-0.87753800	2.08354100
H	0.54183000	1.50473600	2.49734400
H	1.33739000	3.29807200	0.86179400
H	3.19391200	2.65539300	-0.71683800
C	-2.13749400	0.23473000	-1.64919200
H	-1.31440700	-0.46500300	-1.69743900
H	-2.04815700	1.15461200	-2.21111800
C	-3.29087300	-0.04580100	-0.88898300
C	-4.38286400	0.87548200	-0.82328400
C	-3.41877600	-1.26485600	-0.15179800
C	-5.51608600	0.59229100	-0.07373500
H	-4.31330400	1.80632300	-1.37202300
C	-4.55780800	-1.53605200	0.59337100
H	-2.60704600	-1.98064200	-0.18345000
C	-5.61558900	-0.61312700	0.64042700
H	-6.32932900	1.30548000	-0.03988400
H	-4.63139400	-2.46582800	1.14223400
H	-6.50093400	-0.82919600	1.22269800



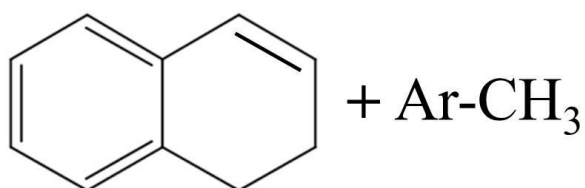
C	-3.84100800	-1.93471400	0.03042200
C	-2.55300000	-1.65549900	0.51961000
C	-2.01089200	-0.37120700	0.45607600
C	-2.79086100	0.69249700	-0.12580800
C	-4.09170900	0.38588400	-0.60489300
C	-4.60693000	-0.90757300	-0.53074700
H	0.21272500	-0.31307500	-0.10585100
H	-4.23617800	-2.93978900	0.09266500
H	-1.96590600	-2.45192400	0.96157100
C	-0.64410300	-0.07502700	0.94229600
C	-2.25883000	2.00680700	-0.21036400
H	-4.68729900	1.18125200	-1.03641100
H	-5.60041400	-1.11419000	-0.90656700
C	-0.88831500	2.36006000	0.28300700
C	-0.37093600	1.36548500	1.34444000
H	-0.18099000	2.37776500	-0.56083300
H	-0.87088600	1.57363000	2.29943700
H	-2.85818400	2.78056900	-0.67667300
H	-0.88032600	3.37735400	0.68585000
H	0.69724600	1.51590300	1.51484500
H	-0.25295000	-0.81541900	1.64031600
C	1.05953100	-0.60949700	-1.11647100
H	0.74451600	-1.63042000	-1.32189700
H	0.72804500	0.08533600	-1.88457400
C	2.44462700	-0.44792900	-0.66152400
C	3.12339800	-1.49926200	-0.00297200
C	3.13217300	0.77689300	-0.82615900
C	4.42589300	-1.33351300	0.46579000
H	2.61991200	-2.44885700	0.13122500
C	4.43500600	0.94004300	-0.35774600
H	2.63557600	1.59581500	-1.33211600
C	5.09012100	-0.11317500	0.29226700
H	4.92605800	-2.15477400	0.96265800
H	4.94257500	1.88519500	-0.50121000
H	6.10149400	0.01399000	0.65422300



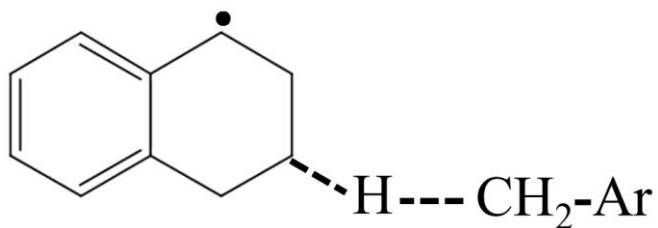
C	-4.26659200	-1.77081900	0.12368500
C	-3.01243300	-1.58721600	0.60503700
C	-2.35526000	-0.28768500	0.53813000
C	-3.06675300	0.80924200	-0.18005100
C	-4.42922400	0.54902600	-0.62854000
C	-4.99709400	-0.67452200	-0.49156400
H	-4.74701800	-2.73741200	0.20044200
H	-2.47704500	-2.39999900	1.08107800
C	-1.16895900	-0.03329300	1.15166100
C	-2.41796300	1.97364600	-0.44482600
H	-4.96773700	1.35983800	-1.10438800
H	-6.00260200	-0.85508800	-0.84838800
C	-0.96483400	2.15690000	-0.08300500
C	-0.58677600	1.35857500	1.17804600
H	1.11864300	-1.71735800	-0.89035000
H	-0.96814000	1.88175300	2.06987500
H	-2.91838300	2.75619200	-1.00445700
H	-0.34482000	1.81792800	-0.92854200
H	0.49828700	1.32453700	1.28758400
C	2.13767500	-1.98827900	-1.18242200
H	2.16885100	-2.00456300	-2.27279900
H	2.32072800	-3.00278900	-0.82537000
H	-0.72886300	3.21325200	0.05847600
H	-0.67147800	-0.81563800	1.71407300
C	3.14470100	-1.01266300	-0.61523800
C	3.73079500	-1.22921700	0.64245700
C	3.50258400	0.14662400	-1.32291100
C	4.64099500	-0.31456100	1.18005700
H	3.47438600	-2.12114100	1.20119000
C	4.41206600	1.06402300	-0.78909500
H	3.06782500	0.32867200	-2.29820800
C	4.98497300	0.83701800	0.46585900
H	5.08281100	-0.50301900	2.14998800
H	4.67538200	1.94969000	-1.35278400
H	5.69176400	1.54436700	0.87889800



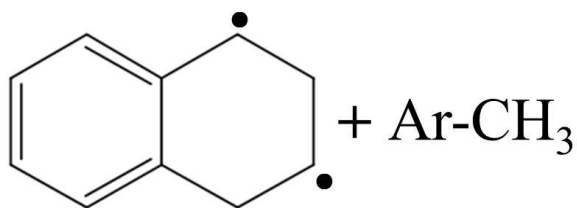
C	4.81548100	0.94588900	-0.57878700
C	3.61601300	1.51410800	-0.11862100
C	2.52012800	0.73015200	0.22274500
C	2.62168600	-0.71383000	0.12509500
C	3.85972300	-1.26732200	-0.35748600
C	4.92239100	-0.45603100	-0.70112400
H	0.58728700	1.52924900	-0.23118000
H	5.65196900	1.58048600	-0.83824900
H	3.53804000	2.59178200	-0.03283900
C	1.20703200	1.34716200	0.65590800
C	1.55051600	-1.52821500	0.49876700
H	3.94410500	-2.34411800	-0.43990200
H	5.84427600	-0.89522500	-1.05976400
C	0.29336200	-0.96580400	1.08581000
C	0.41239300	0.44441100	1.62342900
H	-0.63688100	-0.89091300	-0.04589300
H	0.93232500	0.42340400	2.59234800
H	1.63909800	-2.60310100	0.39421000
H	-0.26611000	-1.65629200	1.71568700
H	-0.57617800	0.86911900	1.81464600
H	1.38529900	2.32454700	1.10995300
C	-1.41014100	-0.89289500	-1.06519900
H	-0.87092700	-0.28192700	-1.78645100
H	-1.39817800	-1.94330400	-1.35186900
C	-2.73522400	-0.37304700	-0.67754600
C	-3.72309300	-1.22730000	-0.13937100
C	-3.04311200	1.00082800	-0.79039400
C	-4.96285000	-0.73087000	0.26258300
H	-3.51132600	-2.28540700	-0.04561400
C	-4.28370900	1.49614600	-0.38934600
H	-2.30281400	1.67500800	-1.20344700
C	-5.25090500	0.63371600	0.14056000
H	-5.70592300	-1.40584600	0.66721800
H	-4.49890000	2.55191300	-0.49173900
H	-6.21329700	1.01803600	0.45073300



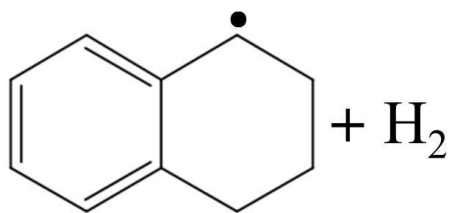
C	-5.45450400	-0.08487400	0.19882400
C	-4.51409000	0.93316000	0.39857000
C	-3.15586500	0.71428400	0.15675200
C	-2.72979300	-0.55602500	-0.30327200
C	-3.67963500	-1.57296200	-0.49182100
C	-5.03459900	-1.34202700	-0.24317400
H	-1.73642800	1.62402300	1.46724800
H	-6.50290700	0.10322100	0.38936500
H	-4.84057000	1.90490900	0.74931300
C	-2.10302500	1.77045100	0.44264900
C	-1.30435900	-0.76941900	-0.59305500
H	-3.35184300	-2.54464600	-0.84121500
H	-5.75541900	-2.13443800	-0.39562000
C	-0.44209000	0.25587400	-0.70095000
C	-0.90205900	1.68521500	-0.51987600
H	1.62777000	-1.10060900	1.75658800
H	-1.17668700	2.10205100	-1.49878500
H	-0.97456900	-1.78769200	-0.76493900
H	0.59298400	0.07873600	-0.96709100
H	-0.08453800	2.30490100	-0.14597100
H	-2.54635500	2.76750300	0.41033300
C	2.69150100	-1.17834500	2.00016800
H	2.84476700	-0.66517500	2.95098000
H	2.91650100	-2.23526100	2.14839700
C	3.54589100	-0.58006600	0.90477200
C	4.08497200	-1.38375800	-0.11247700
C	3.80373900	0.80048400	0.86640500
C	4.85260800	-0.82672200	-1.13979400
H	3.90407200	-2.45159900	-0.09749800
C	4.57077700	1.36144200	-0.15826500
H	3.40347300	1.43687900	1.64630600
C	5.09807700	0.54899400	-1.16688900
H	5.26031500	-1.46530700	-1.91269500
H	4.75971200	2.42713000	-0.16673700
H	5.69445400	0.98113700	-1.95937700



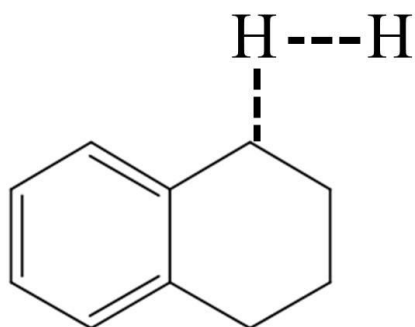
C	-5.20868000	-0.75912200	0.19750300
C	-3.95322700	-1.34952800	-0.00893700
C	-2.79643100	-0.58010600	-0.10154100
C	-2.88067200	0.84851200	0.03594200
C	-4.17129800	1.42591800	0.23775600
C	-5.30916300	0.63696300	0.31570000
H	-1.28742400	-1.25840400	-1.46706500
H	-6.09382000	-1.37731100	0.26487900
H	-3.87920800	-2.42647000	-0.10434100
C	-1.43790500	-1.21122600	-0.37923800
C	-1.71728600	1.65005500	-0.01850400
H	-4.24768200	2.50185200	0.33726900
H	-6.27579500	1.09766500	0.47240200
C	-0.33312300	1.06471700	-0.15313800
C	-0.31199100	-0.40313800	0.24405400
H	0.00835400	1.17011800	-1.19659500
H	-0.18637700	-0.57050900	1.31427300
H	-1.81690600	2.72804600	0.04234000
H	0.37850400	1.63947600	0.44526200
H	0.89885600	-0.94251400	-0.25441100
H	-1.42732900	-2.24221100	-0.01974800
C	1.97880900	-1.47718400	-0.75623100
H	1.92919800	-2.48946700	-0.35846100
H	1.77356000	-1.45670200	-1.82535800
C	3.15909300	-0.69974600	-0.33390200
C	3.64324200	0.37348600	-1.11302800
C	3.81388300	-0.97501200	0.88636900
C	4.73405500	1.13474800	-0.69245200
H	3.16037600	0.60117700	-2.05550900
C	4.90395400	-0.21278200	1.30671700
H	3.46293400	-1.79551300	1.50029400
C	5.37054500	0.84701100	0.52039500
H	5.09058800	1.94893200	-1.31016700
H	5.39204300	-0.44588100	2.24428300
H	6.21729300	1.43631000	0.84587100



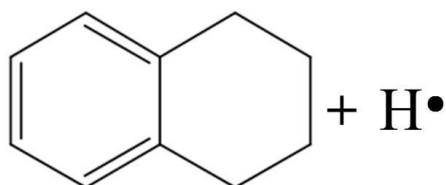
C	4.78170800	-1.49816300	0.12626200
C	3.39821800	-1.62329000	0.31223000
C	2.55044200	-0.51916200	0.24693000
C	3.10003600	0.77821600	-0.02727500
C	4.51464000	0.88128300	-0.20795700
C	5.33538700	-0.23260400	-0.13183800
H	0.90322400	-0.77940300	1.58580200
H	5.41772500	-2.37150300	0.18077300
H	2.97418900	-2.60014200	0.51451400
C	1.05827000	-0.67032700	0.49444900
C	2.27282800	1.91937300	-0.11814400
H	4.93927600	1.85666900	-0.41262700
H	6.40314900	-0.12823200	-0.27432900
C	0.77743000	1.86408100	-0.00401500
C	0.23792100	0.46803400	-0.02527700
H	0.46457400	2.38930400	0.92396000
H	-0.81004300	0.30799700	-0.24440500
H	2.73431400	2.88537000	-0.28920900
H	0.31692600	2.46041500	-0.80303200
H	-3.54366500	0.73706100	2.71983200
H	0.70617300	-1.61516000	0.06961500
C	-4.42549000	0.38464900	2.17636400
H	-4.82681100	-0.46781900	2.72591600
H	-5.16665900	1.18469500	2.20756700
C	-4.07632100	0.00951000	0.75315700
C	-4.07478400	0.97540000	-0.26656600
C	-3.72440200	-1.30816300	0.41958600
C	-3.72579000	0.63779700	-1.57720900
H	-4.35067600	1.99620300	-0.03144800
C	-3.37492400	-1.65051700	-0.89011700
H	-3.72708100	-2.06945200	1.19009200
C	-3.37312100	-0.67768000	-1.89403400
H	-3.73298700	1.39729700	-2.34817400
H	-3.10964600	-2.67295000	-1.12590300
H	-3.10427100	-0.94097000	-2.90822800



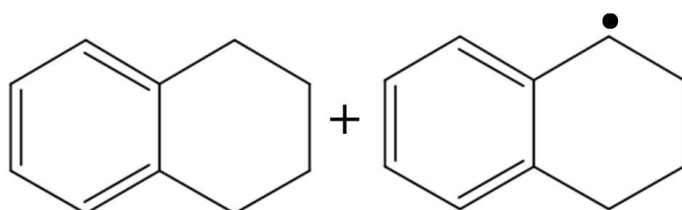
C	2.57351600	-0.74135100	0.05594700
C	1.35846900	-1.40472300	0.28265400
C	0.13667300	-0.74611800	0.16636900
C	0.11559100	0.64212200	-0.20811000
C	1.36554000	1.29636600	-0.43138100
C	2.56764700	0.61758500	-0.29943100
H	-1.42865000	-1.33239200	1.51306200
H	3.50921200	-1.27542900	0.15341100
H	1.36642000	-2.45290200	0.55798800
C	-1.17721200	-1.44752400	0.45035800
C	-1.11127500	1.33064700	-0.35390400
H	1.35926200	2.34270600	-0.71215600
H	3.50224600	1.13460800	-0.47415700
C	-2.44128900	0.65220800	-0.19455600
C	-2.33020400	-0.87286700	-0.39330200
H	-0.46433000	2.93726700	2.94311000
H	-2.85174800	0.85415600	0.80724700
H	-2.14380800	-1.08579600	-1.45015600
H	-1.09123500	2.38790600	-0.59333300
H	-3.16677500	1.07505500	-0.89627500
H	-3.27145200	-1.35840000	-0.12736800
H	-1.07226100	-2.52075800	0.27475800
H	-0.59161700	3.33590700	3.55599600



C	2.60954200	-0.67407800	0.02889500
C	1.41646100	-1.38848900	0.13421700
C	0.17116100	-0.74132300	0.10529500
C	0.13223500	0.66379900	-0.04085300
C	1.34364600	1.37174700	-0.16099700
C	2.57203300	0.71701000	-0.12320900
H	-1.34964500	-1.74099400	1.25336700
H	3.55770900	-1.19473800	0.05536300
H	1.44402200	-2.46715300	0.23354300
C	-1.11256000	-1.54848800	0.19950300
C	-1.16626800	1.41378700	-0.07645100
H	1.31207000	2.44848500	-0.27769900
H	3.49090100	1.28120800	-0.21266400
C	-2.43883800	0.58952100	0.14467400
C	-2.30297600	-0.82400100	-0.44894400
H	-1.13708100	2.24218400	0.82764500
H	-2.63323800	0.49420700	1.21844200
H	-2.15180100	-0.76074900	-1.53113800
H	-1.23027000	2.06593900	-0.95090600
H	-3.29735100	1.11017900	-0.28330600
H	-3.22305900	-1.38976600	-0.28509600
H	-0.96237500	-2.52706400	-0.26295900
H	-1.16650200	2.96135300	1.64263100

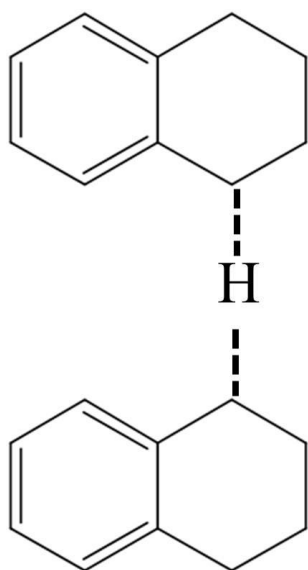


C	2.61381500	-0.68104200	0.07644200
C	1.42285600	-1.40158000	0.15496500
C	0.17306600	-0.76527200	0.06544600
C	0.12873600	0.63300600	-0.11076700
C	1.33575800	1.34876400	-0.18670900
C	2.56989000	0.70671300	-0.09481800
H	-1.24722100	-1.85585000	1.24441900
H	3.56440700	-1.19348000	0.14698100
H	1.45456700	-2.47691500	0.28743500
C	-1.09926100	-1.59215000	0.18972600
C	-1.19290600	1.37572400	-0.24966200
H	1.29945800	2.42394300	-0.31912000
H	3.48617100	1.27941200	-0.15495400
C	-2.40342600	0.56685700	0.24447000
C	-2.35414900	-0.86273300	-0.31729000
H	-1.13315700	2.32928200	0.28241600
H	-2.39971900	0.52465000	1.33905600
H	-2.34158200	-0.81982800	-1.41179800
H	-1.34610200	1.62913700	-1.30611500
H	-3.32853700	1.06762200	-0.05065500
H	-3.24814500	-1.42238900	-0.03210700
H	-0.97205500	-2.53916000	-0.34178300
H	-0.95435000	5.08384700	1.68539800



C	4.23704300	2.36780900	-0.20934100
C	4.72773400	1.16039700	0.28567400
C	4.01983800	-0.04249800	0.12107900
C	2.78764000	-0.02242200	-0.56388000
C	2.30203500	1.20107600	-1.05669600
C	3.01253600	2.38864300	-0.88559100
H	4.42296500	-1.32063800	1.79447600
H	4.80133400	3.28092700	-0.07159400
H	5.67655100	1.14213800	0.80951000
C	4.58235800	-1.32924300	0.70893800

C	1.99090300	-1.29670700	-0.80617300
H	2.61823200	3.31857400	-1.27416000
C	2.41033700	-2.46186800	0.10497200
C	3.94070000	-2.59940500	0.12646000
H	2.04993000	-2.28382300	1.12407700
H	4.30275600	-2.76348400	-0.89429200
H	0.92443500	-1.08878800	-0.68648300
H	1.94266400	-3.38723500	-0.23939200
H	4.24360900	-3.46948900	0.71385500
H	5.66590900	-1.35276700	0.56451500
H	2.12312700	-1.60180400	-1.85170600
H	1.35417100	1.21393600	-1.58224900
C	-1.86143400	1.87523900	1.29964400
C	-2.05074600	0.38801700	1.37849400
C	-3.01953400	-0.29713000	0.60899300
C	-3.83257100	0.41025400	-0.34316300
C	-3.60223100	1.89555300	-0.54275700
C	-3.11569000	2.58137800	0.74748500
H	-2.61507700	-2.24447500	1.46717200
H	-1.60317400	2.27477500	2.28503700
C	-3.22400400	-1.70340400	0.75299900
C	-4.79143600	-0.28653900	-1.07462200
H	-2.84691700	2.04418800	-1.32592900
H	-3.91121800	2.54221900	1.49764300
C	-4.97526900	-1.66796100	-0.91435700
C	-4.18081300	-2.37271800	0.00488800
H	-5.40618800	0.25368600	-1.78518500
H	-5.72677000	-2.18569600	-1.49525700
H	-4.31804600	-3.43868600	0.13219100
H	-1.42121000	-0.18144300	2.05288700
H	-1.00089000	2.11240700	0.65493600
H	-2.90323900	3.63556400	0.55765500
H	-4.51734100	2.36909200	-0.90598600



C	-4.21521000	-1.72761200	-0.33914600
C	-4.16954900	-0.53121500	0.38462000
C	-3.09410400	0.35281500	0.25512900
C	-2.03165900	0.03772600	-0.63348700
C	-2.10200500	-1.16466100	-1.37049400
C	-3.17660000	-2.03956700	-1.22449900
H	-2.40887600	1.59769500	1.88151000
H	-5.05514900	-2.39988000	-0.22380200
H	-4.98292500	-0.27713100	1.05413800
C	-3.04588500	1.67492200	0.99113300
C	-0.86625800	0.93158200	-0.74399000
H	-3.21005400	-2.95527900	-1.80043300
C	-1.04910200	2.41824900	-0.39132000
C	-2.48033200	2.76944200	0.06459200
H	-0.35288100	2.69565700	0.40864100
H	-3.13643700	2.86143800	-0.80582800
H	0.05477000	0.49062900	0.15148600
H	-0.77482500	3.03529000	-1.25106500
H	-2.48062500	3.73756100	0.57070300
H	-4.04345500	1.94445000	1.34466300
H	-0.27724400	0.76152800	-1.64496000
H	-1.30482700	-1.40170700	-2.06481200
C	0.58348600	-1.19987800	1.60712500
C	1.00177100	0.17345600	1.10507400
C	2.32093400	0.29186600	0.45657300
C	3.06172700	-0.85899800	0.07685700
C	2.56441200	-2.24992800	0.43440500
C	1.04277200	-2.30768500	0.64396500
H	2.29914500	2.44778400	0.45488100
H	1.01977200	-1.38077100	2.59930800

C	2.85557300	1.56636000	0.15914600
C	4.28389200	-0.69675600	-0.58833300
H	2.86773600	-2.95966800	-0.33965200
H	0.75583400	-3.28825800	1.03055300
C	4.79430300	0.57027900	-0.88099200
C	4.07411400	1.70859500	-0.49832800
H	4.84437400	-1.57877300	-0.87600000
H	5.73992200	0.66936100	-1.39749400
H	4.46201200	2.69605000	-0.71232700
H	0.77615900	0.98883400	1.79359400
H	-0.50113000	-1.23632200	1.73790400
H	0.53417600	-2.18492500	-0.31617900
H	3.06084300	-2.57752200	1.35699900