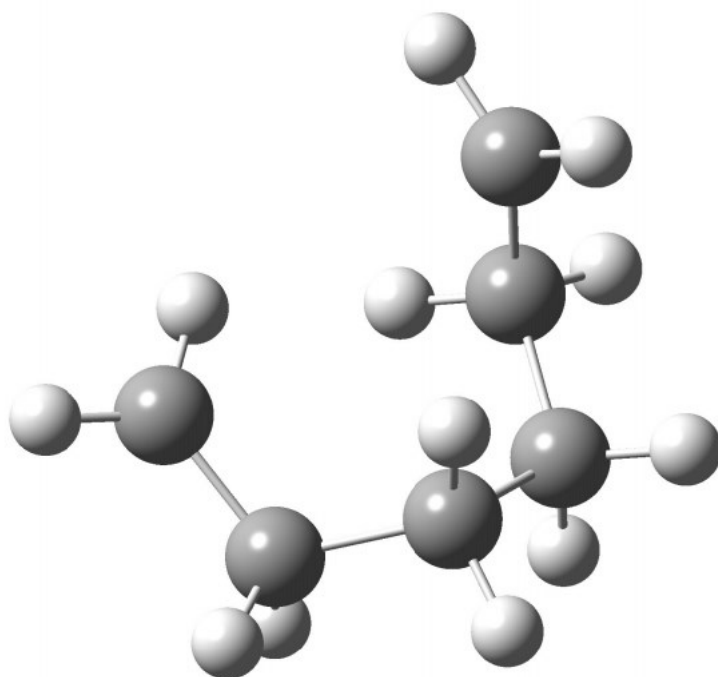


Supplementary Materials

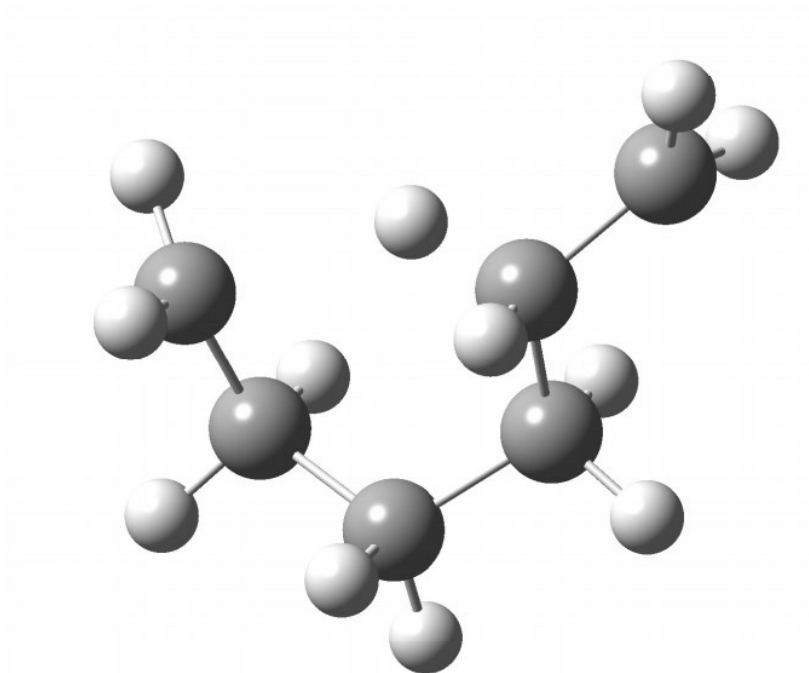
Geometries of some species involved in this work.

1. TS1



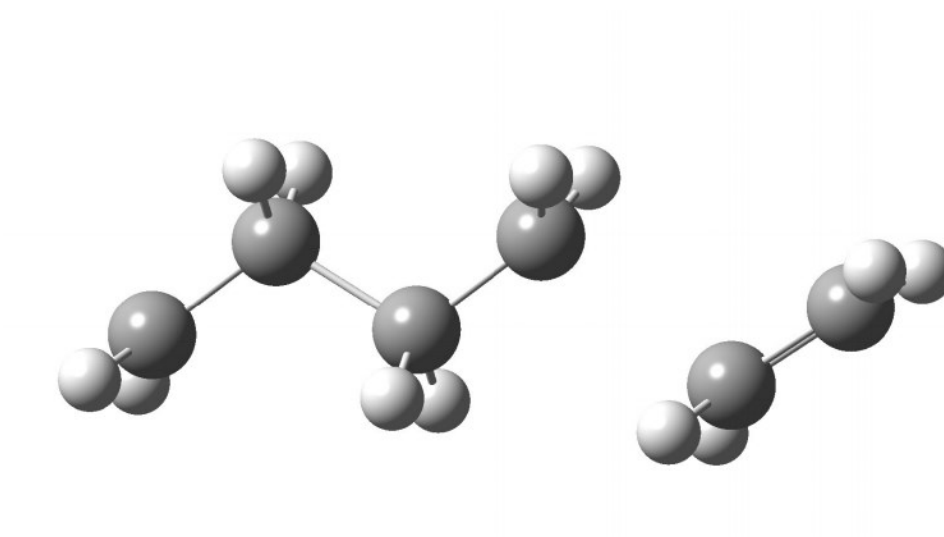
C	-1.29806100	0.09425500	0.89567800
C	-0.63040200	-1.16185900	0.30187400
C	0.47280300	-0.93343100	-0.74346400
C	1.75002600	-0.20749000	-0.25161600
C	1.66812400	1.28173100	-0.16125400
C	-1.92978900	0.99280700	-0.11184900
H	0.77632300	-1.92628900	-1.12001400
H	-0.22097000	-1.76669600	1.13163200
H	-1.41781900	-1.78243900	-0.16453200
H	-0.57738800	0.66114100	1.51172300
H	2.02550300	-0.63800800	0.73765300
H	2.58350900	-0.47483700	-0.92321700
H	-2.06813000	-0.25154600	1.62191200
H	0.06263500	-0.38608800	-1.60993500
H	-2.09171800	2.05223500	0.10059300
H	-2.40623900	0.57716000	-1.00484300
H	2.47391700	1.90774200	-0.55166000
H	0.85477600	1.78091100	0.36681900

2. TS2



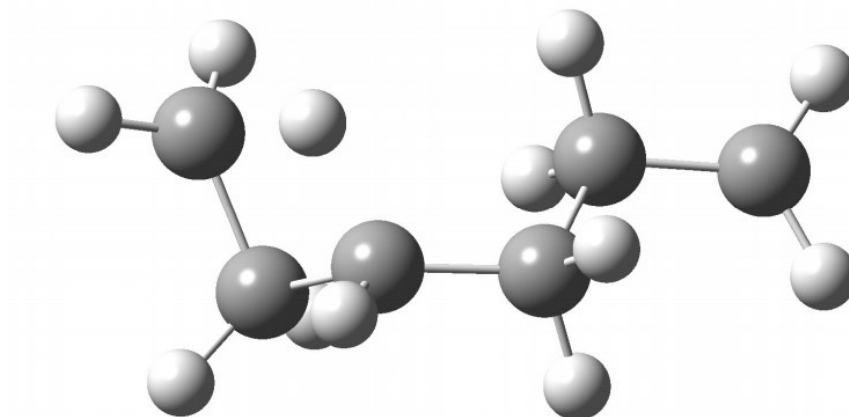
C	-1.46071400	1.47757200	0.10710200
H	-1.49170500	2.33904700	-0.56510400
H	-1.47205100	1.68664900	1.18181200
C	-1.82958700	0.11213000	-0.37798800
H	-2.90609500	-0.07800500	-0.17208400
H	-1.72759200	0.06193800	-1.47730500
C	-1.01546600	-1.03410700	0.25925500
H	-1.10298000	-0.97504900	1.36079400
H	-1.47264700	-1.99482700	-0.03330900
C	0.46605300	-1.04482500	-0.14136100
H	0.53930800	-1.08661500	-1.24485900
H	0.94010600	-1.96958900	0.23122100
C	1.25700400	0.17059400	0.36572700
H	1.29669200	0.16807800	1.47121400
H	0.61476800	1.07912000	0.13182000
C	2.60320900	0.34012300	-0.20808600
H	2.80492200	0.05468000	-1.24522200
H	3.35729000	0.94347300	0.30319400

3. TS3



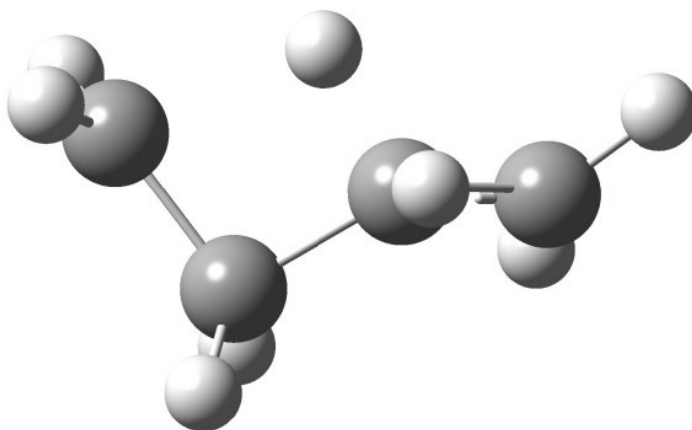
C	-3.41879000	0.88501600	-0.00523100
H	-3.88048300	0.57281100	0.93622500
H	-3.87967100	0.52333500	-0.92923500
C	-2.05282900	1.45595900	-0.01992200
H	-1.88945200	2.06644700	-0.92413200
H	-1.88850000	2.10949300	0.85347800
C	-0.92258000	0.33507900	0.00597100
H	-1.08519500	-0.27902800	0.90809400
H	-1.08571600	-0.31964300	-0.86710700
C	0.45316900	0.90628300	-0.00756200
H	0.80751200	1.40570900	0.90112800
H	0.80240600	1.37341600	-0.93523400
C	1.91283600	-0.88216400	0.01769300
H	1.44408100	-1.23939300	-0.90270800
H	1.44656400	-1.21227100	0.94940300
C	3.20148500	-0.44020700	0.00941100
H	3.73060800	-0.20531500	0.93714500
H	3.72790800	-0.23249900	-0.92631200

4. TS4



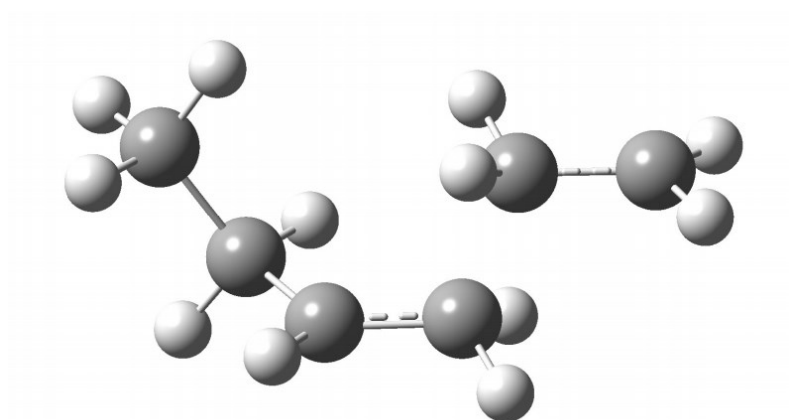
C	-2.20138000	-0.91472100	-0.28767000
H	-1.83638200	-1.94308700	-0.17571900
H	-3.22369500	-0.82480700	-0.67459900
C	-1.71853000	0.13372100	0.71913700
H	-2.51748400	0.76191600	1.14080500
H	-1.14611100	-0.29448300	1.55669300
C	-0.83922800	0.85053500	-0.31940800
H	-1.32240500	-0.18826100	-1.13557300
H	-1.29287900	1.75980200	-0.73721200
C	0.66531500	0.89896800	-0.17087800
H	0.92337500	1.48618400	0.73628700
H	1.09800200	1.45088400	-1.02263100
C	1.35654100	-0.47367800	-0.06858900
H	1.12831400	-1.07189400	-0.97113700
H	0.90079400	-1.04598200	0.77046200
C	2.83083300	-0.38452600	0.12830800
H	3.27629500	0.47951200	0.62964200
H	3.47570200	-1.24011400	-0.08487900

5. TS5



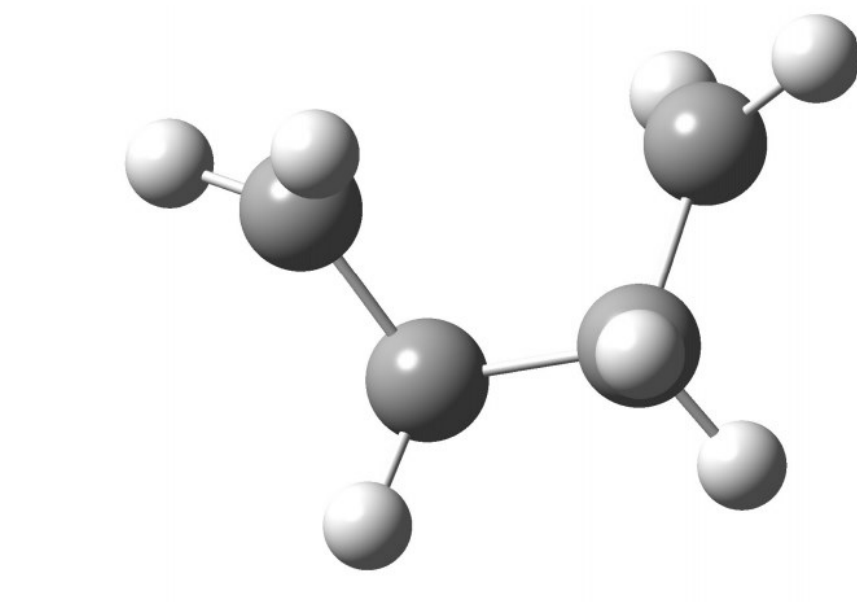
C	-2.24720100	-0.91847000	-0.27997400
H	-1.87448300	-1.94604600	-0.31724200
H	-3.22350800	-0.72394300	-0.73408400
C	-1.67283100	0.05255100	0.72862400
H	-2.42212400	0.66728300	1.25070900
H	-1.05659800	-0.44748100	1.49244700
C	-0.80581400	0.83930700	-0.26343300
H	-1.06612500	0.01013100	-1.16715700
H	-1.33882300	1.69857400	-0.69976900
C	0.60192000	0.98635100	-0.09176700
H	1.13523300	0.41362300	0.67214900
H	1.20357100	1.45291900	-0.87627700

6. TS6



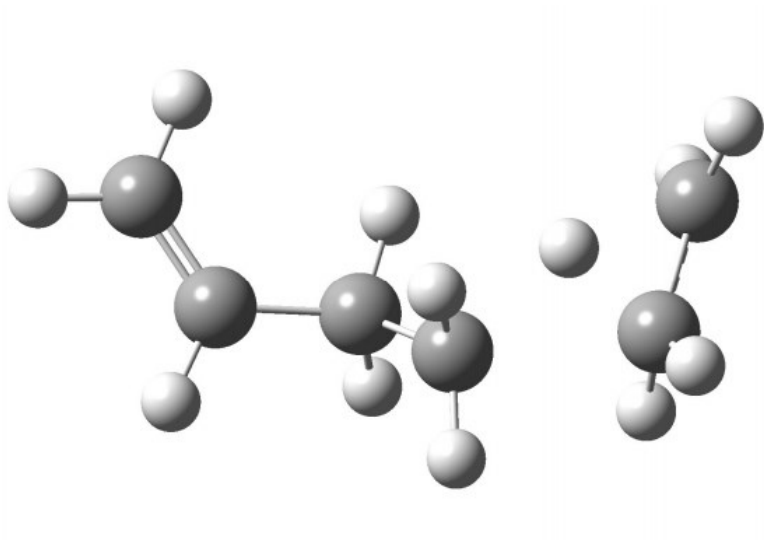
C	-2.41150400	-0.95591600	-0.12209100
H	-1.66924200	-1.76658700	-0.20670800
H	-3.23643600	-1.31646400	0.51465000
C	-1.78318900	0.32617300	0.45739200
H	-2.58881500	1.08040500	0.56966400
H	-1.40882400	0.13199600	1.47841000
C	-0.68460400	0.90390400	-0.38188900
H	-2.82108100	-0.77409700	-1.12994800
H	-0.91233100	1.06504300	-1.44376100
C	0.68443600	0.98493800	0.03897900
H	0.81630600	1.15174600	1.11690600
H	1.29423200	1.68670000	-0.54297700
C	1.53139200	-0.56594400	-0.20480400
H	1.36934500	-0.76237400	-1.27255100
H	0.93417600	-1.25109800	0.41175700
C	2.90885400	-0.47621900	0.17733700
H	3.20167700	-0.53950200	1.22979300
H	3.65604500	-0.07780800	-0.51552500

7. TS7



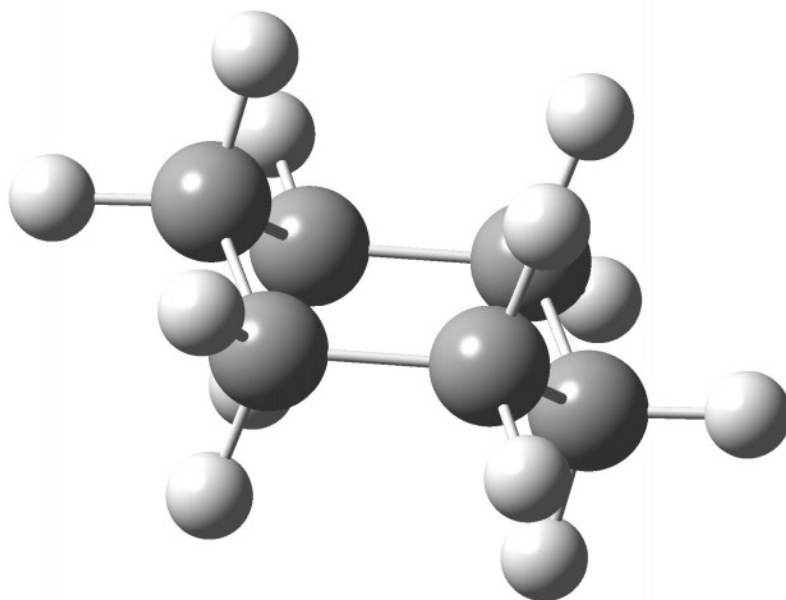
C	-0.61540900	1.24709500	-0.64573800
C	-0.61708200	0.45388800	0.62246600
C	0.61708200	-0.45388800	0.62246600
C	0.61540900	-1.24709500	-0.64573800
H	-1.54431700	1.61328300	-1.09107700
H	0.31876200	1.69516200	-0.99606300
H	-1.53056200	-0.16616000	0.67957300
H	-0.64157100	1.10504100	1.52333900
H	0.64157100	-1.10504100	1.52333900
H	1.53056200	0.16616000	0.67957300
H	-0.31876200	-1.69516200	-0.99606300
H	1.54431700	-1.61328300	-1.09107700

8. TS8



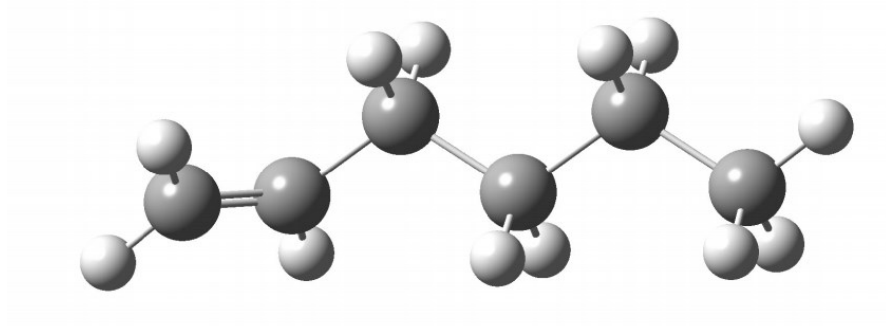
C	2.16598000	-0.53590900	-1.22020000
C	1.49186100	-0.11171900	-0.14605500
H	3.20067200	-0.88089600	-1.14773900
H	1.70442500	-0.55360100	-2.21324400
C	0.05620000	0.34811600	-0.14491300
H	1.98928900	-0.11518600	0.83247300
C	-0.87582800	-0.55699300	0.64418500
H	-0.00113500	1.37331500	0.26861700
H	-0.29150500	0.41796300	-1.19887900
H	-0.77680400	-1.62467200	0.38463600
H	-0.85308900	-0.41655200	1.73385000
C	-2.93860400	0.03354000	0.36266500
C	-3.39266000	0.04273400	-1.01132700
H	-2.74445500	0.99407400	0.84543000
H	-3.30355700	-0.75108800	1.02904600
H	-3.25955600	0.93349700	-1.62272600
H	-2.09529300	-0.33887500	-0.46110300
H	-3.81877800	-0.85883700	-1.44899300

9. Cyclohexane



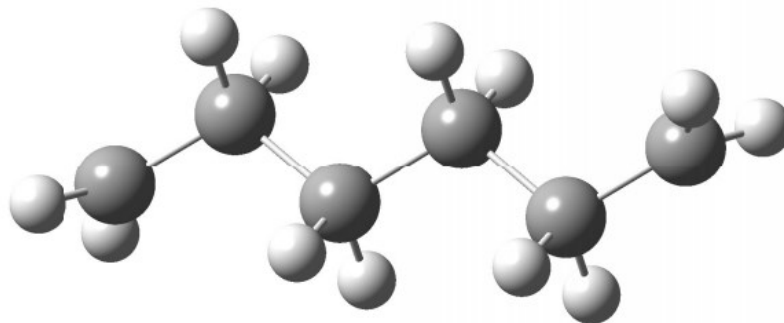
C	-1.26926800	0.73306700	0.22898200
C	0.00000000	1.46620100	-0.22940900
C	1.26926800	0.73306700	0.22898200
C	1.26926800	-0.73306700	-0.22898200
C	0.00000000	-1.46620100	0.22940900
C	-1.26926800	-0.73306700	-0.22898200
H	2.16795900	1.25152300	-0.14673400
H	0.00000000	1.53580600	-1.33414500
H	0.00000000	2.50348600	0.14701000
H	-1.32846400	0.76767700	1.33380500
H	-2.16795900	1.25152300	-0.14673400
H	1.32846400	-0.76767700	-1.33380500
H	2.16795900	-1.25152300	0.14673400
H	0.00000000	-2.50348600	-0.14701000
H	0.00000000	-1.53580600	1.33414500
H	-1.32846400	-0.76767700	-1.33380500
H	-2.16795900	-1.25152300	0.14673400
H	1.32846400	0.76767700	1.33380500

10. 1-hexene



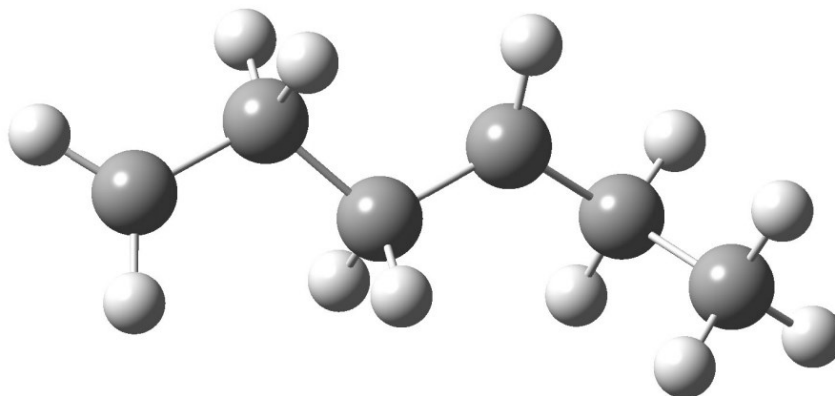
C	-0.55576000	2.23882300	5.34411800
C	-0.70110800	1.10284000	-0.66656600
C	-0.44554200	0.56597400	0.53003400
C	0.31753500	1.23342700	1.64067600
C	-0.51199700	1.41334400	2.92383600
C	0.27418000	2.05513600	4.07161800
H	-0.82433100	-0.44161600	0.74947600
H	-0.34638000	2.10479000	-0.93021300
H	-1.26940000	0.56205000	-1.42779200
H	-1.43141400	2.88475700	5.16097800
H	0.03672200	2.70113800	6.15009400
H	1.21050400	0.62496700	1.88318400
H	0.69119800	2.21401700	1.29665900
H	-1.40195700	2.02775000	2.69444500
H	-0.89832400	0.42931100	3.25057200
H	1.16250000	1.43549000	4.29532100
H	0.66523700	3.03506200	3.74072800
H	-0.93255100	1.27202000	5.71964700

11. 1,6-hexyl diradical



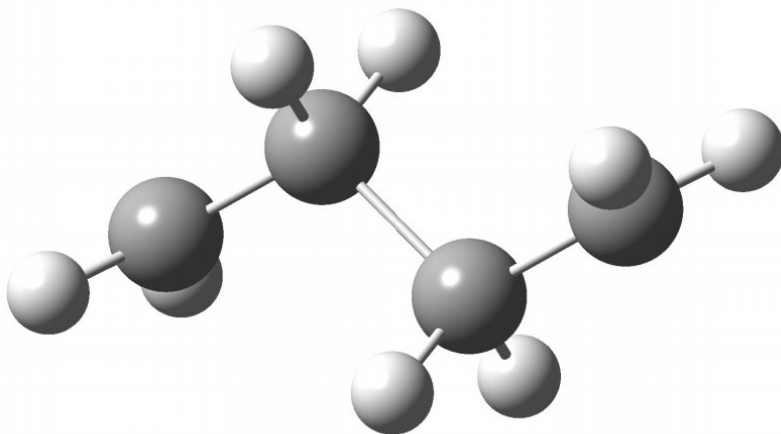
C	-3.19998200	-0.19134000	-0.00000800
H	-3.64123900	-0.54820900	0.93480100
H	-3.64128400	-0.54785400	-0.93493100
C	-1.90263200	0.54502500	0.00010300
H	-1.84092000	1.20368000	-0.88602900
H	-1.84091300	1.20340100	0.88644400
C	-0.66276900	-0.38452200	-0.00004600
H	-0.70780200	-1.04778500	0.88307200
H	-0.70780600	-1.04750900	-0.88337300
C	0.66276900	0.38452200	0.00007100
H	0.70781100	1.04750400	0.88340000
H	0.70779700	1.04779000	-0.88304500
C	1.90263100	-0.54502500	-0.00009200
H	1.84088400	-1.20339300	-0.88644200
H	1.84094900	-1.20368800	0.88603100
C	3.19998200	0.19134000	-0.00002700
H	3.64160100	0.54740300	0.93491700
H	3.64092200	0.54866000	-0.93481500

12. 1,4-hexyl diradical



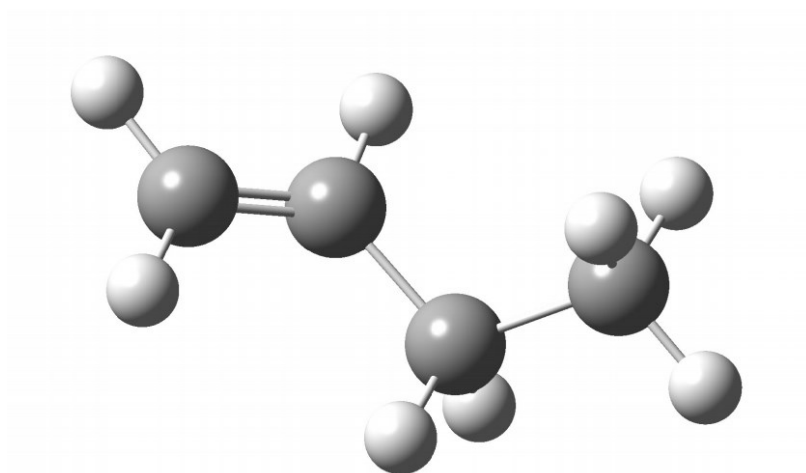
C	-2.25841000	-1.07446500	-0.06655800
H	-1.40021600	-1.76525000	-0.02266700
H	-3.06257900	-1.49317300	0.56164000
C	-1.86344500	0.34135200	0.41232000
H	-2.76706800	0.97821300	0.39261300
H	-1.54460800	0.28135500	1.46931700
C	-0.78067900	0.97345300	-0.40454500
H	-2.61820500	-1.05430700	-1.10862700
H	-1.04876000	1.39595800	-1.38073300
C	0.66603100	0.80126300	-0.08651700
H	0.99876100	-0.24147900	-0.29799500
H	0.83032400	0.92884300	1.00259000
C	1.58449500	1.76030300	-0.86019900
H	1.24830300	2.80406400	-0.70068600
H	1.43205000	1.58493900	-1.94962000
C	3.02287800	1.62301000	-0.50732200
H	3.40545300	0.69990700	-0.06307400
H	3.74553700	2.39104700	-0.79252700

13. 1,4-butyl diradical



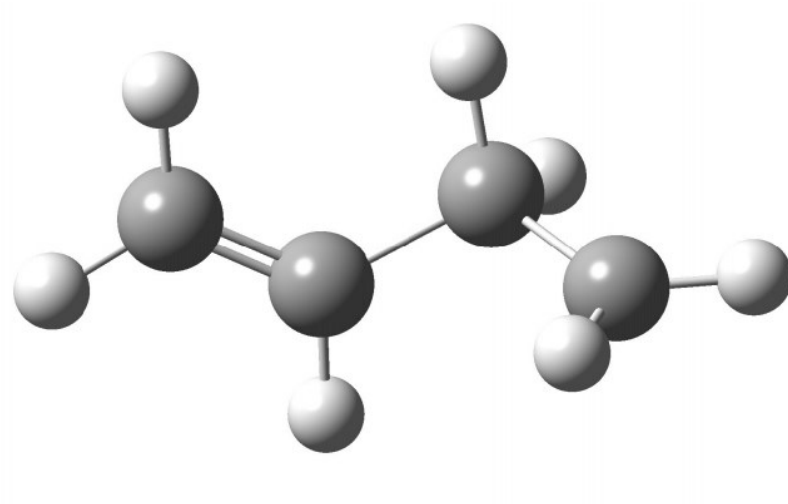
C	1.93414000	0.06934400	0.00016000
H	2.38364600	0.42292200	0.93315400
H	2.38275900	0.42471700	-0.93259000
C	0.59154500	-0.54472200	0.00015000
H	0.44355400	-1.17871400	-0.88993400
H	0.44336300	-1.17822000	0.89052900
C	-0.59171700	0.54496200	-0.00046400
H	-0.44357400	1.17942100	0.88923500
H	-0.44365200	1.17798800	-0.89122300
C	-1.93434400	-0.06905200	0.00012400
H	-2.38392900	-0.42154900	0.93349900
H	-2.38269400	-0.42579700	-0.93224300

14. 1-butene



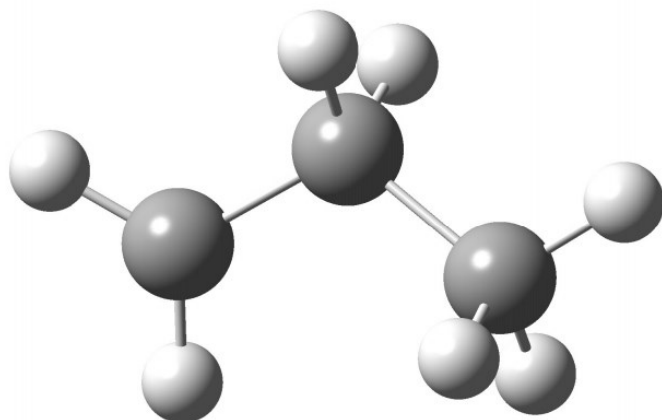
C	-2.35809700	-0.95831800	-0.15099600
H	-1.44023500	-1.53979300	-0.33667800
H	-3.02211800	-1.56224600	0.48843800
C	-2.03285500	0.39136400	0.50749100
H	-2.98177200	0.92037000	0.71859400
H	-1.54141300	0.22809900	1.48210900
C	-1.16528300	1.26850200	-0.35324800
H	-2.86507100	-0.81793800	-1.12083900
H	-1.57766700	1.52596600	-1.33861600
C	0.04241500	1.73227200	-0.01926100
H	0.49492700	1.49956000	0.95047400
H	0.62202300	2.36321400	-0.69811000

15. C₄H₇



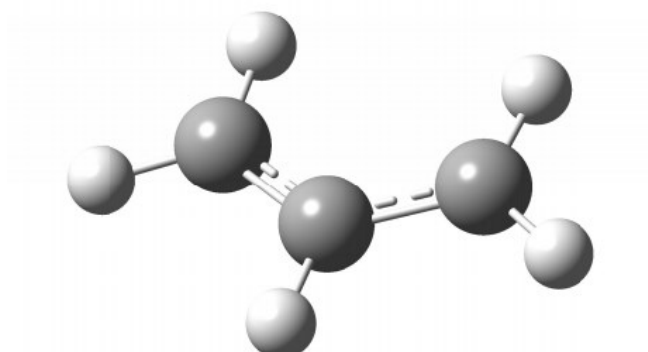
C	-0.21453200	-0.21415600	-0.68256500
C	0.08566300	-0.13605200	0.61674300
C	0.08933100	1.13278000	1.43327600
C	-0.87347300	1.10482600	2.57793300
H	0.34049700	-1.05219000	1.16448400
H	-0.48021000	0.67591600	-1.26268200
H	-0.20266700	-1.16830600	-1.21568700
H	1.10946600	1.32035300	1.81967700
H	-0.13394000	1.98967900	0.76045500
H	-0.67856000	1.67537800	3.48895300
H	-1.85290900	0.63369800	2.46055300

16. C₃H₇



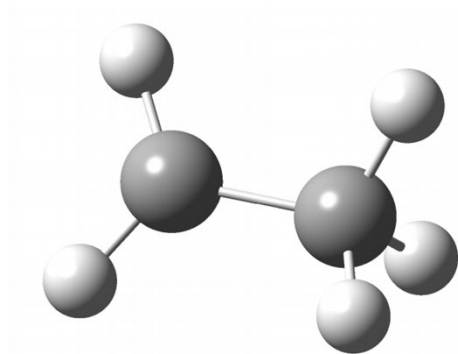
C	-0.10638000	1.62699600	5.56628600
C	-0.75859000	1.42167400	3.12572900
C	0.15141300	2.06155400	4.11885600
H	-1.12749500	1.89408900	5.88502600
H	0.60249600	2.10438900	6.26183400
H	-0.87908100	1.84229500	2.12422300
H	-1.19195700	0.43619000	3.32059400
H	1.21006600	1.83144100	3.85971200
H	0.08067900	3.16300300	4.03556900
H	0.00120800	0.53440100	5.67595700

17. C₃H₅



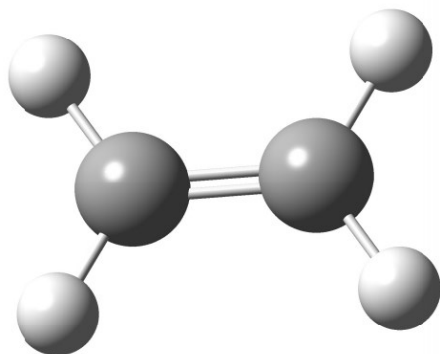
C	-0.95382300	1.36459100	-0.88774800
C	-0.29187400	0.68636000	0.12653900
C	0.65981000	1.24126900	0.97047300
H	-0.54139600	-0.37190600	0.27249300
H	-0.75024600	2.42124300	-1.08429200
H	-1.69379500	0.86632600	-1.51632400
H	1.14255000	0.64877000	1.74950900
H	0.95194800	2.29110600	0.87627700

18. C₂H₅



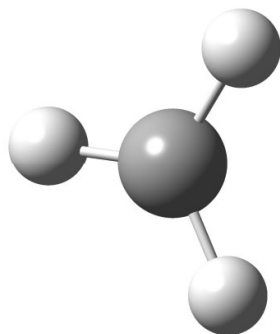
C	-0.25821600	2.45742900	5.81163900
C	0.72728500	2.44197100	4.69566900
H	-1.16406500	3.03380500	5.55617100
H	0.16033600	2.92822300	6.72850500
H	1.46320400	1.63819400	4.60955100
H	0.84144600	3.30713100	4.03724700
H	-0.56937900	1.43954500	6.10334900

19. C₂H₄



C	2.19887800	-1.32980200	-0.19142000
H	1.69208300	-0.87168100	-1.04625000
H	1.65740200	-2.12345600	0.33245000
C	3.41441800	-0.93971300	0.19354300
H	3.92062100	-1.39717800	1.04907800
H	3.95561400	-0.14542700	-0.32964500

20. CH₃



C	-0.93646500	2.30744800	6.07914800
H	-1.69667600	2.87923600	5.54529400
H	-0.07936100	2.81771800	6.52058500
H	-1.03194300	1.22449500	6.16916600