Computed Enthalpies for Multiple Conformations

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Energies and geometries for other compounds reported in this paper will be found in the supporting information for references 15 and 16.

Table S1:

Full citations for Reference 21

Gaussian 98, Revision A.11.3, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2002.

Full citation for Reference 22

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Table S2: Standard state element entropies in J mol^{-1} K^{-1}.

Element	S
C (graphite)	5.686
H_2	130.68

Hydrogen is from from reference 24; graphite is from the JANAF Thermochemical Tables, 2nd edition

Table S3: G3MP2 absolute energies for undecane through eicosane.

decane	-393.510007	-393.566666
undecane	-432.743025	-432.803455
dodecane	-471.975965	-472.040117
tridecane	-511.208931	-511.276809
tetradecane	-550.441897	-550.513496
pentadecane	-589.674864	-589.750187
hexadecane	-628.907830	-628.986894
heptadecane	-668.140799	-668.223553
octadecane	-707.373748	-707.460145
nonadecane	-746.606715	-746.696818
eicosane	-785.839684	-785.933493

Table S3: Corrected, experimental, and corrected enthalpies of formation for all compounds represented by the summary in Manuscript Table 3..

		Enthalpies of Formation		
Molecule	Source	Uncorr	Expt	corrected
methane	CC	-74.8	-74.6	
ethane	CC	-84.4	-84.0	
propane	CC	-104.8	-104.7	
butane	CC	-124.8	-125.8	-124.2
pentane	CC	-147.1	-146.8	-145.9
hexane	CC	-168.3	-166.9	-166.5
heptane	DH	-189.5	-187.7	-187.1
octane	WB	-210.7	-208.4	-207.7
nonane	DH	-232.0	-228.2	-228.4
decane	WB	-253.1	-249.7	-248.9
undecane	WB	-274.6	-270.3	-269.8
dodecane	WB	-295.8	-290.9	-290.4
tridecane	WB	-317.1	-311.5	-311.1
tetradecane	WB	-338.3	-332.1	-331.7
pentadecane	WB	-359.6	-354.8	-352.4
hexadecane	DH	-380.9	-374.8	-373.1
heptadecane	DH	-402.2	-393.9	-393.8
octadecane	DH	-423.5	-414.6	-414.5
nonadecane	DH	-444.7	-435.1	-435.1
eicosane	DH	-466.0	-455.8	-455.8
methylpropane	CC	-134.0	-135.0	-134.0
2-methylbutane	CC	-153.1	-153.7	-152.5
2-methylpentane	CC	-174.4	-174.6	-173.2
2-methylhexane	WB	-195.7	-195.0	-193.9
2-methylheptane	WB	-217.0	-215.5	-214.6
2-methyloctane	GA	-238.3	-235.6	-235.3

2-methylnonane	GA	-259.6	-256.3	-256.0
3-methylpentane	CC	-171.7	-172.0	-170.5
3-methylhexane	DH	-192.9	-191.3	-191.1
3-methylheptane	WB	-214.3	-212.6	-211.9
3-methyloctane	GA	-235.6	-233.4	-232.6
3-methylnonane	GA	-256.9	-254.0	-253.3
4-methylheptane	DH	-214.2	-212.0	-211.8
4-methyloctane	GA	-235.6	-233.4	-232.6
4-methylnonane	GA	-256.9	-254.0	-253.3
3-ethylpentane	WB	-190.0	-189.7	-188.2
3-ethylhexane	GA	-211.7	-210.5	-209.3
3-ethylheptane	GA	-233.2	-231.0	-230.2
2,2-dimethylpropane	CC	-168.7	-167.9	-168.7
2,2-dimethylbutane	CC	-185.2	-184.0	-185.2
2,2-dimethylpentane	WB	-206.4	-206.2	-205.8
2,2-dimethylhexane	DH	-227.9	-224.6	-226.7
2,2-dimethylheptane	DH	-249.3	-246.2	-247.5
2,2-dimethyloctane	DH	-270.6	-266.2	-268.2
2,3-dimethylbutane	CC	-177.1	-175.9	-176.5
2,3-dimethylpentane	DH	-195.7	-198.9	-194.5
2,3-dimethylhexane	DH	-217.2	-213.8	-215.4
2,3-dimethylheptane	AG	-238.6	-235.7	-236.2
2,3-dimethyloctane	AG	-260.0	-256.1	-257.0
2,4-dimethylpentane	WB	-203.1	-202.1	-201.9
2,4-dimethylhexane	DH	-222.0	-219.2	-220.2
2,4-dimethylheptane	AG	-243.3	-240.7	-240.9
2,4-dimethyloctane	AG	-264.7	-261.3	-261.7
2,5-dimethylhexane	DH	-222.7	-222.5	-220.9
2,5-dimethylheptane	AG	-241.3	-240.1	-238.9
2,5-dimethyloctane	AG	-262.6	-261.0	-259.6
2,6-dimethylheptane	AG	-244.7	-242.6	-242.3
2,6-dimethyloctane	AG	-263.4	-260.8	-260.4
2,7-dimethyloctane	DH	-264.4	-264.0	-261.4
3,3-dimethylpentane	WB	-200.5	-201.5	-199.3
3,3-dimethylhexane	DH	-221.7	-220.0	-219.9
3,3-dimethylheptane	AG	-243.3	-241.1	-240.9
3,3-dimethyloctane	AG	-265.0	-266.9	-262.0
3,4-dimethylhexane	DH	-210.8	-212.8	-209.0
3,4-dimethylheptane	AG	-232.4	-232.8	-230.0
3,4-dimethyloctane	AG	-253.9	-253.3	-250.9
3-ethyl-2-methylpentane	DH	-213.0	-211.0	-211.8
3-ethyl-2-methylheptane	AG	-256.5	-253.8	-254.1
3-ethyl-3-methylhexane	AG	-242.3	-235.7	-242.3

3,3-diethylpentane	DH	-238.5	-232.3	-238.5
2,2,3-trimethylbutane	DH	-205.8	-204.5	-205.2
2,2,3-trimethylpentane	DH	-222.7	-220.0	-221.5
2,2,3-trimethylhexane	AG	-244.4	-241.8	-242.6
2,2,3-trimethylheptane	AG	-266.0	-262.4	-263.6
2,3,3-trimethylpentane	DH	-223.8	-216.3	-222.6
2,3,3-trimethylhexane	AG	-241.5	-239.1	-239.7
2,3,3-trimethylheptane	AG	-263.1	-259.7	-260.7
2,2,4-trimethylpentane	DH	-224.7	-224.0	-224.1
2,2,4-trimethylhexane	AG	-242.9	-243.3	-241.7
2,2,4-trimethylheptane	AG	-264.2	-264.1	-262.4
2,3,4-trimethylpentane	WB	-219.5	-217.4	-218.3
2,3,4-trimethylhexane	AG	-239.0	-234.1	-237.2
2,3,4-trimethylheptane	AG	-260.7	-255.1	-258.3
2,2,3,3-tetramethylbutane	WB	-230.4	-225.9	-230.4
2,2,3,3-tetramethylpentane	DH	-243.9	-237.1	-242.7
2,2,4,4-tetramethylpentane	WB	-246.9	-241.5	-245.7

Table S4: Input geometries for undecane through eicosane.

undecane

C,0,0.314817,-6.384452,0.22362
H,0,0.328639,-6.428798,1.309071
H,0,1.344280,-6.428798,-0.120753
H,0,-0.192718,-7.27396,-0.136892
C,0,-0.376909,-5.113235,-0.267728
H,0,-0.405232,-5.115577,-1.3553
H,0,-1.413216,-5.1155770647,0.063677063
C,0,0.306665,-3.8336952221,0.2178327133
H,0,1.343987,-3.8339860366,-0.113298
H,0,0.33558,-3.8339860366,1.3063399267
C,0,-0.379834,-2.5566116319,-0.269806
H,0,-1.417023,-2.5574080189,0.061408
H,0,-0.408628,-2.5574080189,-1.358215
C,0,0.304526,-1.2776239089,0.2163133576
H,0,1.341698,-1.2769306432,-0.114883
H,0,0.333331,-1.2769306432,1.30470072
C,0,-0.382145,-0.0005178065,-0.271447487
H,0,-1.419324,-0.0012400126,0.059749018
H,0,-0.4109525929,-0.0012400126,-1.35984
C,0,0.30222,1.2784460577,0.2146782015
H,0,1.3393967256,1.2791971895,-0.116518
H,0,0.331029,1.2791971894,1.303065527
C,0,-0.384438,2.5555760418,-0.273076
H,0,-1.421627,2.5549280227,0.0581377594
H,0,-0.4132323381,2.554928,-1.361486
C,0,0.2997599991,3.834516,0.2129272437
H,0,1.337079,3.8362524935,-0.1182048916
H,0,0.32867,3.8362524935,1.3014331609
C,0,-0.386118,5.1122017833,-0.274270
H,0,-1.422428,5.113100,0.0571336255
H,0,-0.414444,5.1131005856,-1.361911
C,0,0.303316,6.3852895897,0.215453717
H,0,1.332699417,6.4310501036,-0.128979
H,0,-0.2058197036,7.273428162,-0.146199
H,0,0.317058,6.4310501036,1.3008450098

dodecane

C,0,0.360513,-7.0230102483,0.2560819291
H,0,0.374374,-7.0667175169,1.341556891
H,0,1.39001,-7.0667175169,-0.0882655114
H,0,-0.146288,-7.9131574609,-0.103912
C,0,-0.332246,-5.7526378935,-0.236002
H,0,-0.36056,-5.7556321918,-1.3236400833
H,0,-1.368550,-5.7556321918,0.095401
C,0,0.350276,-4.4722480642,0.2488104129
H,0,1.387598999,-4.471885,-0.0823182779
H,0,0.379195,-4.4718854209,1.3373176004
C,0,-0.337261,-3.1960010809,-0.239565
H,0,-1.37445,-3.1974532646,0.091646324
H,0,-0.366057,-3.1974532646,-1.327974
C,0,0.34604,-1.9161674304,0.2458076128
H,0,1.383222,-1.9148212601,-0.085387
H,0,0.374856,-1.9148212601,1.334195448
C,0,-0.341660,-0.6399027076,-0.242689
H,0,-1.378841,-0.6412838431,0.088502809
H,0,-0.370471,-0.6412838431,-1.331084
C,0,0.341660,0.6399027076,0.2426899132
H,0,1.3788411912,0.6412838431,-0.08850
H,0,0.370471,0.6412838431,1.3310847292
C,0,-0.34604,1.9161674304,-0.2458076128
H,0,-1.383222,1.9148212601,0.0853871086
H,0,-0.374856,1.9148212601,-1.334195448
C,0,0.337261,3.1960010809,0.2395658368
H,0,1.374450862,3.1974532646,-0.09164
H,0,0.366057,3.1974532646,1.3279743814
C,0,-0.350276,4.4722480642,-0.248810
H,0,-1.387598999,4.471885,0.0823182779
H,0,-0.379195,4.4718854209,-1.337317
C,0,0.332246,5.7526378935,0.2360029411
H,0,1.3685509623,5.7556321918,-0.095401
H,0,0.36056,5.7556321918,1.3236400833
C,0,-0.360513,7.0230102483,-0.256081
H,0,-1.39001,7.0667175169,0.0882655114
H,0,0.146288,7.9131574609,0.1039126706
H,0,-0.3743749905,7.0667175169,-1.34155

tridecane

C,0,0.381341,-6.3902944607,0.270876763
H,0,0.409672,-6.3911749822,1.358517672
H,0,1.417652,-6.3911749821,-0.060521365
C,0,-0.304520,-5.1126022387,-0.216308873
H,0,-0.333439,-5.1143561941,-1.304814
H,0,-1.341841,-5.1143561942,0.114818
C,0,0.379662,-3.8336382982,0.269684294
H,0,1.416854,-3.832982,-0.0615223902
H,0,0.408464,-3.8329825625,1.3580938055
C,0,-0.306995,-2.5565020882,-0.218067
H,0,-1.344169,-2.5572611874,0.113124
H,0,-0.335806,-2.5572611873,-1.306454
C,0,0.377356,-1.2775252215,0.2680463738
H,0,1.41454,-1.2768046696,-0.0631421007
H,0,0.406173,-1.2768046697,1.3564425302
C,0,-0.309310,-0.0004213631,-0.219710864
H,0,-1.346494,-0.0011474533,0.111476
H,0,-0.3381276327,-0.001147,-1.308106
C,0,0.375042,1.2785501914,0.2664024432
H,0,1.4122266944,1.279281,-0.0647860384
H,0,0.403859,1.2792818181,1.3547985925
C,0,-0.311624,2.5556593614,-0.221354
H,0,-1.348798,2.554966304,0.1098365519
H,0,-0.340434963,2.554966,-1.3097426529
C,0,0.3727197778,3.83466,0.2647524539
H,0,1.4099115072,3.835459,-0.0664543208
H,0,0.4015215762,3.835459,1.3531618748
C,0,-0.3137780607,5.111759,-0.222884
H,0,-1.3511006587,5.112061,0.1082417734
H,0,-0.3426988377,5.112061,-1.311391161
C,0,0.3697688243,6.391317,0.2626563158
H,0,1.4060770093,6.3936,-0.0687438775
H,0,0.398097049,6.393648,1.3502951594
C,0,-0.321957319,7.662544,-0.2286945718
H,0,-1.3514235981,7.706894,0.1156741673
H,0,0.185563338,8.552076,0.1318104167
H,0,-0.3357872978,7.706894,-1.314143502
C,0,-0.3080808291,-7.663402,-0.218837
H,0,-0.3218292102,-7.70917,-1.304228714
H,0,0.20104,-8.5515496666,0.1428105514
H,0,-1.337465,-7.7091737621,0.125588

tetradecane

C,0,0.351250,-5.7504330697,0.2495021045
H,0,0.380172,-5.7502414093,1.3380091987
H,0,1.388573,-5.7502414093,-0.081622
C,0,-0.336003,-4.4739570061,-0.238671631
H,0,-0.364806,-4.4752479592,-1.327080
H,0,-1.373194,-4.4752479592,0.092533901
C,0,0.347567,-3.1943242089,0.2468863246
H,0,1.384743,-3.1931433563,-0.084301
H,0,0.37638,-3.1931433563,1.3352745353
C,0,-0.339863,-1.9178337024,-0.241413
H,0,-1.377047,-1.919050,0.0897733772
H,0,-0.3686813166,-1.919050,-1.329809
C,0,0.3437153414,-0.6382401216,0.244149
H,0,1.380901,-0.637032,-0.0870354356
H,0,0.372535,-0.637032,1.3325468211
C,0,-0.343715,0.6382401216,-0.244149
H,0,-1.380901,0.637032,0.0870354356
H,0,-0.372535,0.6370323351,-1.332546
C,0,0.339863,1.9178337024,0.2414139146
H,0,1.377047,1.9190504633,-0.0897733772
H,0,0.368681,1.9190504633,1.3298096097
C,0,-0.347567,3.1943242089,-0.246886
H,0,-1.384743,3.1931433563,0.0843017505
H,0,-0.37638,3.1931433563,-1.3352745353
C,0,0.336003,4.4739570061,0.238671631
H,0,1.373194,4.4752479592,-0.092533901
H,0,0.364806,4.4752479592,1.3270805762
C,0,-0.351250,5.7504330697,-0.249502
H,0,-1.388573,5.7502414093,0.0816229854
H,0,-0.380172,5.7502414093,-1.338009
C,0,0.331524,7.0306196616,0.2354904265
H,0,1.3678324125,7.0334350962,-0.095907
H,0,0.359855,7.0334350962,1.3231280788
C,0,-0.360961622,8.3012245693,-0.256400
H,0,-1.390455544,8.34510,0.087947802
H,0,0.146017,9.1912224687,0.10372
H,0,-0.374820,8.345102912,-1.3418685793
C,0,-0.331524,-7.0306196616,-0.235490
H,0,-0.359855,-7.0334350962,-1.323128
H,0,-1.367832,-7.033435,0.0959070898
C,0,0.36096,-8.301224,0.2564003328
H,0,0.374820,-8.34510,1.3418685793
H,0,-0.1460175151,-9.191222,-0.10372
H,0,1.390455544,-8.34510,-0.087947802

pentadecane

C,0,0.376426,-5.1117042629,0.2673851348
H,0,0.405231,-5.1110472527,1.3557955398
H,0,1.413619,-5.1110472527,-0.063818
C,0,-0.310216,-3.8345595697,-0.220354
H,0,-0.339033,-3.8353266501,-1.308743
H,0,-1.347393,-3.8353266501,0.110831
C,0,0.374128,-2.5555712055,0.2657533026
H,0,1.4113159535,-2.554846,-0.065429
H,0,0.4029513873,-2.5548468446,1.354150
C,0,-0.312531,-1.2784643218,-0.221999
H,0,-1.34971,-1.2791946748,0.1091840058
H,0,-0.341354,-1.2791946748,-1.310397
C,0,0.371813,0.0005069129,0.2641084527
H,0,1.4090021132,0.001233589,-0.067074
H,0,0.400636,0.0012335891,1.3525073652
C,0,-0.314848,1.2776089808,-0.223644
H,0,-1.35203,1.2768859852,0.1075387613
H,0,-0.343670,1.2768859852,-1.312042
C,0,0.369496,2.5565850298,0.2624628169
H,0,1.4066835879,2.5573140175,-0.068720
H,0,0.398319,2.5573140175,1.3508601548
C,0,-0.317165,3.8337042259,-0.225290
H,0,-1.3543425718,3.833017,0.1058955034
H,0,-0.3459817866,3.833017,-1.313679
C,0,0.367161,5.1127180356,0.2608040927
H,0,1.4043550422,5.1135143598,-0.070399
H,0,0.395966,5.1135143599,1.3492144081
C,0,-0.319324,6.3898247743,-0.22682432
H,0,-1.356649,6.3901217105,0.1042975169
H,0,-0.348250,6.3901217105,-1.315331
C,0,0.364213,7.6693995246,0.2587103811
H,0,1.400524,7.6717304985,-0.0726843352
H,0,0.392547,7.6717304985,1.3463494714
C,0,-0.32750,8.9406374519,-0.2326325644
H,0,-1.3569695416,8.984990,0.1117325919
H,0,0.180010996,9.830179,0.1278664441
H,0,-0.341335,8.9849907968,-1.318082
C,0,-0.307743,-6.3906796895,-0.218598
H,0,-0.336667,-6.3924302999,-1.307103702
H,0,-1.345066,-6.3924302999,0.112525
C,0,0.378111,-7.6683874719,0.2685826867
H,0,0.406449,-7.6692669547,1.3562238435
H,0,1.4144252649,-7.669266,-0.062809
C,0,-0.3112974038,-8.941508,-0.221122
H,0,0.197825,-9.8296647697,0.1405206813
H,0,-1.340684,-8.9872839843,0.123300
H,0,-0.3250497636,-8.987283,-1.306514

hexadecane

C,0,0.,0.,0.
H,0,0.,0.,1.08879635
H,0,1.0455912969,0.,-0.3036714206
C,0,-0.672511,1.2779786721,-0.504982
H,0,-0.672524,1.277871186,-1.5937571609
H,0,-1.7180853745,1.277871186,-0.201329
C,0,-0.000207,2.5561167053,-0.000156
H,0,1.045376432,2.556173004,-0.303801
H,0,-0.0001849596,2.55617,1.0886263245
C,0,-0.672715,3.8340889836,-0.505136
H,0,-1.7183019731,3.834016,-0.201494
H,0,-0.6727429844,3.834016,-1.593919
C,0,-0.0004219089,5.112236,-0.000316
H,0,1.045165642,5.11230,-0.3039571957
H,0,-0.000393,5.112302993,1.08846729
C,0,-0.6728616199,6.39019,-0.5052456284
H,0,-1.718449,6.3901258567,-0.201605
H,0,-0.672890,6.3901258567,-1.594029726
C,0,-0.000567,7.6683398661,-0.000426
H,0,1.045018,7.6684123181,-0.3040679272
H,0,-0.000540,7.6684123182,1.0883568169
C,0,-0.67307,8.9463121444,-0.5054063222
H,0,-1.718659,8.9462558457,-0.201760
H,0,-0.673098,8.9462558457,-1.594188
C,0,-0.000771,10.2244501776,-0.000579
H,0,1.044801,10.2245576637,-0.304232
H,0,-0.000759,10.224557,1.0881947249
C,0,-0.673283,11.5024288497,-0.50556
H,0,-1.718874,11.5024288498,-0.201891
H,0,-0.673283,11.5024288497,-1.59435
C,0,-0.001168,12.7805137614,-0.000877
H,0,1.044550,12.7815915588,-0.304464
H,0,-0.001051,12.781591,1.0880181008
C,0,-0.672852,14.0590433523,-0.505238
H,0,-1.717564,14.0606082583,-0.201344
H,0,-0.672393,14.0606082583,-1.593252
C,0,-0.672115,-1.2780849117,-0.504685
H,0,-0.672231,-1.2791627091,-1.593580
H,0,-1.717834,-1.2791627091,-0.201097
C,0,-0.000431,-2.5566145026,-0.000323
H,0,-0.000889,-2.558179,1.087690
H,0,1.044280,-2.5581794086,-0.304217
C,0,-0.677518,-3.8288663881,-0.508742
H,0,-0.178750,-4.7175598497,-0.134222
H,0,-1.715681,-3.8739908568,-0.191660
H,0,-0.662568,-3.8739908568,-1.594145
C,0,0.004234,15.3312952378,0.0031797656
H,0,-0.494532,16.2199886994,-0.371340
H,0,-0.010715,15.376419,1.0885830138
H,0,1.042397,15.3764197065,-0.313902

heptadecane
C,0,0.,0.,0.
H,0,0.,0.,1.08879765
H,0,1.045593,0.0000000001,-0.3036688783
C,0,-0.672507,1.2779820924,-0.504981
H,0,-0.672520,1.277874167,-1.5937566194
H,0,-1.718083,1.2778741669,-0.201331
C,0,-0.000209,2.5561244446,-0.000157034
H,0,1.045377,2.5561806706,-0.3037997917
H,0,-0.000185,2.5561806705,1.0886268042
C,0,-0.672712,3.8340998615,-0.505135
H,0,-1.718301,3.8340268525,-0.201496
H,0,-0.6727405073,3.8340268526,-1.59391
C,0,-0.0004238762,5.112250308,-0.000318
H,0,1.0451664186,5.1123165791,-0.303955
H,0,-0.00039447,5.112311.0884676022
C,0,-0.672926,6.3902057888,-0.505295
H,0,-1.718516,6.3901416747,-0.201658
H,0,-0.672956,6.3901416748,-1.594081
C,0,-0.000624,7.6683261876,-0.000468
H,0,1.044965,7.6683881445,-0.304106
H,0,-0.0005949124,7.668388,1.0883170915
C,0,-0.673113,8.9463117193,-0.505436
H,0,-1.7187020263,8.946256,-0.201797
H,0,-0.673141,8.9462565008,-1.594220
C,0,-0.00081,10.2244520545,-0.000608
H,0,1.044776,10.2245240552,-0.304251
H,0,-0.000787,10.224524,1.0881752646
C,0,-0.673309,11.5024294896,-0.505583
H,0,-1.718884,11.5024091908,-0.201933
H,0,-0.673322,11.5024091909,-1.594358
C,0,-0.001002,12.7805765012,-0.000752
H,0,1.044591,12.7807047259,-0.304421
H,0,-0.001002,12.780704,1.0880450761
C,0,-0.67328,14.0584931377,-0.505566
H,0,-1.719006,14.0594549912,-0.201980
H,0,-0.673401,14.0594549913,-1.594461
C,0,-0.672084,-1.2780815012,-0.504663
H,0,-0.672198,-1.2791716088,-1.593558
H,0,-1.717803,-1.2791716088,-0.201077
C,0,-0.000331,-2.5565984893,-0.000248627
H,0,-0.000802,-2.558165,1.0877661629
H,0,1.044379,-2.558165201,-0.3041518261
C,0,-0.677514,-3.8288737555,-0.50874125
H,0,-0.178752,-4.7175729104,-0.134223
H,0,-1.715679,-3.8739958794,-0.191661
H,0,-0.662564,-3.8739958793,-1.594145
C,0,-0.001734,15.3371748601,-0.001302
H,0,-0.0022059277,15.338869,1.086712
H,0,1.0429755669,15.3388696305,-0.30520
C,0,-0.679117,16.6092840111,-0.509944
H,0,-1.717289,16.6542806537,-0.192870
H,0,-0.18049,17.4981054788,-0.135532
H,0,-0.664174,16.6542806538,-1.595354

octadecane
C,0,-0.001359,-0.0288132671,-0.001019
H,0,-0.000770,-0.028932,1.0878030858
H,0,1.044105,-0.0289326785,-0.305219
C,0,-0.673939,1.2493213069,-0.50550722
H,0,-0.674543,1.2493203172,-1.594305
H,0,-1.7193854712,1.2493203174,-0.20132
C,0,-0.001240,2.5273571125,-0.000930
H,0,1.044214,2.5272983788,-0.305100
H,0,-0.0006257656,2.52729,1.0878739446
C,0,-0.673793,3.8055329133,-0.505397
H,0,-1.719251,3.8055516104,-0.201238
H,0,-0.674419,3.8055516102,-1.594202
C,0,-0.001119,5.0835921262,-0.000840
H,0,1.044336,5.0836159311,-0.3050045053
H,0,-0.000499,5.0836159313,1.0879645012
C,0,-0.673770,6.3616853758,-0.505380
H,0,-1.719226,6.361734206,-0.2012044346
H,0,-0.67437,6.3617342058,-1.5941882955
C,0,-0.001261,7.639684,-0.0009463042
H,0,1.0441948849,7.63963,-0.3051225255
H,0,-0.00065,7.6396354722,1.0878613354
C,0,-0.673911,8.9177775518,-0.505486
H,0,-1.719368,8.9177537469,-0.201322
H,0,-0.674532,8.9177537467,-1.594291
C,0,-0.001238,10.1958367647,-0.000929
H,0,1.044219,10.1958180676,-0.305088
H,0,-0.000612,10.195818,1.0878756748
C,0,-0.673791,11.4740125655,-0.505396
H,0,-1.719246,11.4740712992,-0.201226
H,0,-0.674406,11.474071299,-1.594200
C,0,-0.001092,12.7520483711,-0.000819
H,0,1.044353,12.7520493606,-0.304998
H,0,-0.000488,12.752049,1.0879788976
C,0,-0.673672,14.0301829451,-0.505307
H,0,-1.719137,14.0303023565,-0.201107
H,0,-0.674261,14.0303023563,-1.594130
C,0,-0.673918-1.3067598863,-0.505492
H,0,-0.674603,-1.3077980753,-1.594410
H,0,-1.719503,-1.3077980751,-0.201357
C,0,-0.002080,-2.585412669,-0.001560
H,0,-0.001995,-2.5871225895,1.086470
H,0,1.042483,-2.587122,-0.306022
C,0,-0.679691,-3.8575090342,-0.509821
H,0,-0.1808580562,-4.7463787251,-0.13565
H,0,-1.717724,-3.9025015782,-0.192206
H,0,-0.665321,-3.9025015784,-1.595264

C,0,-0.00111,15.3081295643,-0.000834
H,0,-0.000428,15.309167,1.0880838414
H,0,1.044471,15.3091677531,-0.304969
C,0,-0.672951,16.586782347,-0.504766
H,0,-1.717515,16.5884922677,-0.200304
H,0,-0.673036,16.588492,-1.592797
C,0,0.004659,17.8588787122,0.0034946204
H,0,-0.494173,18.7477484031,-0.370669
H,0,-0.009710,17.9038712564,1.088937616
H,0,1.0426926486,17.9038712562,-0.314120

nonadecane

C,0,0.001150,-0.0340824867,0.0008627649
H,0,0.001746,-0.0335121085,1.0896884221
H,0,1.046620,-0.0335121084,-0.303331
C,0,-0.672500,1.2431626508,-0.504427
H,0,-0.673111,1.2424712807,-1.593229
H,0,-1.717951,1.2424712806,-0.200255
C,0,-0.000889,2.5220859868,-0.000666
H,0,1.044570,2.522717512,-0.3048296047
H,0,-0.000265,2.5227175119,1.0881401438
C,0,-0.6745058663,3.7993793691,-0.50593
H,0,-1.719967,3.7987152299,-0.201780
H,0,-0.675139,3.79871523,-1.5947380423
C,0,-0.002917,5.0783311857,-0.002188
H,0,1.042544,5.079008848,-0.3063408235
H,0,-0.002283,5.0790088479,1.0866183032
C,0,-0.676607,6.3555407058,-0.507508
H,0,-1.722072,6.3549190087,-0.203344
H,0,-0.677230,6.3549190088,-1.596321
C,0,-0.005033,7.6343922649,-0.003775
H,0,1.040437,7.6350453824,-0.3079400545
H,0,-0.00440891.6350453823,1.085042
C,0,-0.678650,8.9115641134,-0.509041
H,0,-1.724114,8.9108795852,-0.204876
H,0,-0.679272,8.9108795853,-1.597853
C,0,-0.007002,10.1904535257,-0.00525
H,0,1.038459,10.1910821008,-0.309404
H,0,-0.006368,10.1910821007,1.083554
C,0,-0.6806,11.4677255983,-0.5105286222
H,0,-1.726095,11.4670835021,-0.206376
H,0,-0.681267,11.4670835022,-1.599334
C,0,-0.00905,12.7466986899,-0.006795
H,0,1.036400,12.7473733846,-0.310958
H,0,-0.008436411,12.747373,1.0820116631
C,0,-0.682713,14.0239422245,-0.512088
H,0,-1.728164,14.0233274001,-0.207916
H,0,-0.683324,14.0233274002,-1.60088
C,0,-0.670325,-1.312910806,-0.5027970377
H,0,-0.671017,-1.3146377488,-1.591718
H,0,-1.715914,-1.3146377489,-0.198667
C,0,0.002583,-2.5906765475,0.0019380087
H,0,0.002677,-2.5916978405,1.0899725199
H,0,1.047153,-2.5916978404,-0.302516307
C,0,-0.673958,-3.8636515802,-0.505521
H,0,-0.174385,-4.7518703432,-0.130802
H,0,-1.711955,-3.9093180054,-0.187880
H,0,-0.659553,-3.9093180053,-1.590936
C,0,-0.0111,15.3028671551,-0.0083299357
H,0,-0.010509,15.303602,1.0804956224
H,0,1.034364,15.3036029759,-0.312523
C,0,-0.684624,16.5800160101,-0.513521
H,0,-1.730213,16.5804364855,-0.209393
H,0,-0.685316,16.5804364856,-1.602444
C,0,-0.013757,17.8594596939,-0.010319
H,0,-0.013666,17.861785,1.0777130581
H,0,1.030809,17.861785432,-0.3147757688
C,0,-0.692332,19.1307426226,-0.519304
H,0,-1.730402,19.175130822,-0.201716
H,0,-0.194180,20.0202072216,-0.145650
H,0,-0.677999,19.1751308221,-1.604773

eicosane

C,0,-0.001372,-0.0399129291,-0.001029122
H,0,-0.000771,-0.039599,1.0877991691
H,0,1.044101,-0.039599883,-0.3052197683
C,0,-0.674613,1.2376679411,-0.506012
H,0,-0.675228,1.2372335849,-1.594816
H,0,-1.720067,1.237233585,-0.2018436785
C,0,-0.002608,2.5162687337,-0.001956
H,0,1.042854,2.5166419672,-0.3061158813
H,0,-0.001981,2.5166419673,1.0868529952
C,0,-0.675808,3.793907103,-0.5069091162
H,0,-1.721270,3.7935055464,-0.202759
H,0,-0.676444,3.7935055463,-1.595715
C,0,-0.003848,5.0725868592,-0.002886
H,0,1.041618,5.0729716933,-0.3070222358
H,0,-0.003197,5.0729716934,1.085919584
C,0,-0.677080,6.3501456534,-0.507863
H,0,-1.722542,6.3498263219,-0.203701
H,0,-0.677705,6.3498263218,-1.596672
C,0,-0.004966,7.6286556746,-0.003724
H,0,1.040515,7.6289826131,-0.3078887498
H,0,-0.004337,7.6289826132,1.0851030381
C,0,-0.67812,8.9061332974,-0.5086488751
H,0,-1.723608,8.9058063589,-0.204485
H,0,-0.678755,8.9058063588,-1.597476
C,0,-0.006013,10.1846433186,-0.004510
H,0,1.039449,10.1849626501,-0.308671
H,0,-0.005388,10.184962,1.0842988385
C,0,-0.679245,11.4622021128,-0.509487

H,0,-1.724712,11.4618172787,-0.205351
H,0,-0.679896,11.4618172786,-1.598293
C,0,-0.007285,12.740881869,-0.005464
H,0,1.038177,12.7412834256,-0.309614
H,0,-0.006649,12.741283,1.0833417148
C,0,-0.680484,14.0185202383,-0.510417
H,0,-1.725948,14.0181470048,-0.206257
H,0,-0.681112,14.0181470047,-1.599226
C,0,-0.67324621,-1.318412,-0.504987
H,0,-0.673941,-1.3198809732,-1.593911
H,0,-1.718838,-1.3198809731,-0.200861
C,0,-0.000744,-2.5965135783,-0.000558
H,0,-0.00064,-2.5977916989,1.0874783437
H,0,1.043828,-2.597791699,-0.3050094808
C,0,-0.677689,-3.869149635,-0.5083205815
H,0,-0.178405,-4.7576220893,-0.133818
H,0,-1.715703,-3.9145613947,-0.190691
H,0,-0.663300,-3.9145613948,-1.593748
C,0,-0.00848,15.297121,-0.006361
H,0,-0.007864,15.297555,1.0824428195
H,0,1.036974,15.297555387,-0.3105301522
C,0,-0.68172161,16.5747019011,-0.511344
H,0,-1.727195,16.574388855,-0.207154
H,0,-0.682321,16.5743888549,-1.600172
C,0,-0.009847,17.8532016053,-0.007386
H,0,-0.009151,17.854669,1.0815377065
H,0,1.035745,17.8546699451,-0.311512159
C,0,-0.682349,19.1313025503,-0.511815
H,0,-1.726922,19.132580671,-0.207364
H,0,-0.682447,19.1325806709,-1.599852
C,0,-0.005403,20.403938607,-0.004053
H,0,-0.504688,21.2924110613,-0.378555
H,0,-0.019793,20.449350,1.0813743321
H,0,1.032609,20.449350,-0.3216824231