Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information.

Gas-phase Thermochemistry of Polycyclic Aromatic Hydrocarbons: An Approach Integrating Quantum Chemistry Composite Scheme and Reaction Generator.

Irina Minenkova,[a] Arseniy A. Otlyotov,[b] Luigi Cavallo[c] and Yury Minenkov*[b,d]*

[a] Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninskii pr. 31, Moscow 119071, Russian Federation

[b] N. N. Semenov Federal Research Center for Chemical Physics RAS, Kosygina Street 4, 119991 Moscow, Russian Federation

[c] KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology, Thuwal-23955-6900, Saudi Arabia

[d] Joint Institute for High Temperatures, Russian Academy of Sciences, 13-2 Izhorskaya Street, Moscow 125412, Russian Federation

E-mail: Luigi.Cavallo@kaust.edu.sa

E-mail: Yury.Minenkov@chph.ras.ru

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Automatic generation of reactions

The chemical reactions and corresponding enthalpies of formations were obtained via following steps:

1) Four distinct carbon atom types were introduced depending on hybridization state and bonding situation: sp, sp^2, sp^2 (aromatic), sp^3. For each molecule the quantities of each carbon atom types were counted and specified manually. All hydrogen atoms were considered to be equal.

2) For every species in the present work apart from naphthalene, we initiated the two separate lists termed “pre-reactants” and “pre-products”. The “pre-reactants” list has been populated with a number of variable-size lists. Each such list apart from one species with to-be-calculated enthalpy of formation included up to 4 unique combinations of reference molecules from Table S1 as well as naphthalene and pyrene. In similar fashion, the “pre-product” list has been enlarged with the variable-size lists containing up 5 unique combinations of reference species. We have to stress, that in both “pre-reactants” and “pre-products” cases we considered absolutely all possible combinations up to 4 and 5 reference species. Afterwards, we iterated over all possible combinations of the lists in “pre-reactants” and “pre-products” sets. Each combination that contained unique set of the references (i.e. no species from “pre-product” list was found in “pre-reactant” list and vice versa) was kept as “pre-reaction” and utilized to populate another list termed “pre-reactions”.

3) The initial set of “pre-reactions” was further reduced to ensure that “pre-reactant” and “pre-product” lists in “pre-reaction” list contained identical sets of carbon atom types. For instance, if

sp^3 carbon type was in “pre-product” list and missing in “pre-reactant” list, such “pre-reaction” was ruled out.

4) Each “pre-reaction” in the “pre-reactions” list was subjected to brute force balancing procedure under constraint of maximum number of each individual species being less or equal 15. Each successfully balanced “pre-reaction” was kept as “reaction” only in case of equal numbers of each carbon type on the both sides of the equation. Otherwise, the balanced “pre-reaction” was ruled out.

5) All constructed reactions were written to files corresponding to each molecule and contained following information: a) balanced reaction with all species represented in form of molecular formulas; b) difference between the sums of coefficients of products and that of reactants (ΔN); c) sum of all reaction coefficients (number of species involved, N); d) sum of all reaction coefficients and the absolute value of ΔN, i.e. N + |ΔN|; e) enthalpy of formation of target species; f) reaction correlation energy change; g) reaction enthalpic correction change, $^{\Delta H_{corr}}$; h) sum of f) and g); i) uncertainty (0.95 confidence level) in enthalpy of formation; j) double uncertainty in enthalpy of formation; k) total reaction enthalpy change; l) $^{\Delta E_{AUG}}$; m) $^{\Delta E_{CV}}$; n) $^{\Delta E_{IT}}$; o) balanced chemical reaction with all species represented with their chemical names.

The steps 2) – 5) were completed with help of in-house developed scripts written in the Python programming language.

The scripts and generated data are available at: https://drive.google.com/file/d/11vHRGLzQaKxEpgu82XionvwpbZVBmy82/view?usp=sharing
After download: tar xvf PAH.tar.gz
cd PAH
All scripts are in folder Parallel_9
Example of usage:
python Parallel_9/formation_enthalpie_fpd.py TEMP m1_00_959-02-4-C18H14_ 3
where the last number specifies the maximum number of products in generates reactants. The reference species should be uncommented in the file: Parallel_9/reference.py
After script is completed the file *.all is generated where all generated reactions are provided together with all information in step 5) above.
Afterwards another script is used to get the best reaction:
python Parallel_9/analyze.py m1_00_959-02-4-C18H14_B3LYP-D3.all kj

the last argument indicates the units to be used throughout: kj is kJ mol^{-1} and kcal is kcal/mol. More comments on usage the scripts and information in the files can be obtained from Dr. Yury Minenkov (E-mail: Yury.Minenkov@chph.ras.ru)

Tables mentioned in the main text

Table S1. Reference gas phase formation enthalpies in kJ mol^{-1} used in this work

Molecule	$\Delta_f H_m^\circ(g, 298.15\ K)$
H	217.998±0.000
C	716.883±0.045
CH_4 (methane)	-74.526±0.049[a]
C_2H_6 (ethane)	-84.04±0.13[a]
C_2H_4 (ethylene)	52.32±0.12[a]
C_6H_6 (benzene)	83.12±0.22[a]
C_8H_{10} (Ethylbenzene)	29.73±0.55[a]
C_8H_8 (Phenylethene)	148.34±0.55[a]
C_4H_6 (1,3-Butadiene)	110.90±0.33[a]
C_6H_{12} (Cyclohexane)	-122.94±0.30[a]

C_4H_8 (Isobutene)	-17.01±0.39[a]
C_5H_{12} (neo-Pentane)	-167.39±0.39[a]
C_5H_6 (Cyclopentadiene)	134.15±0.63[a]
C_4H_{10} (iso-Butane)	-134.62±0.30[a]
C_7H_8 (toluene)	50.11±0.33[a]
$C_{10}H_8$ (naphthalene)	149.0±0.4[a,b]
$C_{16}H_{10}$ (pyrene)	224.7±2.9[a,b]

[a] Retrieved from the ATcT database. [b] Obtained from the reaction-based Feller-Peterson-Dixon approach and the ATcT reference values, see Section 3.1

Table S2. Gas phase entropies predicted in this work for a series of polycyclic aromatic compounds

Name	CAS[a]	Formula[b]	$S_m^\circ(g, 298.15\ K)_c$ J (mol K)$^{-1}$
Pyrene	129-00-0	$C_{16}H_{10}$	413.1
Indene	95-13-6	C_9H_8	336.0
Indane	496-11-7	C_9H_{10}	345.6
Acenaphthylene	208-96-8	$C_{12}H_8$	364.8
biphenylene	259-79-0	$C_{12}H_8$	377.0
Acenaphthene	83-32-9	$C_{12}H_{10}$	380.7
Biphenyl	92-52-4	$C_{12}H_{10}$	396.6
1,8-dimethylnaphthalene	569-41-5	$C_{12}H_{12}$	412.1
1,4-Dimethylnaphthalene	571-58-4	$C_{12}H_{12}$	407.9
1,5-Dimethylnaphthalene	571-61-9	$C_{12}H_{12}$	407.9
1,2-Dimethylnaphthalene	573-98-8	$C_{12}H_{12}$	413.0
1,7-Dimethylnaphthalene	575-37-1	$C_{12}H_{12}$	414.6
1,3-Dimethylnaphthalene	575-41-7	$C_{12}H_{12}$	414.6
1,6-Dimethylnaphthalene	575-43-9	$C_{12}H_{12}$	415.1
2,3-dimethylnaphthalene	581-40-8	$C_{12}H_{12}$	410.5
2,6-dimethylnaphthalene	581-42-0	$C_{12}H_{12}$	421.7
2,7-dimethylnaphthalene	582-16-1	$C_{12}H_{12}$	421.7
1H-benz[e]indene	232-54-2	$C_{13}H_{10}$	392.0
1H-benz[f]indene	268-40-6	$C_{13}H_{10}$	392.0
fluorene	86-73-7	$C_{13}H_{10}$	392.5
Diphenylmethane	101-81-5	$C_{13}H_{12}$	444.8
2-phenyltoluene	643-58-3	$C_{13}H_{12}$	431.8
anthracene	120-12-7	$C_{14}H_{10}$	403.3
phenanthrene	85-01-8	$C_{14}H_{10}$	404.2
Pyracene	567-79-3	$C_{14}H_{12}$	402.9
1,4-Dihydrophenanthrene	20244-28-4	$C_{14}H_{12}$	420.5
3,4-Dihydrophenanthrene	38399-10-9	$C_{14}H_{12}$	416.3
1,2-dihydrophenanthrene	56179-83-0	$C_{14}H_{12}$	415.5
9,10-dihydrophenanthrene	776-35-2	$C_{14}H_{12}$	412.5
1,4,5,8-tetramethylnaphthalene	2717-39-7	$C_{14}H_{16}$	466.1
4-methylphenanthrene	832-64-4	$C_{15}H_{12}$	434.3
Acephenanthrylene	201-06-9	$C_{16}H_{10}$	420.9
aceanthrylene	202-03-9	$C_{16}H_{10}$	421.7

fluoranthene	206-44-0	$C_{16}H_{10}$	420.9
1-Phenylnaphthalene	605-02-7	$C_{16}H_{12}$	453.5
4,5-dihydroacephenanthrylene	6232-48-0	$C_{16}H_{12}$	438.1
1,2-Dihydroaceanthrylene	641-48-5	$C_{16}H_{12}$	435.6
2,7-Dimethylphenanthrene	1576-69-8	$C_{16}H_{14}$	482.8
9,10-Dimethylphenanthrene	604-83-1	$C_{16}H_{14}$	474.5
11H-Benzo[a]fluorene	238-84-6	$C_{17}H_{12}$	448.5
11H-Benzo[b]fluorene	243-17-4	$C_{17}H_{12}$	448.9
17H-cyclopenta[a]phenanthrene	219-08-9	$C_{17}H_{12}$	450.6
1H-cyclopenta[l]phenanthrene	235-92-7	$C_{17}H_{12}$	450.6
1H-cyclopent[b]anthracene	259-06-3	$C_{17}H_{12}$	448.9
benzo[ghi]fluoranthene	203-12-3	$C_{18}H_{10}$	435.1
cyclopenta[cd]pyrene	27208-37-3	$C_{18}H_{10}$	431.4
benzo[c]phenanthrene	195-19-7	$C_{18}H_{12}$	455.2
triphenylene	217-59-4	$C_{18}H_{12}$	472.0
chrysene	218-01-9	$C_{18}H_{12}$	463.2
benz[a]anthracene	56-55-3	$C_{18}H_{12}$	460.7
naphthacene	92-24-0	$C_{18}H_{12}$	460.2
1,2-diphenylbenzene	84-15-1	$C_{18}H_{14}$	500.0
1,3-diphenylbenzene	92-06-8	$C_{18}H_{14}$	503.8
1,4-diphenylbenzene	92-94-4	$C_{18}H_{14}$	503.3
5,12-dihydrotetracene	959-02-4	$C_{18}H_{14}$	471.5
3,4,5,6-Tetramethylphenanthrene	"7343-06-8"	$C_{18}H_{18}$	513.0
2,4,5,7-Tetramethylphenanthrene	7396-38-5	$C_{18}H_{18}$	534.7
Triphenylmethane	519-73-3	$C_{19}H_{16}$	550.2
Dicyclopenta[cd,fg]pyrene	173678-72-3	$C_{20}H_{10}$	451.9
corannulene	5821-51-2	$C_{20}H_{10}$	438.1
Perylene	198-55-0	$C_{20}H_{12}$	470.3
Benzo[b]fluoranthene	205-99-2	$C_{20}H_{12}$	477.4
benzo[e]pyrene	192-97-2	$C_{20}H_{12}$	476.6
Benz[j]aceanthrylene	202-33-5	$C_{20}H_{12}$	480.7
benzo[k]fluoranthene	207-08-9	$C_{20}H_{12}$	477.0
benzo[a]pyrene	50-32-8	$C_{20}H_{12}$	471.1
9-Phenylanthracene	602-55-1	$C_{20}H_{14}$	535.1
9,10-dihydro-9,10[1',2']-	477-75-8	$C_{20}H_{14}$	480.3

benzenoanthracene			
1,2-dihydrobenz[j]aceanthrylene cholanthrene	479-23-2	$C_{20}H_{14}$	494.5
3,9-Dimethylbenz[a]anthracene	316-51-8	$C_{20}H_{16}$	538.9
5,6-dimethyl-Chrysene	3697-27-6	$C_{20}H_{16}$	516.3
7,12-Dimethyl-1,2-benzanthracene	56-56-4	$C_{20}H_{16}$	524.7
benzo[ghi]perylene	191-24-2	$C_{22}H_{12}$	483.3
anthanthrene	191-26-4	$C_{22}H_{12}$	480.3
Indeno[1,2,3-cd]fluoranthene	193-43-1	$C_{22}H_{12}$	499.2
pentacene	135-48-8	$C_{22}H_{14}$	517.6
benzo[c]chrysene	194-69-4	$C_{22}H_{14}$	512.5
dibenzo[b,g]phenanthrene	195-06-2	$C_{22}H_{14}$	512.1
benzo[g]chrysene	196-78-1	$C_{22}H_{14}$	513.8
picene	213-46-7	$C_{22}H_{14}$	523.4
benzo[b]chrysene	214-17-5	$C_{22}H_{14}$	520.1
benzo[b]triphenylene	215-58-7	$C_{22}H_{14}$	534.3
pentaphene	222-93-5	$C_{22}H_{14}$	518.8

ibenz[a,j]anthracene	224-41-9	$C_{22}H_{14}$	520.5
benzo[a]naphthacene	226-88-0	$C_{22}H_{14}$	518.4
dibenz[a,h]anthracene	53-70-3	$C_{22}H_{14}$	519.2
benzo[ghi]cyclopenta[cd]perylene	190-88-5	$C_{24}H_{12}$	499.6
coronene	191-07-1	$C_{24}H_{12}$	490.4
Dibenzo(a,i)pyrene	189-55-9	$C_{24}H_{14}$	530.1
Dibenzo[fg,op]naphthacene	192-51-8	$C_{24}H_{14}$	538.5
Naphtho[1,2,3,4-def]chrysene	192-65-4	$C_{24}H_{14}$	538.5
dibenzo[a,h]pyrene	189-64-0	$C_{24}H_{14}$	529.3
dibenzo[de,qr]naphthacene	193-09-9	$C_{24}H_{14}$	535.6
dibenzo[de,mn]naphthacene	214-63-1	$C_{24}H_{14}$	541.4
Tetraphenylene	212-74-8	$C_{24}H_{16}$	556.5
p-Tetraphenyl	135-70-6	$C_{24}H_{18}$	612.5
Triphenylbenzene	612-71-5	$C_{24}H_{18}$	611.3
Tetraphenylmethane	630-76-2	$C_{25}H_{20}$	625.9
Dibenzo[cd,lm]perylene	188-96-5	$C_{26}H_{14}$	543.5
Rubicene	197-61-5	$C_{26}H_{14}$	553.5
[6]helicene	187-83-7	$C_{26}H_{16}$	560.2
dibenzo[g,p]chrysene	191-68-4	$C_{26}H_{16}$	562.7
9,10-Diphenylanthracene	1499-10-1	$C_{26}H_{18}$	633.9
Bifluorenyl	1530-12-7	$C_{26}H_{18}$	591.2
Pentacyclo[18.2.2.2(9,12).0(4,15).0(6,17)]hexacosa-4,6(17),9,11,15,20,22,23,25-nonane	35117-21-6	$C_{26}H_{26}$	601.2
phenanthro[1,10,9,8-opqra]perylene	190-39-6	$C_{28}H_{14}$	561.9
benzo[pqr]naphtho[8,1,2-bcd]perylene	190-71-6	$C_{28}H_{14}$	554.0
9,9'-Bianthracene	1055-23-8	$C_{28}H_{18}$	623.0
9,9'-Biphenanthrene	20532-03-0	$C_{28}H_{18}$	628.4
Dibenzo[bc,ef]coronene	190-31-8	$C_{30}H_{14}$	574.9
Dibenzo[bc,kl]coronene	190-55-6	$C_{30}H_{14}$	559.8
Pyranthrene	191-13-9	$C_{30}H_{16}$	597.1
Ovalene	190-26-1	$C_{32}H_{14}$	570.3
Naphthaceno[2,1,12-qra]naphthacene	189-45-7	$C_{32}H_{18}$	645.2

[a] CAS registry number; [b] Molecular formula; c B3LYP-D3 ideal gas – rigid rotor – harmonic oscillator S^o (298.15 K), see Section 2.1.1

Table S3. Theoretical gas-phase reaction enthalpies, $^{\Delta E_{corr}}$, $^{\Delta\Delta H_{corr}}$, $^{\Delta E_{IT}}$, $^{\Delta E_{CV}}$, $^{\Delta E_{AUG}}$ contributions in kJ mol^{-1} for reactions utilized to derive our recommended enthalpies of formation given in Table 1.

CAS	Reaction (brutto)	Reaction (name)	N	ΔN+N	ΔH_r	ΔE_{corr}	$\Delta\Delta H_{corr}$	ΔE_{AUG}	ΔE_{CV}	ΔE_{IT}
129-00-0	C16H10+C4H8+C2H4→C7H8+C5H6+C10H8	1"Ethylene" + 1"Isobutene" + 1"Pyrene" → 1"Cyclopentadiene" + 1"Naphthalene" + 1"Toluene"	6	6	72.8	15.9	0.8	2.5	-0.4	1.3
95-13-6	C9H8+C2H4→C6H6+C5H6	1"Ethylene" + 1"95-13-6_C9H8" → 1"Cyclopentadiene" + 1"Benzene"	4	4	4.2	3.8	1.3	1.7	0.0	0.0
496-11-7	C9H10+C4H10→C7H8+C6H12	1"496-11-7_C9H10" + 1"iso-Butane" → 1"Cyclohexane" + 1"Toluene"	4	4	3.3	4.6	4.2	0.4	0.0	0.4
208-96-8	C12H8+2C5H12→2C6H12+C10H8	2"neo-Pentane" + 1"208-96-8_C12H8" → 2"Cyclohexane" + 1"Naphthalene"	6	6	-24.3	24.7	17.6	0.8	1.7	2.1
259-79-0	C12H8+C10H8→C6H6+C16H10	1"Naphthalene" + 1"259-79-0-C12H8" → 1"Pyrene" + 1"Benzene"	4	4	-260.7	-1.3	4.6	-2.1	-0.8	0.0
83-32-9	C12H10+C4H10→C6H12+C10H8	1"iso-Butane" + 1"83-32-9-C12H10" → 1"Cyclohexane" + 1"Naphthalene"	4	4	5.4	9.6	5.9	1.3	0.4	0.4
92-52-4	C12H10+C2H4→C6H6+C8H8	1"Ethylene" + 1"92-52-4-C12H10" → 1"Phenylethene" + 1"Benzene"	4	4	2.1	10.5	0.8	1.7	0.0	0.0
569-41-5	C12H12+C2H6→C4H10+C10H8	1"Ethane" + 1"569-41-5-C12H12" → 1"iso-Butane" + 1"Naphthalene"	4	4	-10.0	21.8	-0.4	2.1	0.0	0.4
571-58-4	C12H12+C2H4→C4H8+C10H8	1"571-58-4-C12H12" + 1"Ethylene" → 1"Isobutene" + 1"Naphthalene"	4	4	-4.2	17.2	0.4	2.1	-0.4	0.4
571-61-9	C12H12+C2H4→C4H8+C10H8	1"571-61-9-C12H12" + 1"Ethylene" → 1"Isobutene" + 1"Naphthalene"	4	4	-3.8	17.6	0.4	2.5	-0.4	0.4
573-98-8		1"573-98-8-C12H12" +	4	4	6.7	14.6	0.8	1.7	0.0	0.4

	C12H12+C6H6→C8H10+C10H8	1"Benzene" → 1"Ethylbenzene" + 1"Naphthalene"								
575-37-1	C12H12+C2H4→C4H8+C10H8	1"Ethylene" + 1"575-37-1-C12H12" → 1"Isobutene" + 1"Naphthalene"	4	4	-2.1	13.0	0.8	1.7	-0.4	0.0
575-41-7	C12H12+C2H4→C4H8+C10H8	1"575-41-7-C12H12" + 1"Ethylene" → 1"Isobutene" + 1"Naphthalene"	4	4	-2.1	12.1	0.8	1.7	-0.4	0.0
575-43-9	C12H12+C2H4→C4H8+C10H8	1"575-43-9-C12H12" + 1"Ethylene" → 1"Isobutene" + 1"Naphthalene"	4	4	-2.5	12.1	0.8	1.7	-0.4	0.0
581-40-8	C12H12+C2H4→C4H8+C10H8	1"Ethylene" + 1"581-40-8-C12H12" → 1"Isobutene" + 1"Naphthalene"	4	4	-1.3	13.0	1.3	1.7	0.0	0.0
581-42-0	C12H12+C2H4→C4H8+C10H8	1"Ethylene" + 1"581-42-0-C12H12" → 1"Isobutene" + 1"Naphthalene"	4	4	-1.7	7.9	1.3	1.3	0.0	0.0
582-16-1	C12H12+C2H4→C4H8+C10H8	1"582-16-1-C12H12" + 1"Ethylene" → 1"Isobutene" + 1"Naphthalene"	4	4	-1.3	7.9	1.7	1.3	0.0	0.0
232-54-2	C13H10+C2H4→C5H6+C10H8	1"232-54-2-C13H10" + 1"Ethylene" → 1"Cyclopentadiene" + 1"Naphthalene"	4	4	6.3	8.4	1.3	2.1	-0.4	0.0
268-40-6	C13H10+C2H4→C5H6+C10H8	1"268-40-6-C13H10" + 1"Ethylene" → 1"Cyclopentadiene" + 1"Naphthalene"	4	4	6.3	3.3	0.8	1.7	0.0	0.0
86-73-7	C13H10+C10H8→C7H8+C16H10	1"86-73-7-C13H10" + 1"Naphthalene" → 1"Pyrene" + 1"Toluene"	4	4	-58.2	-11.3	0.8	-0.4	0.0	-1.3
101-81-5	C13H12+C2H6→C7H8+C8H10	1"Ethane" + 1"101-81-5_C13H12" → 1"Ethylbenzene" + 1"Toluene"	4	4	0.8	7.5	-0.4	0.8	-0.4	0.0
643-58-3	C13H12+C2H4→C7H8+C8H8	1"Ethylene" + 1"643-58-3-C13H12" → 1"Phenylethene" + 1"Toluene"	4	4	-2.5	17.2	0.8	2.1	0.0	0.0
120-12-7	C14H10+C6H6→2C1	1"120-12-7-C14H10" + 1"Benzene" → 2"Naphthalene"	4	4	-14.6	6.7	0.0	0.8	0.0	0.4

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85-01-8	C14H10+C6H6→2C10H8	1"85-01-8-C14H10" + 1"Benzene" → 2"Naphthalene"	4	4	9.6	2.9	-0.4	0.8	0.0	-0.4
567-79	C14H12+C8H10→C6H12+C16H10	1"Ethylbenzene" + 1"567-79-3_C14H12" → 1"Cyclohexane" + 1"Pyrene"	4	4	-120.9	-3.3	5.0	0.4	0.4	-0.8
20244-28-4	C14H12+C6H6→C4H8+C16H10	1"Benzene" + 1"20244-28-4-C14H12" → 1"Isobutene" + 1"Pyrene"	4	4	-74.1	-12.1	-2.9	0.0	0.4	-1.7
38399-10-9	C14H12+C6H6→C4H8+C16H10	1"38399-10-9-C14H12" + 1"Benzene" → 1"Isobutene" + 1"Pyrene"	4	4	-69.5	-7.5	-3.8	-0.4	0.0	-1.3
56179-83-0	C14H12+C6H6→C4H8+C16H10	1"56179-83-0-C14H12" + 1"Benzene" → 1"Isobutene" + 1"Pyrene"	4	4	-70.7	-7.9	-3.8	-0.8	0.0	-1.3
776-35-2	C14H12+C10H8→C8H10+C16H10	1"776-35-2-C14H12" + 1"Naphthalene" → 1"Ethylbenzene" + 1"Pyrene"	4	4	-44.8	-3.3	-0.8	0.0	0.4	-1.3
2717-39-7	C14H16+CH4→C10H8+C5H12	1"Methane" + 1"2717-39-7-C14H16" → 1"neo-Pentane" + 1"Naphthalene"	4	4	-24.3	47.3	0.4	4.2	0.0	0.8
832-64-4	C15H12+C7H8+C2H6→C4H10+2C10H8	1"832-64-4-C15H12" + 1"Ethane" + 1"Toluene" → 1"iso-Butane" + 2"Naphthalene"	6	6	-0.8	20.5	-0.8	2.5	0.0	0.0
201-06-9	C16H10+2C6H6→C16H10+C10H8+C2H4	1"201-06-9-C16H10" + 2"Benzene" → 1"Ethylene" + 1"Pyrene" + 1"Naphthalene"	6	6	-49.8	-8.8	-1.7	-1.3	0.0	-0.8
202-03-9	C16H10+2C6H6→C16H10+C10H8+C2H4	1"202-03-9-C16H10" + 2"Benzene" → 1"Ethylene" + 1"Pyrene" + 1"Naphthalene"	6	6	-79.1	0.0	-0.8	-0.4	0.0	0.0
206-44-0	C16H10→C16H10	1"Fluoranthene" → 1"Pyrene"	2	2	-59.0	-2.9	1.7	-0.4	-0.4	-0.4
605-02-7	C16H12+C2H4→C8H8+C10H8	1"Ethylene" + 1"605-02-7_C16H12" → 1"Phenylethene" + 1"Naphthalene"	4	4	-2.1	18.4	0.4	2.5	-0.4	0.0
6232-48-0	C16H12+C4H10+C6H6→C6H12+2C10H8	1"iso-Butane" + 1"6232-48-0-C16H12" + 1"Benzene" → 1"Cyclohexane" +	6	6	19.7	11.7	5.0	2.1	0.4	0.4

		2"Naphthalene"								
641-48-5	C16H12+C4H10+C6H6→C6H12+2C10H8	1"iso-Butane" + 1"641-48-5-C16H12" + 1"Benzene" → 1"Cyclohexane" + 2"Naphthalene"	6	6	-5.9	18.4	5.9	2.5	0.0	0.8
1576-69-8	C16H14+C6H6+C2H4→C4H8+2C10H8	1"Ethylene" + 1"1576-69-8-C16H14" + 1"Benzene" → 1"Isobutene" + 2"Naphthalene"	6	6	7.5	10.9	0.8	1.7	-0.4	0.0
604-83-1	C16H14+2C6H6→C8H10+2C10H8	1"604-83-1-C16H14" + 2"Benzene" → 1"Ethylbenzene" + 2"Naphthalene"	6	6	7.1	24.3	-0.8	2.1	-0.4	0.0
238-84-6	C17H12+CH4→C16H10+C2H6	1"Methane" + 1"238-84-6_C17H12" → 1"Ethane" + 1"Pyrene"	4	4	-33.1	3.8	3.8	1.3	0.0	-0.8
243-17-4	C17H12+CH4→C16H10+C2H6	1"Methane" + 1"243-17-4_C17H12" → 1"Ethane" + 1"Pyrene"	4	4	-34.3	1.3	3.8	0.8	0.4	-0.8
219-08-9	C17H12+C7H8+C6H6→C4H8+C16H10+C10H8	1"Benzene" + 1"219-08-9-C17H12" + 1"Toluene" → 1"Isobutene" + 1"Pyrene" + 1"Naphthalene"	6	6	-58.6	-4.2	0.0	0.0	0.0	-1.3
235-92-7	C17H12+C7H8+C6H6→C4H8+C16H10+C10H8	1"Benzene" + 1"235-92-7-C17H12" + 1"Toluene" → 1"Isobutene" + 1"Pyrene" + 1"Naphthalene"	6	6	-57.3	-0.4	0.0	0.4	0.0	-1.3
259-06-3	C17H12+C7H8+C6H6→C4H8+C16H10+C10H8	1"259-06-3-C17H12" + 1"Benzene" + 1"Toluene" → 1"Isobutene" + 1"Pyrene" + 1"Naphthalene"	6	6	-80.8	-6.7	0.4	-0.4	0.4	-0.8
203-12-3	C18H10+2C10H8→C6H6+2C16H10	1"203-12-3-C18H10" + 2"Naphthalene" → 2"Pyrene" + 1"Benzene"	6	6	-126.4	0.8	2.1	-0.4	-0.4	-0.4
27208-37-3	C18H10+C4H8+C4H10→C5H6+C16H10+C5H12	1"iso-Butane" + 1"27208-37-3-C18H10" + 1"Isobutene" → 1"Cyclopentadiene" + 1"neo-Pentane" + 1"Pyrene"	6	6	0.0	1.3	-0.4	0.8	-0.4	0.8
195-19-7	C18H12+CH4+C10H8→C7H8+C6H6+C16H	1"Methane" + 1"195-19-7-C18H12" + 1"Naphthalene" → 1"Benzene" + 1"Pyrene" +	6	6	-3.8	31.4	1.7	2.5	0.0	0.8

	10	1"Toluene"								
217-59-4	C18H12+C4H6+C10H8→C16H10+2C8H8	1"1,3-Butadiene" + 1"217-59-4-C18H12" + 1"Naphthalene" → 1"Pyrene" + 2"Phenylethene"	6	6	-1.7	7.5	0.4	0.4	-0.4	0.0
218-01-9	C18H12+C4H6+C10H8→C16H10+2C8H8	1"218-01-9-C18H12" + 1"1,3-Butadiene" + 1"Naphthalene" → 1"Pyrene" + 2"Phenylethene"	6	6	-2.5	4.6	0.0	0.8	0.0	0.0
56-55-3	C18H12+2C6H6→3C10H8	1"56-55-3-C18H12" + 2"Benzene" → 3"Naphthalene"	6	6	1.3	7.5	-0.8	1.3	-0.4	0.0
92-24-0	C18H12+CH4+C10H8→C7H8+C6H6+C16H10	1"Methane" + 1"92-24-0-C18H12" + 1"Naphthalene" → 1"Benzene" + 1"Pyrene" + 1"Toluene"	6	6	-31.8	28.9	4.2	1.3	0.0	1.7
84-15-1	C18H14+C2H6+C2H4→2C7H8+C8H8	1"Ethylene" + 1"Ethane" + 1"84-15-1-C18H14" → 1"Phenylethene" + 2"Toluene"	6	6	7.1	35.1	0.0	4.6	-0.4	0.8
92-06-8	C18H14+C2H6+C2H4→2C7H8+C8H8	1"Ethylene" + 1"Ethane" + 1"92-06-8-C18H14" → 1"Phenylethene" + 2"Toluene"	6	6	11.3	20.1	-0.4	2.5	-0.4	0.4
92-94-4	C18H14+C2H6+C2H4→2C7H8+C8H8	1"Ethylene" + 1"92-94-4-C18H14" + 1"Ethane" → 1"Phenylethene" + 2"Toluene"	6	6	10.5	19.2	-0.4	2.1	-0.4	0.4
959-02-4	C18H14+C2H6→C4H10+C16H10	1"959-02-4-C18H14" + 1"Ethane" → 1"iso-Butane" + 1"Pyrene"	4	4	-47.7	-1.3	-0.4	1.3	1.3	-1.3
7343-06-8	C18H18+C6H6+CH4→2C10H8+C5H12	1"Methane" + 1"7343-06-8-C18H18" + 1"Benzene" → 1"neo-Pentane" + 2"Naphthalene"	6	6	-7.9	61.9	2.5	5.9	0.4	0.8
7396-38-5	C18H18+C6H6+CH4→2C10H8+C5H12	1"Methane" + 1"7396-38-5-C18H18" + 1"Benzene" → 1"neo-Pentane" + 2"Naphthalene"	6	6	-5.4	46.4	2.9	4.2	0.4	0.8
519-73-3	C19H16+CH4+C2H4→2C7H8+C8H8	1"Methane" + 1"Ethylene" + 1"519-73-3_C19H16" → 1"Phenylethene" + 2"Toluene"	6	6	4.2	45.6	1.3	6.3	-0.4	0.4
173678-		1"173678-72-3-C20H10" +	6	6	-1.7	19.7	-0.4	1.7	-1.3	2.1

72-3	C20H10+C4H6+C2H6→2C5H6+C16H10	1"Ethane" + 1"1,3-Butadiene" → 2"Cyclopentadiene" + 1"Pyrene"								
5821-51-2	C20H10+C7H8+C5H12→C6H12+C16H10+C10H8	1"5821-51-2-C20H10" + 1"neo-Pentane" + 1"Toluene" → 1"Cyclohexane" + 1"Pyrene" + 1"Naphthalene"	6	6	-111.3	59.8	9.6	3.8	1.3	1.3
198-55-0	C20H12+C6H6→C16H10+C10H8	1"198-55-0_C20H12" + 1"Benzene" → 1"Pyrene" + 1"Naphthalene"	4	4	-23.8	14.2	0.0	0.8	-0.8	0.0
205-99-2	C20H12+C6H6→C16H10+C10H8	1"205-99-2_C20H12" + 1"Benzene" → 1"Pyrene" + 1"Naphthalene"	4	4	-43.1	-1.3	0.8	0.4	-0.8	-0.4
192-97-2	C20H12+C6H6→C16H10+C10H8	1"192-97-2-C20H12" + 1"Benzene" → 1"Pyrene" + 1"Naphthalene"	4	4	8.8	7.9	-0.4	0.8	-0.4	-0.4
202-33-5	C20H12+2C10H8→2C16H10+C8H8	1"202-33-5-C20H12" + 2"Naphthalene" → 2"Pyrene" + 1"Phenylethene"	6	6	-88.3	5.0	0.8	-0.4	0.0	0.0
207-08-9	C20H12+C6H6→C16H10+C10H8	1"207-08-9-C20H12" + 1"Benzene" → 1"Pyrene" + 1"Naphthalene"	4	4	-54.4	-1.3	1.3	0.0	-0.4	-0.4
50-32-8	C20H12+C6H6→C16H10+C10H8	1"Benzene" + 1"50-32-8-C20H12" → 1"Pyrene" + 1"Naphthalene"	4	4	-3.3	7.9	-0.4	1.3	0.0	0.0
602-55-1	C20H14+2C2H6→C4H10+2C10H8	1"602-55-1_C20H14" + 2"Ethane" → 1"iso-Butane" + 2"Naphthalene"	6	6	3.3	34.3	0.0	4.6	-0.4	1.3
477-75-8	C20H14+2C10H8→C8H10+2C16H10	1"477-75-8-C20H14" + 2"Naphthalene" → 1"Ethylbenzene" + 2"Pyrene"	6	6	-140.2	7.9	1.3	0.8	0.4	-2.1
479-23-2	C20H14+2C10H8→C8H10+2C16H10	2"Naphthalene" + 1"479-23-2-C20H14" → 1"Ethylbenzene" + 2"Pyrene"	6	6	-100.8	-3.3	1.3	0.0	0.0	-0.8
316-51-8	C20H16+C10H8+C2H4→C8H10+C16H10+C8H8	1"Ethylene" + 1"316-51-8-C20H16" + 1"Naphthalene" → 1"Ethylbenzene" + 1"Pyrene" + 1"Phenylethene"	6	6	-6.7	14.2	3.8	1.3	0.4	0.4
3697-27-6	C20H16+CH4+C10H8	1"Methane" + 1"3697-27-6-C20H16" + 1"Naphthalene" →	6	6	-10.0	54.0	2.1	3.8	-0.4	1.3

	→C7H8+C8H10+C16H10	1"Ethylbenzene" + 1"Pyrene" + 1"Toluene"								
56-56-4	C20H16+C10H8+C2H4→C8H10+C16H10+C8H8	1"Ethylene" + 1"Naphthalene" + 1"56-56-4-C20H16" → 1"Ethylbenzene" + 1"Pyrene" + 1"Phenylethene"	6	6	-6.3	19.2	3.3	1.7	0.4	0.4
191-24-2	C22H12+C10H8→2C16H10	1"191-24-2-C22H12" + 1"Naphthalene" → 2"Pyrene"	4	4	6.3	2.5	-0.4	0.0	-0.4	-0.4
191-26-4	C22H12+C10H8→2C16H10	1"191-26-4-C22H12" + 1"Naphthalene" → 2"Pyrene"	4	4	-20.9	8.4	0.4	0.4	0.4	0.8
193-43-1	C22H12+C10H8→2C16H10	1"193-43-1-C22H12" + 1"Naphthalene" → 2"Pyrene"	4	4	-159.4	-2.1	2.9	-1.7	-0.8	-0.4
135-48-8	C22H14+CH4→C7H8+C16H10	1"Methane" + 1"135-48-8-C22H14" → 1"Pyrene" + 1"Toluene"	4	4	-56.9	41.8	4.6	1.7	0.0	2.5
194-69-4	C22H14+CH4→C7H8+C16H10	1"Methane" + 1"194-69-4-C22H14" → 1"Pyrene" + 1"Toluene"	4	4	0.8	36.8	1.3	3.3	-0.4	0.8
195-06-2	C22H14+CH4→C7H8+C16H10	1"Methane" + 1"195-06-2-C22H14" → 1"Pyrene" + 1"Toluene"	4	4	-12.6	37.7	2.1	2.9	0.0	1.3
196-78-1	C22H14+CH4→C7H8+C16H10	1"Methane" + 1"196-78-1-C22H14" → 1"Pyrene" + 1"Toluene"	4	4	0.0	42.3	0.4	3.3	-0.4	0.8
213-46-7	C22H14+C2H4→C16H10+C8H8	1"Ethylene" + 1"213-46-7-C22H14" → 1"Pyrene" + 1"Phenylethene"	4	4	-4.2	17.2	0.8	2.5	-0.8	0.0
214-17-5	C22H14+C2H6→C8H10+C16H10	1"Ethane" + 1"214-17-5-C22H14" → 1"Ethylbenzene" + 1"Pyrene"	4	4	-3.3	18.8	1.3	1.7	-0.4	0.8
215-58-7	C22H14+C2H6→C8H10+C16H10	1"215-58-7-C22H14" + 1"Ethane" → 1"Ethylbenzene" + 1"Pyrene"	4	4	3.8	21.8	0.8	1.7	-0.8	0.4
222-93-5	C22H14+CH4→C7H8+C16H10	1"Methane" + 1"222-93-5-C22H14" → 1"Pyrene" + 1"Toluene"	4	4	2.5	24.3	2.9	2.1	0.0	0.8
224-41-9		1"Ethylene" + 1"224-41-9-	4	4	-7.1	14.6	1.3	1.7	-0.4	0.0

	C22H14+C2H4→C16H10+C8H8	C22H14" → 1"Pyrene" + 1"Phenylethene"								
226-88-0	C22H14+CH4→C7H8+C16H10	1"226-88-0-C22H14" + 1"Methane" → 1"Pyrene" + 1"Toluene"	4	4	-12.1	28.5	3.3	1.7	-0.4	1.3
53-70-3	C22H14+C2H4→C16H10+C8H8	1"Ethylene" + 1"53-70-3-C22H14" → 1"Pyrene" + 1"Phenylethene"	4	4	-7.1	13.4	0.8	1.7	-0.4	0.0
190-88-5	C24H12+2CH4+C10H8→C4H8+2C16H10	2"Methane" + 1"190-88-5-C24H12" + 1"Naphthalene" → 1"Isobutene" + 2"Pyrene"	7	8	24.7	18.4	10.0	0.4	-0.4	1.3
191-07-1	C24H12+C7H8+2C6H6→CH4+2C16H10+C10H8	1"191-07-1-C24H12" + 2"Benzene" + 1"Toluene" → 1"Methane" + 2"Pyrene" + 1"Naphthalene"	8	8	15.9	-16.3	-3.8	-0.8	0.4	-1.3
189-55-9_	C24H14+C7H8+C8H10+C2H6→C16H10+2C10H8+C5H12	1"189-55-9_C24H14" + 1"Ethylbenzene" + 1"Ethane" + 1"Toluene" → 1"neo-Pentane" + 1"Pyrene" + 2"Naphthalene"	8	8	-0.4	8.4	-1.7	2.5	-0.8	0.4
192-51-8	C24H14+C4H8+2C10H8→C8H10+2C16H10+C8H8	1"Isobutene" + 1"192-51-8_C24H14" + 2"Naphthalene" → 1"Ethylbenzene" + 2"Pyrene" + 1"Phenylethene"	8	8	7.9	17.6	1.3	1.3	-0.4	-0.4
192-65-4	C24H14+C4H8+2C10H8→C8H10+2C16H10+C8H8	1"192-65-4_C24H14" + 1"Isobutene" + 2"Naphthalene" → 1"Ethylbenzene" + 2"Pyrene" + 1"Phenylethene"	8	8	0.0	15.5	2.1	0.8	-0.4	0.0
189-64-0	C24H14+CH4+2C8H10→C16H10+2C10H8+C5H12	1"Methane" + 1"189-64-0-C24H14" + 2"Ethylbenzene" → 1"neo-Pentane" + 1"Pyrene" + 2"Naphthalene"	8	8	1.3	23.4	-0.4	3.8	-0.4	0.8
193-09-9	C24H14+C4H8+2C10H8→C8H10+2C16H10+C8H8	1"Isobutene" + 2"Naphthalene" + 1"193-09-9-C24H14" → 1"Ethylbenzene" + 2"Pyrene" + 1"Phenylethene"	8	8	-2.9	12.1	2.1	0.4	0.0	0.0
214-63-1	C24H14+CH4+2C8H10→C16H10+2C10H8+C5H12	1"Methane" + 2"Ethylbenzene" + 1"214-63-1-C24H14" → 1"neo-Pentane" + 1"Pyrene" + 2"Naphthalene"	8	8	-48.5	30.5	0.0	3.3	-0.8	1.3
212-74-8		2"Ethane" + 1"212-74-8-	8	8	-0.4	47.3	-0.4	6.7	0.0	-0.4

	C24H16+C6H6+2C2H6→C4H10+3C10H8	C24H16" + 1"Benzene" → 1"iso-Butane" + 3"Naphthalene"								
135-70-6	C24H18+C6H6→3C10H8	1"135-70-6_C24H18" + 1"Benzene" → 3"Naphthalene"	5	6	-2.1	30.1	-7.5	4.6	0.0	-1.3
612-71-5	C24H18+C6H6→3C10H8	1"612-71-5-C24H18" + 1"Benzene" → 3"Naphthalene"	5	6	0.4	33.9	-7.5	4.6	0.0	-1.3
630-76-2	C25H20+2CH4+C2H4→3C7H8+C8H8	1"630-76-2_C25H20" + 2"Methane" + 1"Ethylene" → 1"Phenylethene" + 3"Toluene"	8	8	1.7	119.2	3.3	13.8	-1.7	1.7
188-96-5	C26H14+C6H6→2C16H10	1"188-96-5-C26H14" + 1"Benzene" → 2"Pyrene"	4	4	-7.9	16.7	-0.4	1.7	-0.4	0.4
197-61-5	C26H14+C6H6→2C16H10	1"Benzene" + 1"197-61-5-C26H14" → 2"Pyrene"	4	4	-122.6	14.2	2.1	1.3	-1.3	0.0
187-83-7	C26H16+C7H8+CH4→C8H10+C16H10+C10H8	1"Methane" + 1"187-83-7-C26H16" + 1"Toluene" → 1"Ethylbenzene" + 1"Pyrene" + 1"Naphthalene"	6	6	-3.8	78.7	4.6	8.4	0.0	1.7
191-68-4	C26H16+C7H8+CH4→C8H10+C16H10+C10H8	1"Methane" + 1"191-68-4-C26H16" + 1"Toluene" → 1"Ethylbenzene" + 1"Pyrene" + 1"Naphthalene"	6	6	1.3	63.2	1.7	5.0	-0.4	0.8
1499-10-1	C26H18→C16H10+C10H8	1"1499-10-1_C26H18" → 1"Pyrene" + 1"Naphthalene"	3	4	-51.9	59.4	-6.7	7.5	-0.8	0.0
1530-12-7	C26H18+C6H6+2C2H6→C6H12+3C10H8	2"Ethane" + 1"1530-12-7-C26H18" + 1"Benzene" → 1"Cyclohexane" + 3"Naphthalene"	8	8	28.5	56.5	5.9	10.0	0.4	0.0
35117-21-6	C26H26+2CH4+C10H8→C6H12+2C8H10+C16H10	2"Methane" + 1"35117-21-6-C26H26" + 1"Naphthalene" → 2"Ethylbenzene" + 1"Cyclohexane" + 1"Pyrene"	8	8	-189.1	205.9	9.6	15.5	-1.3	2.5
190-39-6	C28H14+2C10H8→3C16H10	1"190-39-6-C28H14" + 2"Naphthalene" → 3"Pyrene"	6	6	-79.5	36.4	1.3	0.8	-0.8	1.7

190-71-6	C28H14+2C10H8→3C16H10	1"190-71-6-C28H14" + 2"Naphthalene" → 3"Pyrene"	6	6	10.9	8.4	-0.8	0.4	-0.4	-0.4
1055-23-8	C28H18+CH4+C2H6→C7H8+C8H10+C16H10	1"Methane" + 1"Ethane" + 1"1055-23-8-C28H18" → 1"Ethylbenzene" + 1"Pyrene" + 1"Toluene"	6	6	4.6	78.2	3.8	9.2	-0.8	2.5
20532-03-0	C28H18+2C2H4→C16H10+2C8H8	1"20532-03-0-C28H18" + 2"Ethylene" → 1"Pyrene" + 2"Phenylethene"	6	6	0.0	40.6	1.7	5.0	-0.8	0.4
190-31-8	C30H14+2C6H6+C8H8→3C16H10+C2H4	1"190-31-8-C30H14" + 1"Phenylethene" + 2"Benzene" → 1"Ethylene" + 3"Pyrene"	8	8	-1.7	10.9	-2.1	0.0	0.0	0.0
190-55-6	C30H14+2C6H6+C8H8→3C16H10+C2H4	1"190-55-6-C30H14" + 1"Phenylethene" + 2"Benzene" → 1"Ethylene" + 3"Pyrene"	8	8	-26.8	14.6	-1.7	0.4	0.0	0.8
191-13-9	C30H16+2C6H6→2C16H10+C10H8	1"191-13-9-C30H16" + 2"Benzene" → 2"Pyrene" + 1"Naphthalene"	6	6	-13.0	19.7	-0.8	2.1	-0.4	0.4
190-26-1	C32H14+C7H8+C10H8+C5H12→C6H12+3C16H10	1"neo-Pentane" + 1"190-26-1-C32H14" + 1"Naphthalene" + 1"Toluene" → 1"Cyclohexane" + 3"Pyrene"	8	8	130.5	34.7	6.3	2.1	0.4	1.7
189-45-7	C32H18+2CH4→2C16H10+C2H6	2"Methane" + 1"189-45-7-C32H18" → 1"Ethane" + 2"Pyrene"	6	6	-16.3	62.3	6.7	4.6	0.0	2.5
					Av.[a]	**20.5**	**1.3**	**2.1**	**-0.2**	**0.2**
					Av. (unsigned)[b]	**22.1**	**2.2**	**2.3**	**0.4**	**0.7**
					MIN[c]	-16.3	-7.5	-2.1	-1.7	-2.1
					MAX[d]	205.9	17.6	15.5	1.7	2.5
					[a] Average value; [b] Average unsigned value; [e] Minimal value; [f] Maximal value.					

Table S4. Theoretical gas-phase enthalpies of formation obtained from atomization enthalpies (ΔH_r) and corresponding, $^{\Delta\Delta H_{corr}}$, $^{\Delta E_{corr}}$, $^{\Delta E_{AUG}}$, $^{\Delta E_{CV}}$, $^{\Delta E_{IT}}$, $^{\Delta E_{SO}}$ contributions in kJ mol^{-1}.

	$\Delta_f H_m^\circ(g, 298.15\ K)$	ΔH_r	$\Delta\Delta H_{corr}$	ΔE_{corr}	ΔE_{AUG}	ΔE_{CV}	ΔE_{IT}	ΔE_{SO}
129-00-0	123.9	13526.2	-394.4	3675.8	59.2	94.7	22.5	-5.7
95-13-6	100.1	8095.8	-270.6	2173.9	33.8	52.5	10.6	-3.2
496-11-7	-5.2	8637.1	-320.3	2283.2	35.5	51.3	9.4	-3.2
208-96-8	186.2	10160.4	-303.4	2777.2	44	70.6	16.6	-4.2
259-79-0	344	10002.6	-301.3	2773.7	42	70.1	16.4	-4.2
83-32-9	74.7	10707.9	-351.5	2881.9	46.1	69.8	14.8	-4.2
92-52-4	98.8	10683.7	-350.5	2862.2	44.3	71	14.8	-4.2
569-41-5	25.1	11193.4	-396.5	2996.2	47.7	69.4	14.5	-4.2
571-58-4	-0.4	11219	-395.8	2989.2	47.7	69.6	14.4	-4.2
571-61-9	-0.5	11219.1	-395.8	2989.4	47.8	69.6	14.4	-4.2
573-98-8	4.8	11213.8	-395.5	2991.4	47.8	69.7	14.5	-4.2
575-37-1	-2.2	11220.8	-395.1	2984.8	47.3	69.9	14.4	-4.2
575-41-7	-2.4	11221	-395.2	2984.2	47.2	69.9	14.4	-4.2
575-43-9	-2.1	11220.7	-395.1	2984.2	47.2	69.9	14.4	-4.2
581-40-8	-3.3	11221.8	-395	2985	47.1	70	14.4	-4.2
581-42-0	-2.8	11221.4	-394.6	2980	46.6	70.1	14.3	-4.2
582-16-1	-3.2	11221.8	-394.6	2979.8	46.7	70.1	14.3	-4.2
232-54-2	138.9	11360.5	-359.3	3079.7	49.6	76.2	16.6	-4.6
268-40-6	138.9	11360.6	-359.5	3074.7	49	76.3	16.6	-4.6
86-73-7	100.4	11399	-360.7	3071	49.2	76.5	16	-4.6
101-81-5	75.5	11859.9	-407.4	3166.3	49.6	76.2	15.3	-4.6
643-58-3	62.2	11873.3	-406.4	3176.4	50.2	76.4	15.5	-4.6
120-12-7	138.6	12077.7	-371.5	3272.3	51.8	83	19.1	-5
85-01-8	114.3	12102.1	-372.4	3268.5	51.6	82.8	18.6	-5
567-79-3	98.3	12554	-419.5	3402.3	55.7	80	16.8	-5
20244-28-4	104.9	12547.5	-418.5	3382.3	55.4	81.8	16.7	-5
38399-10-9	100.5	12551.8	-419	3386.7	54.9	81.5	17.2	-5
56179-83-0	101.4	12550.9	-419.1	3386.7	54.8	81.4	17.2	-5
776-35-2	56.3	12596	-420.1	3383.5	54.7	81.7	16.7	-5
2717-39-7	-22	13546.3	-509.9	3631.4	59.2	79.8	16.2	-5
832-64-4	97.5	13271.7	-429.7	3588.6	57.8	87.8	19.5	-5.3
201-06-9	209.1	13441	-392.6	3679.5	59.8	94.3	22.3	-5.7
202-03-9	238.1	13412	-391.9	3688.1	60.3	94.4	23	-5.7
206-44-0	183.1	13467	-393	3673	59	94.4	22.2	-5.7
605-02-7	143.3	13942.8	-439.5	3771.1	60.4	94.6	20.9	-5.7
6232-48-0	101	13985.2	-440.6	3784.9	61.9	93.5	20.5	-5.7
641-48-5	126.6	13959.5	-440.1	3791.8	62.3	93.4	21.1	-5.7
1576-69-8	28.5	14493.6	-483.7	3883.7	62.2	93.6	20.1	-5.7
604-83-1	45.1	14477	-485.7	3902.2	63.8	92.8	20.2	-5.7
238-84-6	138.5	14664.5	-449.6	3975.5	64.7	99.8	22.1	-6
243-17-4	139.7	14663.3	-449.5	3972.9	64.3	100.2	22.1	-6
219-08-9	171.4	14631.6	-448.4	3983.6	65.2	99.6	22.3	-6
235-92-7	170.2	14632.8	-448.4	3987.7	65.7	99.6	22.4	-6
259-06-3	193.4	14609.6	-448	3981.3	64.6	100.2	22.8	-6

203-12-3	250.3	14833.6	-415	4086.9	67.1	106	25.9	-6.4
27208-37-3	230.9	14853	-414.7	4089.9	67.3	106.1	26.3	-6.4
195-19-7	173.9	15345.9	-462	4185	68.4	106.5	24.8	-6.4
217-59-4	149.7	15370.2	-461.4	4178.7	67.8	106	24.3	-6.4
218-01-9	150.6	15369.2	-461.4	4175.9	67.9	106.4	24.6	-6.4
56-55-3	163	15356.9	-461	4174.1	67.4	106.4	24.7	-6.4
92-24-0	201.7	15318.2	-459.7	4182.7	66.8	106.4	25.7	-6.4
84-15-1	157.5	15798.4	-506.3	4277.3	70	106.7	22.8	-6.4
92-06-8	153.4	15802.5	-506.5	4262.4	67.9	106.7	22.7	-6.4
92-94-4	154	15801.9	-506.6	4261.6	67.7	106.7	22.7	-6.4
959-02-4	103.3	15852.5	-507.7	4284.4	70.2	106.3	22.5	-6.4
7343-06-8	2.5	16825.4	-596.2	4546.9	76.1	104.1	22.2	-6.4
7396-38-5	0	16827.9	-595.9	4531.4	74.5	104.3	22.1	-6.4
519-73-3	142.1	16966.6	-563.6	4583.5	75.9	111.6	23.2	-6.7
173678-72-3	344	16173.6	-434.8	4504.4	75.3	117.5	29.9	-7.1
5821-51-2	356.4	16161.3	-436.7	4523.2	76.3	119	30	-7.1
198-55-0	188.2	16765.4	-483.2	4591.1	75	117.6	28.6	-7.1
205-99-2	207.4	16746.2	-482.1	4575.6	74.8	117.8	27.9	-7.1
192-97-2	155.5	16798.1	-483.5	4584.7	75.2	118.1	28.1	-7.1
202-33-5	265.1	16688.6	-481.2	4590.5	75.8	117.8	28.6	-7.1
207-08-9	218.8	16734.9	-481.8	4575.5	74.4	118.2	28.2	-7.1
50-32-8	167.7	16785.9	-483.4	4584.8	75.6	118.5	28.6	-7.1
602-55-1	198.6	17191	-527.9	4685.6	77.3	118.1	27.2	-7.1
477-75-8	192.5	17197.2	-529.2	4705.8	79.2	117.2	25.5	-7.1
479-23-2	152.9	17236.7	-529.4	4694.7	78	117	26.7	-7.1
316-51-8	76.3	17749.3	-572.3	4789.2	77.8	117.4	26.2	-7.1
3697-27-6	108.1	17717.6	-575.1	4819.8	80.1	116.7	26.4	-7.1
56-56-4	75.8	17749.8	-572.8	4794.2	78.2	117.3	26.2	-7.1
191-24-2	158.2	18229.2	-506	4989.4	82.8	130.1	32	-7.8
191-26-4	185.2	18202.2	-505.5	4995.3	83.3	130.6	32.8	-7.8
193-43-1	323.9	18063.5	-502.7	4984.8	81.1	129.5	31.6	-7.8
135-48-8	267.6	18555.8	-547.7	5096.4	82.3	130.3	32.4	-7.8
194-69-4	209.5	18613.9	-551.3	5091.4	84.2	130	30.7	-7.8
195-06-2	223.3	18600.1	-550.4	5092.2	83.9	130.3	31	-7.8
196-78-1	210.7	18612.7	-551.8	5097.2	84.3	129.9	30.6	-7.8
213-46-7	186.3	18637.1	-550.5	5081.1	83.6	129.7	30.5	-7.8
214-17-5	201.8	18621.6	-550	5082.3	83.5	129.9	30.8	-7.8
215-58-7	194.9	18628.5	-550.3	5085.3	83.5	129.7	30.3	-7.8
222-93-5	208.1	18615.3	-549.7	5079.1	83.1	130.5	30.8	-7.8
224-41-9	189.1	18634.3	-550.2	5078.3	83	130.1	30.4	-7.8
226-88-0	222.5	18600.9	-549.2	5083.3	82.6	130.1	31.1	-7.8
53-70-3	188.9	18634.5	-550.3	5077.3	83	130	30.4	-7.8
190-88-5	260	19561.2	-526.5	5403.1	90.9	141.7	35.7	-8.5
191-07-1	142.8	19678.4	-528.8	5393.5	90.5	142.5	35.8	-8.5
189-55-9	207.3	20049.8	-572.4	5490	91.3	141.6	34.5	-8.5
192-51-8	190	20067.1	-573.3	5496.4	91.7	141.4	33.7	-8.5
192-65-4	198	20059.1	-572.6	5494.3	91.5	141.4	34.2	-8.5
189-64-0	217.9	20039.3	-572.2	5496.2	91.6	141.9	34.9	-8.5
193-09-9	201	20056.2	-572.5	5490.7	90.9	141.7	34.2	-8.5

214-63-1	267.5	19989.6	-571.8	5503.6	91.1	141.6	35.2	-8.5
212-74-8	242.9	20450.3	-617	5599.4	94.6	142.4	31.6	-8.5
135-70-6	209.4	20919.7	-662.6	5660.7	91.1	142.2	30.6	-8.5
612-71-5	206.9	20922.2	-662.4	5664.4	91.4	142.3	30.7	-8.5
630-76-2	231	22051	-719.6	6036.2	105.1	146.1	31.7	-8.8
188-96-5	212.9	21478	-594.7	5904.6	99.6	153.5	38.5	-9.2
197-61-5	327.6	21363.4	-592	5902.1	99.3	152.7	38.1	-9.2
187-83-7	265.6	21861.3	-638.5	6031.6	104.2	153.9	37.3	-9.2
191-68-4	260.5	21866.4	-641.4	6016	100.7	153.5	36.6	-9.2
1499-10-1	259.3	22303.6	-684.3	6099.9	102.6	153.3	35.3	-9.2
1530-12-7	210.7	22352.2	-684.9	6116.1	106.8	153.2	33.7	-9.2
35117-21-6	166.8	24140.1	-871.5	6689.5	119.7	146.3	31.5	-9.2
190-39-6	284.3	22840.4	-615.9	6334.3	107.1	165	43.3	-9.9
190-71-6	194.1	22930.6	-617.8	6306.2	106.6	165.4	41.4	-9.9
1055-23-8	280.4	23716.3	-705.2	6520.5	112.7	165.3	39.8	-9.9
20532-03-0	239.9	23756.8	-706.5	6492.3	108.4	165.3	38.5	-9.9
190-31-8	229.6	24328.9	-639.3	6723.1	114.4	177.7	46	-10.6
190-55-6	254.8	24303.7	-639	6726.8	114.7	177.6	47	-10.6
191-13-9	258.3	24736.2	-683.8	6808.4	115.1	177.3	44.5	-10.6
190-26-1	195.6	25796.6	-662.4	7120.1	121.6	189.6	49.4	-11.3
189-45-7	330.9	26533.3	-748.8	7317.5	122.7	189.1	47.7	-11.3
Av.[a]	-123.1[b]		-500.6	4484.5	73.82	112.8	26.1	-6.8
Av. (unsigned)[c]	123.1[d]		500.6	4484.5	73.82	112.8	26.1	6.8
MIN[e]	-200.0		-871.5	2173.9	33.8	51.3	9.4	-11.3
MAX[f]	-60.1		-270.6	7317.5	122.7	189.6	49.4	-3.2

[a] Average value; [b] Average deviation from $\Delta_f H_m^\circ(g, 298.15\ K)$ calculated via composed chemical reactions, see Table 1 in main text; [c] Average unsigned value; [d] Average unsigned deviation from $\Delta_f H_m^\circ(g, 298.15\ K)$ calculated via composed chemical reactions, see Table 1 in main text; [e] Minimal value; [f] Maximal value.

Tables forming the basis of Figures 1 – 3 in the main text

Table S5. Mean absolute deviation (MAD) and mean signed deviation (MSD) of our predicted gas-phase $\Delta_f H_m^\circ(g, 298.15\ K)$ from their experimental and calculated counterparts available in the literature in kJ mol^{-1} (Figure 1). Number of compound with available $\Delta_f H_m^\circ(g, 298.15\ K)$ is given in parenthesis.

	MAD	MSD
G4MP2 (27)	18.5	18.5
G3MP2B3 (34)	1.7	-0.3
B3LYP (86)	8.1	-5.6
M06-2X (17)	4.2	-0.9
ATOMIC (16)	1.9	-1.3
Expt. (50)	12.9	-7.5

Table S6. Mean absolute deviation (MAD), mean signed deviation (MSD), minimum (MIN) and maximum (MAX) deviations of our predicted recommended gas-phase $\Delta_f H_m^\circ(g, 298.15\ K)$ from their counterparts averaged over all reactions of each layer in kJ mol^{-1} (Figure 2).

	MAD	MSD	MIN	MAX
L0 (5)	-0.07	0.49	-2.30	2.10
L1 (57)	-0.04	0.76	-2.40	2.50
L2 (381)	0.11	0.78	-2.60	2.70
L3 (1297)	0.12	0.85	-2.80	2.60
L4 (2556)	0.08	0.89	-3.00	2.70
L5 (3790)	0.08	0.92	-3.10	2.70
L6 (4786)	0.10	0.96	-3.30	2.80
L7 (5501)	0.12	0.98	-3.50	3.00
L8 (5971)	0.14	1.00	-3.60	3.20
L9 (6288)	0.15	1.01	-3.50	3.30
L10 (6508)	0.15	1.02	-3.60	3.30
L11 (6657)	0.16	1.03	-3.60	3.30
L12 (6759)	0.17	1.04	-3.60	3.30
L13 (6833)	0.18	1.04	-3.60	3.40
L14 (6884)	0.19	1.05	-3.50	3.40

L15 (6916)	0.20	1.05	-3.50	3.40

Table S7. Mean absolute (MA), mean signed (MS), minimum (MIN) and maximum (MAX) contributions of $^{\Delta E_{CV}}$, $^{\Delta E_{AUG}}$, $^{\Delta E_{IT}}$ ***and*** $^{\Delta\Delta H_{corr}}$ ***to reaction enthalpies*** $^{\Delta_r H_m^\circ(g,\,298.15\,K)}$ ***utilized to derive our recommended gas-phase*** $^{\Delta_f H_m^\circ(g,\,298.15\,K)}$ ***in kJ mol-1 (Figure 3).***

	MA	MS	MIN	MAX
ΔE_{AUG}	0.4	-0.2	-1.7	1.7
ΔE_{CV}	0.7	0.2	-2.1	2.5
ΔE_{IT}	1.4	-0.8	-7.1	2.5
$\Delta\Delta H_{corr}$	2.2	1.3	-7.5	17.6

Cartesian Coordinates (Å) and Absolute Energies (Hartree) of All Species Studied in Present Work

100-41-40_C8H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -311.026194033 (a.u.)
E(HF/CC-PVTZ) = -308.87671256
E(DLPNO-CCSD(T)/CC-PVTZ) = -310.285790054919
T1 (CC-PVTZ)= 0.009373985
T2 (CC-PVTZ)= 0.034495
E(HF/CC-PVQZ) = -308.8957394
E(DLPNO-CCSD(T)/CC-PVQZ) = -310.374906156173
E(HF/TZ-AUG) = -308.8788921
E(DLPNO-CCSD(T)/TZ-AUG) = -310.306294295
E(HF/TZ-CORE) = -308.87896956
E(DLPNO-CCSD(T)/TZ-CORE) = -310.691707097
E(HF/TZ-IT) = -308.87671256
E(DLPNO-CCSD(T)/TZ-IT) = -310.28893765
T1 (CC-PVQZ)= 0.009533474
T2 (CC-PVQZ)= 0.037408
E(HF/CBS) = -308.900375724
E(DLPNO-CCSD(T)/CBS) = -310.430688697
Enthalpic correction = 0.15981387 (a.u.)
Entropy = 86.13084 (cal/(mol*K))

C	0.238031	0.493508	0.000000
C	0.239003	-0.221759	1.197322
C	0.239003	-0.221759	-1.197322
C	0.239003	-1.611161	1.200632
C	0.239003	-1.611161	-1.200632
C	0.238054	-2.311412	0.000000
H	0.243410	0.317461	2.137649
H	0.243410	0.317461	-2.137649
H	0.243827	-2.147523	2.141150
H	0.243827	-2.147523	-2.141150
H	0.241226	-3.393724	0.000000
C	0.186290	1.999256	0.000000
C	-1.250766	2.533409	0.000000
H	0.714524	2.381950	-0.876762
H	0.714524	2.381950	0.876762
H	-1.263967	3.625114	0.000000
H	-1.793252	2.185653	0.881017
H	-1.793252	2.185653	-0.881017

100-42-50_C8H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -309.793292513 (a.u.)
E(HF/CC-PVTZ) = -307.68757433
E(DLPNO-CCSD(T)/CC-PVTZ) = -309.056222852845
T1 (CC-PVTZ)= 0.010161878
T2 (CC-PVTZ)= 0.040681
E(HF/CC-PVQZ) = -307.70650905
E(DLPNO-CCSD(T)/CC-PVQZ) = -309.143992515586
E(HF/TZ-AUG) = -307.68997507
E(DLPNO-CCSD(T)/TZ-AUG) = -309.075918654
E(HF/TZ-CORE) = -307.68987765
E(DLPNO-CCSD(T)/TZ-CORE) = -309.462500113
E(HF/TZ-IT) = -307.68757433
E(DLPNO-CCSD(T)/TZ-IT) = -309.059750705
T1 (CC-PVQZ)= 0.010256490
T2 (CC-PVQZ)= 0.041940
E(HF/CBS) = -307.711122927
E(DLPNO-CCSD(T)/CBS) = -309.198837296
Enthalpic correction = 0.13667039 (a.u.)
Entropy = 83.90682 (cal/(mol*K))

C	0.000000	0.558324	0.000000
C	-1.001946	-0.420487	0.000000
C	1.332703	0.134043	0.000000
C	-0.679244	-1.767307	0.000000
C	1.658674	-1.215768	0.000000
C	0.653092	-2.173068	0.000000
H	-2.042817	-0.125869	0.000000
H	2.120929	0.877385	0.000000
H	-1.469115	-2.507661	0.000000
H	2.697873	-1.518752	0.000000
H	0.901489	-3.226388	0.000000
C	-0.286109	1.996820	0.000000
C	-1.481552	2.584588	0.000000
H	0.595585	2.631111	0.000000
H	-1.569531	3.662399	0.000000
H	-2.408116	2.024897	0.000000

101-81-5_C13H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -502.850169723 (a.u.)
E(HF/CC-PVTZ) = -499.44401149
E(DLPNO-CCSD(T)/CC-PVTZ) = -501.657818876386
T1 (CC-PVTZ)= 0.009790107
T2 (CC-PVTZ)= 0.035515
E(HF/CC-PVQZ) = -499.47434412
E(DLPNO-CCSD(T)/CC-PVQZ) = -501.799996596068
E(HF/TZ-AUG) = -499.44769738
E(DLPNO-CCSD(T)/TZ-AUG) = -501.690654593
E(HF/TZ-CORE) = -499.44771428
E(DLPNO-CCSD(T)/TZ-CORE) = -502.318102888
E(HF/TZ-IT) = -499.44401149
E(DLPNO-CCSD(T)/TZ-IT) = -501.663631242
T1 (CC-PVQZ)= 0.009874647
T2 (CC-PVQZ)= 0.037973
E(HF/CBS) = -499.481735357
E(DLPNO-CCSD(T)/CBS) = -501.88900452
Enthalpic correction = 0.21419723 (a.u.)
Entropy = 106.30859 (cal/(mol*K))

C	0.000646	-1.462228	-0.187548
C	-1.263689	-0.650154	-0.020839
C	-2.270608	-0.681909	-0.981523
C	-3.433187	0.066135	-0.823157
C	-3.601965	0.858698	0.303801
C	-2.600667	0.899659	1.269664
C	-1.442552	0.153876	1.105947
C	1.263903	-0.632484	-0.143370
C	1.436689	0.437770	-1.022437
C	2.594486	1.201276	-0.992938
C	3.601530	0.910535	-0.077274

C	3.438741	-0.148609	0.805018
C	2.276496	-0.912894	0.769804
H	-0.048269	-2.000940	-1.137436
H	0.050765	-2.223537	0.595212
H	-2.143938	-1.298286	-1.863730
H	-4.204236	0.029520	-1.582272
H	-4.504443	1.442701	0.429788
H	-2.723054	1.517105	2.150540
H	-0.660092	0.201432	1.853568
H	0.649797	0.678197	-1.726994
H	2.712056	2.027248	-1.682945
H	4.503725	1.507864	-0.051939
H	4.214222	-0.381304	1.523766
H	2.154525	-1.738034	1.461563

1055-23-8-C28H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1078.36212349 (a.u.)
E(HF/CC-PVTZ) = -1071.15724695
E(DLPNO-CCSD(T)/CC-PVTZ) = -1075.813088676644
T1 (CC-PVTZ)= 0.010383335
T2 (CC-PVTZ)= 0.039434
E(HF/CC-PVQZ) = -1071.22060004
E(DLPNO-CCSD(T)/CC-PVQZ) = -1076.113237252490
E(HF/TZ-AUG) = -1071.16506458
E(DLPNO-CCSD(T)/TZ-AUG) = -1075.88600413
E(HF/TZ-CORE) = -1071.16514732
E(DLPNO-CCSD(T)/TZ-CORE) = -1077.23565805
E(HF/TZ-IT) = -1071.15724695
E(DLPNO-CCSD(T)/TZ-IT) = -1075.82824361
T1 (CC-PVQZ)= 0.010391914
T2 (CC-PVQZ)= 0.040813
E(HF/CBS) = -1071.23603747
E(DLPNO-CCSD(T)/CBS) = -1076.30147138
Enthalpic correction = 0.37718112 (a.u.)
Entropy = 148.87114 (cal/(mol*K))

C	-0.745063	0.000001	0.000001
C	-1.443670	-0.861683	0.861516
C	-1.443666	0.861686	-0.861515
C	0.745063	-0.000001	0.000002
C	-2.882602	-0.859260	0.859092
C	-0.774070	-1.751915	1.751575
C	-2.882597	0.859268	-0.859095
C	-0.774060	1.751914	-1.751573
C	1.443669	0.861528	0.861671
C	1.443667	-0.861531	-0.861669
C	-3.562617	0.000005	-0.000002
C	-3.573833	-1.740206	1.739861
C	-1.474104	-2.579293	2.578787
C	-3.573824	1.740215	-1.739865
C	-1.474090	2.579295	-2.578788
C	2.882601	0.859105	0.859250
C	0.774068	1.751600	1.751889
C	2.882598	-0.859112	-0.859248
C	0.774063	-1.751601	-1.751887
C	-2.893863	-2.575172	2.574662
C	-2.893849	2.575178	-2.574666
C	3.562617	-0.000004	0.000001
C	3.573831	1.739891	1.740179
C	1.474101	2.578828	2.579253
C	3.573826	-1.739899	-1.740178
C	1.474093	-2.578831	-2.579251
C	2.893860	2.574706	2.575130
C	2.893852	-2.574712	-2.575129
H	0.306677	-1.760451	1.760113
H	0.306687	1.760447	-1.760108
H	-4.646575	0.000007	-0.000003
H	-4.656993	-1.730917	1.730571
H	-0.946184	-3.247482	3.246846
H	-4.656983	1.730930	-1.730578
H	-0.946165	3.247481	-3.246845
H	-0.306680	1.760135	1.760426
H	-0.306685	-1.760134	-1.760423
H	-3.431740	-3.239372	3.238727
H	-3.431722	3.239380	-3.238733
H	4.646575	-0.000005	0.000000
H	4.656991	1.730603	1.730889
H	0.946179	3.246897	3.247431
H	4.656986	-1.730613	-1.730889
H	0.946170	-3.246898	-3.247429
H	3.431736	3.238785	3.239317
H	3.431726	-3.238792	-3.239316

106-97-80_C4H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -158.535062174 (a.u.)
E(HF/CC-PVTZ) = -157.35549235
E(DLPNO-CCSD(T)/CC-PVTZ) = -158.153236754251
T1 (CC-PVTZ)= 0.007805388
T2 (CC-PVTZ)= 0.030611
E(HF/CC-PVQZ) = -157.36556119
E(DLPNO-CCSD(T)/CC-PVQZ) = -158.200829671497
E(HF/TZ-AUG) = -157.35632368
E(DLPNO-CCSD(T)/TZ-AUG) = -158.164531687
E(HF/TZ-CORE) = -157.3565724
E(DLPNO-CCSD(T)/TZ-CORE) = -158.355259901
E(HF/TZ-IT) = -157.35549235
E(DLPNO-CCSD(T)/TZ-IT) = -158.153989716
T1 (CC-PVQZ)= 0.008231821
T2 (CC-PVQZ)= 0.029586
E(HF/CBS) = -157.368014693
E(DLPNO-CCSD(T)/CBS) = -158.230665609
Enthalpic correction = 0.13419750 (a.u.)
Entropy = 72.29375 (cal/(mol*K))

C	0.702010	1.826283	0.000000
C	0.702010	0.300424	0.000000
H	1.717233	2.227386	0.000000
H	0.188950	2.218886	0.881392
H	0.188950	2.218886	-0.881392
C	-0.702010	-0.300424	0.000000
H	1.248889	-0.066797	0.874889
H	1.248889	-0.066797	-0.874889
C	-0.702010	-1.826283	0.000000
H	-1.248889	0.066797	0.874889
H	-1.248889	0.066797	-0.874889
H	-1.717233	-2.227386	0.000000
H	-0.188950	-2.218886	0.881392
H	-0.188950	-2.218886	-0.881392

106-98-90_C4H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -157.298278082 (a.u.)

E(HF/CC-PVTZ) = -156.16405092
E(DLPNO-CCSD(T)/CC-PVTZ) = -156.920792264171
T1 (CC-PVTZ)= 0.009379378
T2 (CC-PVTZ)= 0.060296
E(HF/CC-PVQZ) = -156.1741574
E(DLPNO-CCSD(T)/CC-PVQZ) = -156.967086898528
E(HF/TZ-AUG) = -156.16526554
E(DLPNO-CCSD(T)/TZ-AUG) = -156.931480724
E(HF/TZ-CORE) = -156.16520373
E(DLPNO-CCSD(T)/TZ-CORE) = -157.123271843
E(HF/TZ-IT) = -156.16405092
E(DLPNO-CCSD(T)/TZ-IT) = -156.921827906
T1 (CC-PVQZ)= 0.009673199
T2 (CC-PVQZ)= 0.057974
E(HF/CBS) = -156.176620074
E(DLPNO-CCSD(T)/CBS) = -156.995957145
Enthalpic correction = 0.11101953 (a.u.)
Entropy = 71.34984 (cal/(mol*K))

C	-1.850809	0.015036	-0.279085
C	-0.719018	-0.291212	0.341775
C	0.537428	0.522933	0.303971
H	-1.944815	0.919900	-0.869566
H	-2.723806	-0.622250	-0.219619
H	-0.667818	-1.211402	0.920150
H	0.795716	0.831457	1.323265
H	0.362462	1.438636	-0.266586
C	1.719117	-0.248957	-0.292508
H	2.628909	0.353770	-0.277662
H	1.514441	-0.533026	-1.326216
H	1.914601	-1.163878	0.271322

106-99-00_C4H6

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -156.068589584
(a.u.)
E(HF/CC-PVTZ) = -154.97781053
E(DLPNO-CCSD(T)/CC-PVTZ) = -155.694427438190
T1 (CC-PVTZ)= 0.010994869
T2 (CC-PVTZ)= 0.047562
E(HF/CC-PVQZ) = -154.98784529
E(DLPNO-CCSD(T)/CC-PVQZ) = -155.739349805924
E(HF/TZ-AUG) = -154.97925332
E(DLPNO-CCSD(T)/TZ-AUG) = -155.704276405
E(HF/TZ-CORE) = -154.97901039
E(DLPNO-CCSD(T)/TZ-CORE) = -155.897290258
E(HF/TZ-IT) = -154.97781053
E(DLPNO-CCSD(T)/TZ-IT) = -155.695847914
T1 (CC-PVQZ)= 0.011181498
T2 (CC-PVQZ)= 0.047034
E(HF/CBS) = -154.990290488
E(DLPNO-CCSD(T)/CBS) = -155.767253529
Enthalpic correction = 0.08795689 (a.u.)
Entropy = 66.36953 (cal/(mol*K))

C	0.600146	1.742200	0.000000
C	0.600146	0.408249	0.000000
C	-0.600146	-0.408249	0.000000
H	1.520210	2.310749	0.000000
H	-0.325763	2.305706	0.000000
H	1.546214	-0.126163	0.000000
C	-0.600146	-1.742200	0.000000
H	-1.520210	-2.310749	0.000000
H	0.325763	-2.305706	0.000000
H	-1.546214	0.126163	0.000000

108-88-30_C7H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -271.693049424
(a.u.)
E(HF/CC-PVTZ) = -269.82936259
E(DLPNO-CCSD(T)/CC-PVTZ) = -271.045899876756
T1 (CC-PVTZ)= 0.009608736
T2 (CC-PVTZ)= 0.034545
E(HF/CC-PVQZ) = -269.84601419
E(DLPNO-CCSD(T)/CC-PVQZ) = -271.123538960980
E(HF/TZ-AUG) = -269.83138131
E(DLPNO-CCSD(T)/TZ-AUG) = -271.063356431
E(HF/TZ-CORE) = -269.83134509
E(DLPNO-CCSD(T)/TZ-CORE) = -271.401344881
E(HF/TZ-IT) = -269.82936259
E(DLPNO-CCSD(T)/TZ-IT) = -271.048801725
T1 (CC-PVQZ)= 0.009754479
T2 (CC-PVQZ)= 0.038006
E(HF/CBS) = -269.850071732
E(DLPNO-CCSD(T)/CBS) = -271.172100884
Enthalpic correction = 0.13073693 (a.u.)
Entropy = 81.26297 (cal/(mol*K))

C	2.414476	0.000000	0.009395
C	0.909905	-0.000001	-0.011774
C	0.193892	1.197044	-0.009059
C	0.193892	-1.197043	-0.009059
C	-1.195492	1.200051	0.002057
C	-1.195493	-1.200050	0.002057
C	-1.896352	-0.000000	0.008688
H	2.790561	-0.000032	1.036465
H	2.818776	-0.883570	-0.485949
H	2.818774	0.883602	-0.485895
H	0.731927	2.137763	-0.018116
H	0.731925	-2.137764	-0.018116
H	-1.731152	2.140971	0.001691
H	-1.731152	-2.140971	0.001691
H	-2.978623	0.000001	0.014408

109-66-00_C5H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -197.867865950
(a.u.)
E(HF/CC-PVTZ) = -196.40319743
E(DLPNO-CCSD(T)/CC-PVTZ) = -197.392725038084
T1 (CC-PVTZ)= 0.007888523
T2 (CC-PVTZ)= 0.029847
E(HF/CC-PVQZ) = -196.4156825
E(DLPNO-CCSD(T)/CC-PVQZ) = -197.451955029965
E(HF/TZ-AUG) = -196.40422344
E(DLPNO-CCSD(T)/TZ-AUG) = -197.406991594
E(HF/TZ-CORE) = -196.40453996
E(DLPNO-CCSD(T)/TZ-CORE) = -197.645266884
E(HF/TZ-IT) = -196.40319743
E(DLPNO-CCSD(T)/TZ-IT) = -197.393699242
T1 (CC-PVQZ)= 0.008295583
T2 (CC-PVQZ)= 0.028961
E(HF/CBS) = -196.418724772
E(DLPNO-CCSD(T)/CBS) = -197.489108461
Enthalpic correction = 0.16307145 (a.u.)
Entropy = 80.16037 (cal/(mol*K))

C	0.000000	2.547402	0.323899

C	0.000000	1.277521	-0.522301
C	0.000000	0.000000	0.313348
H	0.000000	3.444167	-0.298534
H	0.881344	2.589550	0.968585
H	-0.881344	2.589550	0.968585
H	0.874879	1.275974	-1.180780
H	-0.874879	1.275974	-1.180780
C	0.000000	-1.277521	-0.522301
H	0.875259	0.000000	0.973290
H	-0.875259	0.000000	0.973290
C	0.000000	-2.547402	0.323899
H	0.874879	-1.275974	-1.180780
H	-0.874879	-1.275974	-1.180780
H	0.000000	-3.444167	-0.298534
H	0.881344	-2.589550	0.968585
H	-0.881344	-2.589550	0.968585

110-82-70_C6H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -235.993378983 (a.u.)
E(HF/CC-PVTZ) = -234.28609461
E(DLPNO-CCSD(T)/CC-PVTZ) = -235.433579093221
T1 (CC-PVTZ)= 0.008157724
T2 (CC-PVTZ)= 0.031258
E(HF/CC-PVQZ) = -234.30058119
E(DLPNO-CCSD(T)/CC-PVQZ) = -235.503078790119
E(HF/TZ-AUG) = -234.28724429
E(DLPNO-CCSD(T)/TZ-AUG) = -235.450563029
E(HF/TZ-CORE) = -234.28769201
E(DLPNO-CCSD(T)/TZ-CORE) = -235.736656825
E(HF/TZ-IT) = -234.28609461
E(DLPNO-CCSD(T)/TZ-IT) = -235.434893784
T1 (CC-PVQZ)= 0.008476941
T2 (CC-PVQZ)= 0.029475
E(HF/CBS) = -234.304111176
E(DLPNO-CCSD(T)/CBS) = -235.546753483
Enthalpic correction = 0.17133775 (a.u.)
Entropy = 71.55215 (cal/(mol*K))

C	1.264378	0.729989	0.229233
H	1.319741	0.761953	1.323449
H	2.154339	1.243808	-0.143014
C	-1.264378	0.729989	0.229233
H	-1.319741	0.761953	1.323449
H	-2.154339	1.243808	-0.143014
C	0.000000	-1.459978	0.229233
H	0.000000	-1.523905	1.323449
H	0.000000	-2.487616	-0.143014
C	0.000000	1.459978	-0.229233
H	0.000000	1.523905	-1.323449
H	0.000000	2.487616	0.143014
C	-1.264378	-0.729989	-0.229233
H	-1.319741	-0.761953	-1.323449
H	-2.154339	-1.243808	0.143014
C	1.264378	-0.729989	-0.229233
H	1.319741	-0.761953	-1.323449
H	2.154339	-1.243808	0.143014

115-07-10_C3H6

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -117.965777450 (a.u.)
E(HF/CC-PVTZ) = -117.11649093
E(DLPNO-CCSD(T)/CC-PVTZ) = -117.681691937370
T1 (CC-PVTZ)= 0.009816223
T2 (CC-PVTZ)= 0.060511
E(HF/CC-PVQZ) = -117.12419278
E(DLPNO-CCSD(T)/CC-PVQZ) = -117.716434703572
E(HF/TZ-AUG) = -117.11752074
E(DLPNO-CCSD(T)/TZ-AUG) = -117.689449398
E(HF/TZ-CORE) = -117.11737291
E(DLPNO-CCSD(T)/TZ-CORE) = -117.833682761
E(HF/TZ-IT) = -117.11649093
E(DLPNO-CCSD(T)/TZ-IT) = -117.682492643
T1 (CC-PVQZ)= 0.010117634
T2 (CC-PVQZ)= 0.058295
E(HF/CBS) = -117.126069511
E(DLPNO-CCSD(T)/CBS) = -117.738043996
Enthalpic correction = 0.08200625 (a.u.)
Entropy = 63.43965 (cal/(mol*K))

C	0.000000	0.472625	0.000000
C	1.286814	0.149673	0.000000
H	2.062176	0.904919	0.000000
H	1.611198	-0.885199	0.000000
H	-0.276063	1.524090	0.000000
C	-1.133510	-0.503222	0.000000
H	-0.773650	-1.533000	0.000000
H	-1.771744	-0.362631	0.877209
H	-1.771744	-0.362631	-0.877209

115-11-70_C4H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -157.304326395 (a.u.)
E(HF/CC-PVTZ) = -156.16855539
E(DLPNO-CCSD(T)/CC-PVTZ) = -156.926304897296
T1 (CC-PVTZ)= 0.009538075
T2 (CC-PVTZ)= 0.058893
E(HF/CC-PVQZ) = -156.17869333
E(DLPNO-CCSD(T)/CC-PVQZ) = -156.972807578762
E(HF/TZ-AUG) = -156.16977681
E(DLPNO-CCSD(T)/TZ-AUG) = -156.937056605
E(HF/TZ-CORE) = -156.16971124
E(DLPNO-CCSD(T)/TZ-CORE) = -157.128942452
E(HF/TZ-IT) = -156.16855539
E(DLPNO-CCSD(T)/TZ-IT) = -156.927370587
T1 (CC-PVQZ)= 0.009824948
T2 (CC-PVQZ)= 0.056480
E(HF/CBS) = -156.18116367
E(DLPNO-CCSD(T)/CBS) = -157.001814352
Enthalpic correction = 0.11046129 (a.u.)
Entropy = 69.65168 (cal/(mol*K))

C	0.000000	0.000000	1.454095
C	0.000000	0.000000	0.123947
H	0.000000	0.923087	2.020617
H	0.000000	-0.923087	2.020617
C	0.000000	-1.270648	-0.676587
H	0.000000	-2.152479	-0.036603
H	-0.877159	-1.317936	-1.329310
H	0.877159	-1.317936	-1.329310
C	0.000000	1.270648	-0.676587
H	0.000000	2.152479	-0.036603
H	0.877159	1.317936	-1.329310
H	-0.877159	1.317936	-1.329310

120-12-7-C14H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -539.777068354 (a.u.)
E(HF/CC-PVTZ) = -536.16455441
E(DLPNO-CCSD(T)/CC-PVTZ) = -538.497595183250
T1 (CC-PVTZ)= 0.010341292
T2 (CC-PVTZ)= 0.035965
E(HF/CC-PVQZ) = -536.19656844
E(DLPNO-CCSD(T)/CC-PVQZ) = -538.648744228791
E(HF/TZ-AUG) = -536.16833386
E(DLPNO-CCSD(T)/TZ-AUG) = -538.532310927
E(HF/TZ-CORE) = -536.16850837
E(DLPNO-CCSD(T)/TZ-CORE) = -539.209020716
E(HF/TZ-IT) = -536.16455441
E(DLPNO-CCSD(T)/TZ-IT) = -538.504866521
T1 (CC-PVQZ)= 0.010373418
T2 (CC-PVQZ)= 0.037558
E(HF/CBS) = -536.204369389
E(DLPNO-CCSD(T)/CBS) = -538.74348154
Enthalpic correction = 0.19815933 (a.u.)
Entropy = 96.36461 (cal/(mol*K))

C	1.217836	-0.719530	0.000000
C	1.217835	0.719530	0.000000
C	0.000000	-1.398122	0.000000
C	2.468555	-1.401162	0.000000
C	-0.000001	1.398122	0.000000
C	2.468555	1.401163	0.000000
C	-1.217834	-0.719531	0.000000
C	3.643806	-0.710490	0.000000
C	-1.217835	0.719530	0.000000
C	3.643805	0.710490	0.000000
C	-2.468556	-1.401163	0.000000
C	-2.468556	1.401163	0.000000
C	-3.643805	-0.710491	0.000000
C	-3.643805	0.710491	0.000000
H	0.000001	-2.482213	0.000000
H	2.466570	-2.484407	0.000000
H	0.000000	2.482213	0.000000
H	2.466571	2.484407	0.000000
H	4.586768	-1.241799	0.000000
H	4.586767	1.241801	0.000000
H	-2.466571	-2.484408	0.000000
H	-2.466570	2.484407	0.000000
H	-4.586768	-1.241799	0.000000
H	-4.586769	1.241798	0.000000

129-00-0-C16H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -616.053139587 (a.u.)
E(HF/CC-PVTZ) = -611.95325975
E(DLPNO-CCSD(T)/CC-PVTZ) = -614.596160427965
T1 (CC-PVTZ)= 0.010207142
T2 (CC-PVTZ)= 0.034203
E(HF/CC-PVQZ) = -611.98944783
E(DLPNO-CCSD(T)/CC-PVQZ) = -614.767750616100
E(HF/TZ-AUG) = -611.95748881
E(DLPNO-CCSD(T)/TZ-AUG) = -614.635851322
E(HF/TZ-CORE) = -611.95774321
E(DLPNO-CCSD(T)/TZ-CORE) = -615.409166584
E(HF/TZ-IT) = -611.95325974
E(DLPNO-CCSD(T)/TZ-IT) = -614.604739781
T1 (CC-PVQZ)= 0.010223271
T2 (CC-PVQZ)= 0.037329
E(HF/CBS) = -611.998265881
E(DLPNO-CCSD(T)/CBS) = -614.875375611
Enthalpic correction = 0.21161021 (a.u.)
Entropy = 98.73724 (cal/(mol*K))

C	-0.710203	0.000001	0.000000
C	0.710203	-0.000001	0.000000
C	1.422735	1.230944	-0.000001
C	1.422737	-1.230941	0.000001
C	-1.422737	-1.230945	0.000000
C	-1.422735	1.230940	0.000000
C	0.677563	2.454055	0.000000
C	2.820723	1.205665	0.000000
C	0.677565	-2.454055	0.000000
C	2.820724	-1.205664	-0.000001
C	-0.677563	-2.454055	0.000001
C	-2.820721	-1.205665	-0.000002
C	-0.677565	2.454054	0.000001
C	-2.820725	1.205664	0.000001
C	3.508394	0.000002	0.000000
C	-3.508394	0.000001	-0.000001
H	1.225325	3.388586	-0.000003
H	3.364947	2.142053	-0.000001
H	1.225327	-3.388585	0.000000
H	3.364947	-2.142052	-0.000005
H	-1.225323	-3.388587	0.000004
H	-3.364951	-2.142050	0.000000
H	-1.225330	3.388583	0.000003
H	-3.364944	2.142055	0.000005
H	4.590805	0.000001	0.000001
H	-4.590805	-0.000001	-0.000003

135-48-8-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.185723166 (a.u.)
E(HF/CC-PVTZ) = -841.53053226
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.179459606004
T1 (CC-PVTZ)= 0.010682938
T2 (CC-PVTZ)= 0.031789
E(HF/CC-PVQZ) = -841.58027992
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.415479616047
E(HF/TZ-AUG) = -841.53622934
E(DLPNO-CCSD(T)/TZ-AUG) = -845.234361646
E(HF/TZ-CORE) = -841.53672129
E(DLPNO-CCSD(T)/TZ-CORE) = -846.297339928
E(HF/TZ-IT) = -841.53053226
E(DLPNO-CCSD(T)/TZ-IT) = -845.191790386
T1 (CC-PVQZ)= 0.010665192
T2 (CC-PVQZ)= 0.037437
E(HF/CBS) = -841.592402072
E(DLPNO-CCSD(T)/CBS) = -845.56353024
Enthalpic correction = 0.29357959 (a.u.)
Entropy = 123.66749 (cal/(mol*K))

C	3.660833	-0.724752	0.000000
C	3.660833	0.724752	0.000000
C	4.919366	-1.404693	0.000000
C	2.456324	-1.402518	0.000000
C	4.919365	1.404692	0.000000
C	2.456324	1.402518	0.000000
C	6.089352	0.714120	0.000000
C	6.089351	-0.714119	0.000000
C	1.220583	-0.725621	0.000000

C	1.220583	0.725621	0.000000
C	0.000000	-1.403007	0.000000
C	0.000000	1.403007	0.000000
C	-1.220583	-0.725621	0.000000
C	-1.220583	0.725621	0.000000
C	-2.456325	-1.402518	0.000000
C	-2.456325	1.402518	0.000000
C	-3.660833	-0.724753	0.000000
C	-3.660833	0.724753	0.000000
C	-4.919366	-1.404693	0.000000
C	-4.919365	1.404693	0.000000
C	-6.089351	-0.714119	0.000000
C	-6.089352	0.714120	0.000000
H	4.918054	-2.487905	0.000000
H	2.456946	-2.486463	0.000000
H	4.918053	2.487905	0.000000
H	2.456946	2.486462	0.000000
H	7.033651	1.242999	0.000000
H	7.033651	-1.242998	-0.000001
H	0.000000	-2.486850	0.000000
H	0.000000	2.486850	0.000000
H	-2.456946	-2.486463	-0.000001
H	-2.456945	2.486462	0.000000
H	-4.918054	-2.487905	-0.000001
H	-4.918053	2.487905	0.000000
H	-7.033651	-1.242998	0.000001
H	-7.033650	1.242999	0.000001

135-70-6_C24H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -925.849387079 (a.u.)
E(HF/CC-PVTZ) = -919.63976165
E(DLPNO-CCSD(T)/CC-PVTZ) = -923.658484441535
T1 (CC-PVTZ)= 0.009851308
T2 (CC-PVTZ)= 0.038945
E(HF/CC-PVQZ) = -919.69482529
E(DLPNO-CCSD(T)/CC-PVQZ) = -923.917901083622
E(HF/TZ-AUG) = -919.64624307
E(DLPNO-CCSD(T)/TZ-AUG) = -923.718906531
E(HF/TZ-CORE) = -919.64663035
E(DLPNO-CCSD(T)/TZ-CORE) = -924.878020304
E(HF/TZ-IT) = -919.63976165
E(DLPNO-CCSD(T)/TZ-IT) = -923.670155472
T1 (CC-PVQZ)= 0.009926022
T2 (CC-PVQZ)= 0.040594
E(HF/CBS) = -919.708242802
E(DLPNO-CCSD(T)/CBS) = -924.080441057
Enthalpic correction = 0.35150457 (a.u.)
Entropy = 146.38940 (cal/(mol*K))

C	1.462225	-1.135036	-0.377395
C	0.737916	-0.000001	0.000003
C	1.462226	1.135035	0.377400
C	-0.737916	0.000000	0.000003
C	2.847230	-1.134319	-0.379194
C	2.847230	1.134318	0.379198
C	-1.462225	1.135034	-0.377399
C	-1.462226	-1.135034	0.377403
C	3.571108	-0.000001	0.000001
C	-2.847229	1.134318	-0.379198
C	-2.847230	-1.134317	0.379201
C	5.048327	0.000000	0.000000
C	-3.571108	0.000000	0.000001
C	5.767025	-0.665596	-0.998407
C	5.767027	0.665596	0.998405
C	-5.048327	0.000000	-0.000001
C	7.154845	-0.665535	-0.999021
C	7.154847	0.665537	0.999016
C	-5.767027	-0.665589	0.998409
C	-5.767025	0.665590	-0.998411
C	7.855682	0.000001	-0.000004
C	-7.154847	-0.665530	0.999020
C	-7.154845	0.665530	-0.999025
C	-7.855682	0.000000	-0.000003
H	0.932569	-2.025136	-0.690730
H	0.932570	2.025135	0.690735
H	3.377516	-2.033849	-0.663310
H	3.377517	2.033847	0.663313
H	-0.932569	2.025133	-0.690736
H	-0.932570	-2.025134	0.690742
H	-3.377516	2.033846	-0.663317
H	-3.377517	-2.033845	0.663319
H	5.231744	-1.165820	-1.794820
H	5.231747	1.165819	1.794819
H	7.690565	-1.179726	-1.786773
H	7.690568	1.179728	1.786766
H	-5.231747	-1.165808	1.794826
H	-5.231744	1.165809	-1.794827
H	8.937884	0.000002	-0.000005
H	-7.690568	-1.179716	1.786774
H	-7.690565	1.179717	-1.786780
H	-8.937884	0.000000	-0.000004

142-29-00_C5H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -195.419021334 (a.u.)
E(HF/CC-PVTZ) = -194.04355623
E(DLPNO-CCSD(T)/CC-PVTZ) = -194.957132999545
T1 (CC-PVTZ)= 0.009384996
T2 (CC-PVTZ)= 0.061265
E(HF/CC-PVQZ) = -194.05567125
E(DLPNO-CCSD(T)/CC-PVQZ) = -195.013868592415
E(HF/TZ-AUG) = -194.04484912
E(DLPNO-CCSD(T)/TZ-AUG) = -194.970234664
E(HF/TZ-CORE) = -194.04495275
E(DLPNO-CCSD(T)/TZ-CORE) = -195.210163144
E(HF/TZ-IT) = -194.04355623
E(DLPNO-CCSD(T)/TZ-IT) = -194.958561911
T1 (CC-PVQZ)= 0.009632777
T2 (CC-PVQZ)= 0.059971
E(HF/CBS) = -194.058623351
E(DLPNO-CCSD(T)/CBS) = -195.049381652
Enthalpic correction = 0.11847213 (a.u.)
Entropy = 69.73450 (cal/(mol*K))

C	0.664437	1.072012	-0.045876
C	-0.664429	1.072016	-0.045876
C	1.231498	-0.317019	0.100841
C	-1.231500	-0.317011	0.100841
C	-0.000004	-1.224062	-0.132377
H	1.285236	1.956952	-0.101809
H	-1.285222	1.956961	-0.101809
H	2.040237	-0.523214	-0.604109
H	-2.040241	-0.523200	-0.604109
H	1.653557	-0.452555	1.103599
H	-1.653560	-0.452544	1.103599
H	-0.000005	-1.571151	-1.167059
H	-0.000007	-2.106861	0.506384

1499-10-1_C26H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1002.09944544 (a.u.)
E(HF/CC-PVTZ) = -995.38963571
E(DLPNO-CCSD(T)/CC-PVTZ) = -999.730987490239
T1 (CC-PVTZ)= 0.010133450
T2 (CC-PVTZ)= 0.039356
E(HF/CC-PVQZ) = -995.44881965
E(DLPNO-CCSD(T)/CC-PVQZ) = -1000.010413812001
E(HF/TZ-AUG) = -995.39682647
E(DLPNO-CCSD(T)/TZ-AUG) = -999.797928791
E(HF/TZ-CORE) = -995.39703038
E(DLPNO-CCSD(T)/TZ-CORE) = -1001.05184973
E(HF/TZ-IT) = -995.38963571
E(DLPNO-CCSD(T)/TZ-IT) = -999.744418084
T1 (CC-PVQZ)= 0.010159979
T2 (CC-PVQZ)= 0.041300
E(HF/CBS) = -995.463241167
E(DLPNO-CCSD(T)/CBS) = -1000.18555274
Enthalpic correction = 0.36450665 (a.u.)
Entropy = 151.48199 (cal/(mol*K))

C	0.720053	-1.216577	0.002427
C	1.419838	-0.000000	-0.000000
C	0.720053	1.216577	-0.002427
C	2.908523	-0.000000	0.000000
C	-0.720054	-1.216577	-0.002442
C	1.397577	-2.472460	0.013835
C	-0.720054	1.216577	0.002442
C	1.397577	2.472460	-0.013835
C	3.618405	-0.126050	-1.193806
C	3.618405	0.126050	1.193806
C	-1.419839	0.000000	-0.000000
C	-1.397575	-2.472461	-0.013875
C	0.708830	-3.648568	0.008981
C	-1.397575	2.472461	0.013875
C	0.708830	3.648568	-0.008981
C	5.007934	-0.125809	-1.195034
C	5.007934	0.125809	1.195034
C	-2.908523	0.000000	0.000000
C	-0.708828	-3.648568	-0.009041
C	-0.708828	3.648568	0.009041
C	5.706590	-0.000000	0.000000
C	-3.618406	-0.126165	1.193794
C	-3.618406	0.126165	-1.193794
C	-5.007935	-0.125922	1.195022
C	-5.007935	0.125923	-1.195022
C	-5.706591	0.000000	0.000000
H	2.477949	-2.476577	0.027060
H	2.477949	2.476577	-0.027060
H	3.073072	-0.224625	-2.123772
H	3.073072	0.224624	2.123771
H	-2.477947	-2.476580	-0.027104
H	1.244069	-4.589368	0.018260
H	-2.477947	2.476580	0.027104
H	1.244069	4.589368	-0.018260
H	5.544821	-0.223303	-2.129981
H	5.544821	0.223303	2.129981
H	-1.244065	-4.589368	-0.018339
H	-1.244065	4.589368	0.018339
H	6.788898	-0.000000	0.000000
H	-3.073073	-0.224829	2.123750
H	-3.073073	0.224829	-2.123750
H	-5.544821	-0.223506	2.129960
H	-5.544822	0.223506	-2.129960
H	-6.788899	0.000000	0.000000

1530-12-7-C26H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1002.10932602 (a.u.)
E(HF/CC-PVTZ) = -995.40259422
E(DLPNO-CCSD(T)/CC-PVTZ) = -999.747982486298
T1 (CC-PVTZ)= 0.009875896
T2 (CC-PVTZ)= 0.033152
E(HF/CC-PVQZ) = -995.46152613
E(DLPNO-CCSD(T)/CC-PVQZ) = -1000.027767866546
E(HF/TZ-AUG) = -995.40972332
E(DLPNO-CCSD(T)/TZ-AUG) = -999.81652462
E(HF/TZ-CORE) = -995.40993585
E(DLPNO-CCSD(T)/TZ-CORE) = -1001.06881492
E(HF/TZ-IT) = -995.40259422
E(DLPNO-CCSD(T)/TZ-IT) = -999.760806161
T1 (CC-PVQZ)= 0.009912010
T2 (CC-PVQZ)= 0.037779
E(HF/CBS) = -995.475886234
E(DLPNO-CCSD(T)/CBS) = -1000.20329131
Enthalpic correction = 0.36471815 (a.u.)
Entropy = 141.28566 (cal/(mol*K))

C	-1.943171	-0.127865	-1.254594
C	-0.503460	-0.593270	-1.224606
C	-0.459280	-1.430618	0.039763
C	0.503460	0.593268	-1.224607
C	-2.625803	-0.583395	-0.116029
C	-2.583309	0.668610	-2.186969
C	-1.706544	-1.392849	0.685544
C	0.588957	-2.151877	0.586649
C	1.943171	0.127862	-1.254594
C	0.459280	1.430618	0.039761
C	-3.954881	-0.233878	0.093620
C	-3.916537	1.017803	-1.977023
C	-1.903986	-2.064393	1.885893
C	0.388854	-2.823078	1.791789
C	2.625803	0.583394	-0.116030
C	2.583308	-0.668614	-2.186969
C	1.706544	1.392850	0.685541
C	-0.588956	2.151879	0.586645
C	-4.593636	0.571387	-0.843756
C	-0.844830	-2.777326	2.436555
C	3.954880	0.233877	0.093619
C	3.916536	-1.017807	-1.977022
C	1.903987	2.064397	1.885889
C	-0.388852	2.823084	1.791783
C	4.593635	-0.571390	-0.843756
C	0.844831	2.777332	2.436548
H	-0.281655	-1.206806	-2.103074
H	0.281655	1.206803	-2.103075
H	-2.060144	1.027197	-3.065437
H	1.551647	-2.192726	0.096860
H	-4.486600	-0.576939	0.972079
H	-4.429401	1.641388	-2.697676
H	-2.863694	-2.035583	2.386286
H	1.202494	-3.385798	2.230854
H	2.060143	-1.027202	-3.065436
H	-1.551647	2.192727	0.096856
H	-5.627580	0.854065	-0.693122
H	-0.980382	-3.304305	3.372310
H	4.486600	0.576938	0.972078
H	4.429400	-1.641393	-2.697675
H	2.863695	2.035588	2.386281
H	-1.202492	3.385805	2.230846

H	5.627578	-0.854068	-0.693122
H	0.980385	3.304313	3.372302

1576-69-8-C16H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -618.460497170 (a.u.)
E(HF/CC-PVTZ) = -614.27594308
E(DLPNO-CCSD(T)/CC-PVTZ) = -616.994314075425
T1 (CC-PVTZ)= 0.009795003
T2 (CC-PVTZ)= 0.036018
E(HF/CC-PVQZ) = -614.31268855
E(DLPNO-CCSD(T)/CC-PVQZ) = -617.168630048637
E(HF/TZ-AUG) = -614.28004133
E(DLPNO-CCSD(T)/TZ-AUG) = -617.035169964
E(HF/TZ-CORE) = -614.28042623
E(DLPNO-CCSD(T)/TZ-CORE) = -617.8068901
E(HF/TZ-IT) = -614.27594308
E(DLPNO-CCSD(T)/TZ-IT) = -617.001972435
T1 (CC-PVQZ)= 0.009870272
T2 (CC-PVQZ)= 0.037412
E(HF/CBS) = -614.321642422
E(DLPNO-CCSD(T)/CBS) = -617.277973207
Enthalpic correction = 0.25505630 (a.u.)
Entropy = 115.42245 (cal/(mol*K))

C	-3.566251	-0.251469	0.000000
C	-5.069144	-0.234314	-0.000002
C	-2.826626	0.909652	0.000000
C	-2.869601	-1.475916	0.000002
C	-1.417232	0.898660	0.000000
C	-1.496127	-1.517549	0.000002
C	-0.723914	-0.338659	0.000000
C	-0.677175	2.120977	0.000000
C	0.723914	-0.338659	-0.000001
C	0.677175	2.120976	0.000001
C	1.417232	0.898660	0.000001
C	1.496127	-1.517549	-0.000001
C	2.826626	0.909652	0.000000
C	2.869601	-1.475916	-0.000001
C	3.566252	-0.251469	-0.000001
C	5.069144	-0.234314	0.000000
H	-5.454053	0.785238	0.000008
H	-5.468703	-0.746095	-0.879093
H	-5.468706	-0.746114	0.879076
H	-3.332267	1.868834	0.000000
H	-3.430527	-2.403239	0.000004
H	-1.007547	-2.481341	0.000005
H	-1.226873	3.054429	0.000001
H	1.226873	3.054429	0.000002
H	1.007548	-2.481341	-0.000002
H	3.332266	1.868834	0.000001
H	3.430527	-2.403238	-0.000002
H	5.468704	-0.746105	-0.879084
H	5.454053	0.785238	0.000000
H	5.468704	-0.746105	0.879084

173678-72-3-C20H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -768.500592637 (a.u.)
E(HF/CC-PVTZ) = -763.42490572
E(DLPNO-CCSD(T)/CC-PVTZ) = -766.695646899847
T1 (CC-PVTZ)= 0.010692921
T2 (CC-PVTZ)= 0.033356
E(HF/CC-PVQZ) = -763.46953838
E(DLPNO-CCSD(T)/CC-PVQZ) = -766.908251031647
E(HF/TZ-AUG) = -763.43025502
E(DLPNO-CCSD(T)/TZ-AUG) = -766.745709905
E(HF/TZ-CORE) = -763.43052277
E(DLPNO-CCSD(T)/TZ-CORE) = -767.711539112
E(HF/TZ-IT) = -763.42490572
E(DLPNO-CCSD(T)/TZ-IT) = -766.707037529
T1 (CC-PVQZ)= 0.010717094
T2 (CC-PVQZ)= 0.037181
E(HF/CBS) = -763.480414146
E(DLPNO-CCSD(T)/CBS) = -767.041700574
Enthalpic correction = 0.23643453 (a.u.)
Entropy = 107.95891 (cal/(mol*K))

C	-2.851920	1.745695	0.000016
C	-3.484766	0.489226	0.000021
C	-2.722467	-0.680365	-0.000002
C	-1.335918	-0.546673	-0.000035
C	-0.688089	-1.835914	-0.000024
C	0.688089	-1.835914	-0.000023
C	1.335918	-0.546673	-0.000034
C	2.722467	-0.680365	-0.000002
C	3.484766	0.489225	0.000023
C	2.851920	1.745695	0.000017
C	1.451963	1.876921	-0.000009
C	0.683009	3.101620	0.000005
C	-0.683009	3.101621	0.000005
C	-1.451963	1.876921	-0.000010
C	-0.703272	0.682761	-0.000037
C	0.703272	0.682761	-0.000036
C	-1.793347	-2.806923	0.000007
C	-2.978070	-2.136189	0.000026
C	2.978070	-2.136189	0.000019
C	1.793347	-2.806923	0.000012
H	-3.467339	2.637304	0.000038
H	-4.567171	0.449787	0.000051
H	4.567171	0.449787	0.000050
H	3.467339	2.637304	0.000040
H	1.213240	4.046381	0.000021
H	-1.213240	4.046382	0.000020
H	-1.678194	-3.879761	0.000018
H	-3.956004	-2.594658	0.000054
H	3.956004	-2.594657	0.000042
H	1.678194	-3.879761	0.000027

1828-89-32_C6H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -230.994279462 (a.u.)
E(HF/CC-PVTZ) = -229.44715119
E(DLPNO-CCSD(T)/CC-PVTZ) = -230.449792275358
T1 (CC-PVTZ)= 0.013526861
T2 (CC-PVTZ)= 0.055885
E(HF/CC-PVQZ) = -229.4614053
E(DLPNO-CCSD(T)/CC-PVQZ) = -230.514848944668
E(HF/TZ-AUG) = -229.44918975
E(DLPNO-CCSD(T)/TZ-AUG) = -230.464582514
E(HF/TZ-CORE) = -229.44916693
E(DLPNO-CCSD(T)/TZ-CORE) = -230.754650582
E(HF/TZ-IT) = -229.44715119
E(DLPNO-CCSD(T)/TZ-IT) = -230.452356089
T1 (CC-PVQZ)= 0.013504053
T2 (CC-PVQZ)= 0.054447

E(HF/CBS) = -229.464878639
E(DLPNO-CCSD(T)/CBS) = -230.555394422
Enthalpic correction = 0.07680675 (a.u.)
Entropy = 68.35840 (cal/(mol*K))

C	0.000000	0.000000	1.742607
C	0.000000	0.803809	0.666591
C	0.000000	-0.803809	0.666591
C	0.000000	1.162999	-0.661933
C	0.000000	-1.162999	-0.661933
C	0.000000	0.000000	-1.453940
H	0.000000	0.000000	2.825268
H	0.000000	2.175166	-1.037023
H	0.000000	-2.175166	-1.037023
H	0.000000	0.000000	-2.539113

187-78-0-C14H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -538.500024459 (a.u.)
E(HF/CC-PVTZ) = -534.93097961
E(DLPNO-CCSD(T)/CC-PVTZ) = -537.237122914210
T1 (CC-PVTZ)= 0.010982685
T2 (CC-PVTZ)= 0.044300
E(HF/CC-PVQZ) = -534.96253854
E(DLPNO-CCSD(T)/CC-PVQZ) = -537.386409549127
E(HF/TZ-AUG) = -534.93485821
E(DLPNO-CCSD(T)/TZ-AUG) = -537.271542752
E(HF/TZ-CORE) = -534.9349739
E(DLPNO-CCSD(T)/TZ-CORE) = -537.948032476
E(HF/TZ-IT) = -534.93097961
E(DLPNO-CCSD(T)/TZ-IT) = -537.244784481
T1 (CC-PVQZ)= 0.010983157
T2 (CC-PVQZ)= 0.044315
E(HF/CBS) = -534.970228593
E(DLPNO-CCSD(T)/CBS) = -537.480009009
Enthalpic correction = 0.17500683 (a.u.)
Entropy = 92.89392 (cal/(mol*K))

C	2.839920	0.680791	0.000002
C	2.839919	-0.680792	-0.000004
C	1.435602	-1.177591	-0.000005
C	0.722937	-2.363190	0.000002
C	-0.722936	-2.363190	0.000006
C	-1.435603	-1.177591	0.000006
C	-0.673981	0.000000	0.000007
C	-1.435603	1.177592	0.000005
C	-0.722938	2.363189	0.000006
C	0.722938	2.363189	0.000002
C	1.435603	1.177592	-0.000004
C	0.673981	0.000000	-0.000009
C	-2.839919	0.680792	-0.000009
C	-2.839919	-0.680792	-0.000004
H	3.723571	1.301245	0.000002
H	3.723570	-1.301246	-0.000007
H	1.224173	-3.323412	0.000004
H	-1.224172	-3.323412	0.000001
H	-1.224171	3.323413	0.000001
H	1.224170	3.323413	0.000006
H	-3.723571	1.301245	-0.000013
H	-3.723570	-1.301246	-0.000005

187-83-7-C26H16

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1000.90972189 (a.u.)
E(HF/CC-PVTZ) = -994.2304627
E(DLPNO-CCSD(T)/CC-PVTZ) = -998.545079632673
T1 (CC-PVTZ)= 0.010072331
T2 (CC-PVTZ)= 0.035315
E(HF/CC-PVQZ) = -994.28915619
E(DLPNO-CCSD(T)/CC-PVQZ) = -998.823449797613
E(HF/TZ-AUG) = -994.23760197
E(DLPNO-CCSD(T)/TZ-AUG) = -998.612574942
E(HF/TZ-CORE) = -994.23779114
E(DLPNO-CCSD(T)/TZ-CORE) = -999.866202933
E(HF/TZ-IT) = -994.2304627
E(DLPNO-CCSD(T)/TZ-IT) = -998.559298086
T1 (CC-PVQZ)= 0.010087287
T2 (CC-PVQZ)= 0.037272
E(HF/CBS) = -994.303458198
E(DLPNO-CCSD(T)/CBS) = -998.998056406
Enthalpic correction = 0.34234030 (a.u.)
Entropy = 133.89550 (cal/(mol*K))

C	1.542424	-0.531339	0.513958
C	2.777411	-1.176101	0.225712
C	1.284758	0.785339	-0.034593
C	0.658807	-1.185895	1.398129
C	3.787846	-0.474440	-0.493111
C	3.016974	-2.478078	0.712753
C	3.620204	0.832983	-0.807704
C	2.389470	1.504358	-0.545325
C	2.292258	2.905255	-0.752903
C	-0.000001	1.445124	0.000000
C	-0.000003	2.865956	0.000000
C	1.165313	3.574219	-0.393542
C	-1.165320	3.574217	0.393542
C	-1.284760	0.785336	0.034594
C	-2.292264	2.905251	0.752903
C	-2.389473	1.504353	0.545325
C	-3.620206	0.832977	0.807704
C	-1.542423	-0.531341	-0.513958
C	-3.787846	-0.474447	0.493109
C	-2.777409	-1.176106	-0.225713
C	-3.016970	-2.478083	-0.712755
C	-0.658804	-1.185897	-1.398127
C	-0.928913	-2.440216	-1.888753
C	-2.104388	-3.111654	-1.518757
C	0.928920	-2.440215	1.888754
C	2.104394	-3.111650	1.518757
H	-0.244225	-0.686367	1.709344
H	4.715675	-0.985241	-0.718975
H	3.953639	-2.959615	0.459243
H	4.421005	1.397695	-1.269014
H	3.158625	3.435924	-1.127379
H	1.122015	4.655291	-0.437835
H	-1.122024	4.655289	0.437834
H	-3.158632	3.435918	1.127379
H	-4.421008	1.397686	1.269014
H	-4.715674	-0.985249	0.718973
H	-3.953634	-2.959622	-0.459246
H	0.244228	-0.686366	-1.709341
H	-0.229820	-2.909628	-2.568439
H	-2.302381	-4.107766	-1.892602
H	0.229827	-2.909628	2.568441
H	2.302390	-4.107762	1.892601

188-96-5-C26H14

Charge of molecule: 0

Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -999.745946543 (a.u.)
E(HF/CC-PVTZ) = -993.11722958
E(DLPNO-CCSD(T)/CC-PVTZ) = -997.385662807776
T1 (CC-PVTZ)= 0.010244873
T2 (CC-PVTZ)= 0.034830
E(HF/CC-PVQZ) = -993.17537625
E(DLPNO-CCSD(T)/CC-PVQZ) = -997.662832019476
E(HF/TZ-AUG) = -993.12408075
E(DLPNO-CCSD(T)/TZ-AUG) = -997.451405335
E(HF/TZ-CORE) = -993.12447847
E(DLPNO-CCSD(T)/TZ-CORE) = -998.706630072
E(HF/TZ-IT) = -993.11722958
E(DLPNO-CCSD(T)/TZ-IT) = -997.400335966
T1 (CC-PVQZ)= 0.010249343
T2 (CC-PVQZ)= 0.037290
E(HF/CBS) = -993.189545013
E(DLPNO-CCSD(T)/CBS) = -997.836828042
Enthalpic correction = 0.32091019 (a.u.)
Entropy = 129.94596 (cal/(mol*K))

C	-0.709255	1.237453	0.000008
C	0.709255	1.237453	-0.000008
C	1.414053	-0.000001	-0.000004
C	1.471758	2.447692	-0.000030
C	-1.414053	-0.000001	0.000004
C	-1.471758	2.447692	0.000030
C	-0.709256	-1.237454	0.000002
C	-2.842687	0.000000	0.000003
C	0.709256	-1.237454	-0.000002
C	-1.471759	-2.447693	0.000005
C	1.471759	-2.447693	-0.000005
C	2.842687	0.000000	-0.000003
C	-2.826910	2.444996	0.000030
C	-3.564528	1.224443	0.000009
C	-4.963530	1.202304	-0.000001
C	-3.564528	-1.224443	-0.000006
C	3.564528	1.224443	-0.000009
C	3.564528	-1.224443	0.000006
C	2.826910	2.444996	-0.000030
C	4.963530	1.202304	0.000001
C	2.826911	-2.444996	0.000000
C	4.963531	-1.202303	0.000016
C	-2.826911	-2.444996	0.000000
C	-4.963531	-1.202303	-0.000016
C	-5.654558	0.000000	-0.000015
C	5.654558	0.000001	0.000015
H	0.959503	3.397267	-0.000061
H	-0.959503	3.397267	0.000062
H	-0.959506	-3.397268	0.000018
H	0.959505	-3.397268	-0.000017
H	-3.373492	3.380056	0.000050
H	-5.502774	2.141469	0.000003
H	3.373492	3.380056	-0.000050
H	5.502774	2.141469	-0.000003
H	3.373494	-3.380055	-0.000002
H	5.502775	-2.141468	0.000024
H	-3.373494	-3.380055	0.000002
H	-5.502775	-2.141468	-0.000024
H	-6.736898	0.000001	-0.000024
H	6.736898	0.000001	0.000023

189-45-7-C32H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1230.88791052 (a.u.)
E(HF/CC-PVTZ) = -1222.70756013
E(DLPNO-CCSD(T)/CC-PVTZ) = -1227.979415722360
T1 (CC-PVTZ)= 0.010424731
T2 (CC-PVTZ)= 0.034494
E(HF/CC-PVQZ) = -1222.77926431
E(DLPNO-CCSD(T)/CC-PVQZ) = -1228.320964731211
E(HF/TZ-AUG) = -1222.71589918
E(DLPNO-CCSD(T)/TZ-AUG) = -1228.0603775
E(HF/TZ-CORE) = -1222.71650802
E(DLPNO-CCSD(T)/TZ-CORE) = -1229.60527344
E(HF/TZ-IT) = -1222.70756013
E(DLPNO-CCSD(T)/TZ-IT) = -1227.99759194
T1 (CC-PVQZ)= 0.010427318
T2 (CC-PVQZ)= 0.037464
E(HF/CBS) = -1222.79673667
E(DLPNO-CCSD(T)/CBS) = -1228.53535088
Enthalpic correction = 0.40323410 (a.u.)
Entropy = 154.22339 (cal/(mol*K))

C	8.151619	-0.312747	0.000046
C	7.900427	1.087609	0.000067
C	7.118108	-1.199864	0.000018
C	6.622365	1.560333	0.000058
C	5.511058	0.668695	0.000028
C	5.765866	-0.747345	0.000009
C	4.195719	1.127370	0.000017
C	4.684500	-1.617869	-0.000014
C	3.361867	-1.158108	-0.000022
C	3.100015	0.261205	-0.000011
C	1.735400	0.718450	-0.000026
C	2.280090	-2.059599	-0.000035
C	0.971890	-1.625298	-0.000035
C	0.683071	-0.215768	-0.000030
C	-0.683071	0.215768	-0.000030
C	-0.123546	-2.542561	-0.000042
C	1.406716	2.112165	-0.000039
C	-1.735400	-0.718450	-0.000026
C	-1.406716	-2.112165	-0.000037
C	-3.100015	-0.261205	-0.000011
C	-0.971890	1.625298	-0.000036
C	-2.280090	2.059599	-0.000035
C	-3.361867	1.158108	-0.000021
C	-4.684500	1.617869	-0.000013
C	-4.195719	-1.127370	0.000015
C	0.123546	2.542561	-0.000045
C	-5.511058	-0.668695	0.000027
C	-5.765866	0.747345	0.000010
C	-7.118108	1.199864	0.000020
C	-6.622366	-1.560333	0.000056
C	-8.151619	0.312747	0.000047
C	-7.900427	-1.087610	0.000066
H	9.173862	-0.668364	0.000053
H	8.735135	1.776514	0.000090
H	7.306376	-2.266566	0.000003
H	6.429914	2.626406	0.000074
H	4.043402	2.197056	0.000037
H	4.863906	-2.686811	-0.000024
H	2.487134	-3.123247	-0.000044
H	0.096517	-3.603015	-0.000054
H	2.199588	2.844660	-0.000052
H	-2.199588	-2.844660	-0.000048
H	-2.487134	3.123247	-0.000044
H	-4.863906	2.686811	-0.000022
H	-4.043401	-2.197056	0.000033
H	-0.096517	3.603015	-0.000058
H	-7.306376	2.266566	0.000006
H	-6.429914	-2.626406	0.000070
H	-9.173862	0.668364	0.000055
H	-8.735135	-1.776514	0.000088

189-55-9_C24H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -923.477665101 (a.u.)
E(HF/CC-PVTZ) = -917.34080591
E(DLPNO-CCSD(T)/CC-PVTZ) = -921.295946343930
T1 (CC-PVTZ)= 0.010250397
T2 (CC-PVTZ)= 0.035342
E(HF/CC-PVQZ) = -917.39477461
E(DLPNO-CCSD(T)/CC-PVQZ) = -921.552528058462
E(HF/TZ-AUG) = -917.34715108
E(DLPNO-CCSD(T)/TZ-AUG) = -921.356413125
E(HF/TZ-CORE) = -917.34752473
E(DLPNO-CCSD(T)/TZ-CORE) = -922.515252854
E(HF/TZ-IT) = -917.34080591
E(DLPNO-CCSD(T)/TZ-IT) = -921.309082987
T1 (CC-PVQZ)= 0.010250952
T2 (CC-PVQZ)= 0.037624
E(HF/CBS) = -917.407925315
E(DLPNO-CCSD(T)/CBS) = -921.713531504
Enthalpic correction = 0.30771415 (a.u.)
Entropy = 126.69126 (cal/(mol*K))

C	-3.546958	0.525458	0.000002
C	-2.871036	-0.728571	-0.000004
C	-3.655356	-1.902118	0.000005
C	-1.429520	-0.744429	-0.000015
C	-4.961178	0.553362	0.000013
C	-2.797412	1.723088	0.000001
C	-5.691244	-0.606425	0.000020
C	-5.028331	-1.846572	0.000017
C	-0.712475	0.472373	-0.000009
C	-0.682067	-1.947794	-0.000032
C	-1.423887	1.723145	-0.000002
C	0.712476	0.472373	-0.000010
C	-0.673380	2.951216	0.000000
C	1.423887	1.723145	-0.000006
C	1.429520	-0.744429	-0.000014
C	0.673381	2.951216	-0.000002
C	2.797412	1.723087	-0.000006
C	2.871036	-0.728571	-0.000003
C	0.682067	-1.947794	-0.000031
C	3.546958	0.525458	-0.000002
C	3.655355	-1.902118	0.000013
C	4.961178	0.553362	0.000006
C	5.028331	-1.846572	0.000025
C	5.691244	-0.606425	0.000019
H	-3.176323	-2.870092	0.000006
H	-5.458624	1.515569	0.000018
H	-3.328763	2.667749	0.000006
H	-6.772904	-0.571589	0.000029
H	-5.602990	-2.763656	0.000025
H	-1.195864	-2.897476	-0.000049
H	-1.225407	3.883106	0.000005
H	1.225408	3.883106	0.000001
H	3.328763	2.667748	-0.000005
H	1.195864	-2.897475	-0.000048
H	3.176322	-2.870092	0.000021
H	5.458623	1.515569	0.000005
H	5.602990	-2.763656	0.000039
H	6.772904	-0.571589	0.000027

189-64-0-C24H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -923.473750268 (a.u.)
E(HF/CC-PVTZ) = -917.33427477
E(DLPNO-CCSD(T)/CC-PVTZ) = -921.291546775407
T1 (CC-PVTZ)= 0.010292435
T2 (CC-PVTZ)= 0.034754
E(HF/CC-PVQZ) = -917.38825492
E(DLPNO-CCSD(T)/CC-PVQZ) = -921.548108491567
E(HF/TZ-AUG) = -917.34067327
E(DLPNO-CCSD(T)/TZ-AUG) = -921.352092299
E(HF/TZ-CORE) = -917.34098779
E(DLPNO-CCSD(T)/TZ-CORE) = -922.51095529
E(HF/TZ-IT) = -917.33427477
E(DLPNO-CCSD(T)/TZ-IT) = -921.30485639
T1 (CC-PVQZ)= 0.010282657
T2 (CC-PVQZ)= 0.037624
E(HF/CBS) = -917.401408415
E(DLPNO-CCSD(T)/CBS) = -921.709091778
Enthalpic correction = 0.30763811 (a.u.)
Entropy = 126.52728 (cal/(mol*K))

C	0.695132	-0.167840	-0.000015
C	1.081951	-1.547643	-0.000019
C	-0.695132	0.167840	-0.000015
C	1.684010	0.841510	-0.000011
C	0.056624	-2.542699	-0.000026
C	2.422890	-1.883822	-0.000020
C	-1.254838	-2.207864	-0.000020
C	-1.684010	-0.841510	-0.000009
C	-3.068160	-0.479632	0.000005
C	-1.081951	1.547643	-0.000020
C	3.068160	0.479632	0.000005
C	1.254838	2.207864	-0.000026
C	3.427895	-0.905530	-0.000005
C	4.118039	1.431982	0.000036
C	4.800130	-1.268950	0.000002
C	5.433016	1.048486	0.000046
C	5.782009	-0.319142	0.000025
C	-3.427895	0.905530	-0.000003
C	-4.118039	-1.431982	0.000029
C	-2.422890	1.883822	-0.000017
C	-4.800130	1.268949	0.000007
C	-0.056624	2.542700	-0.000031
C	-5.433016	-1.048486	0.000040
C	-5.782009	0.319142	0.000027
H	0.353733	-3.584253	-0.000036
H	2.708220	-2.929316	-0.000029
H	-1.992322	-2.996096	-0.000030
H	1.992322	2.996096	-0.000043
H	3.887050	2.486668	0.000060
H	5.052737	-2.322244	-0.000009
H	6.211739	1.800105	0.000072
H	6.824606	-0.609317	0.000031
H	-3.887050	-2.486668	0.000045
H	-2.708221	2.929315	-0.000025
H	-5.052737	2.322244	-0.000001
H	-0.353733	3.584253	-0.000046
H	-6.211739	-1.800105	0.000061
H	-6.824606	0.609318	0.000035

190-26-1-C32H14

Charge of molecule: 0

Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1228.56319542 (a.u.)
E(HF/CC-PVTZ) = -1220.4713091
E(DLPNO-CCSD(T)/CC-PVTZ) = -1225.670494845291
T1 (CC-PVTZ)= 0.010097653
T2 (CC-PVTZ)= 0.034129
E(HF/CC-PVQZ) = -1220.54180812
E(DLPNO-CCSD(T)/CC-PVQZ) = -1226.008883248215
E(HF/TZ-AUG) = -1220.479144
E(DLPNO-CCSD(T)/TZ-AUG) = -1225.75098206
E(HF/TZ-CORE) = -1220.48020869
E(DLPNO-CCSD(T)/TZ-CORE) = -1227.29654547
E(HF/TZ-IT) = -1220.4713091
E(DLPNO-CCSD(T)/TZ-IT) = -1225.68929241
T1 (CC-PVQZ)= 0.010093014
T2 (CC-PVQZ)= 0.037139
E(HF/CBS) = -1220.55898681
E(DLPNO-CCSD(T)/CBS) = -1226.22154879
Enthalpic correction = 0.36087408 (a.u.)
Entropy = 136.28175 (cal/(mol*K))

C	-2.454226	-0.710470	-0.000001
C	-2.454223	0.710475	0.000002
C	-3.681630	-1.417149	-0.000001
C	-1.223016	-1.420704	-0.000001
C	-3.681635	1.417153	0.000005
C	-1.223019	1.420702	-0.000002
C	-4.886866	0.687260	0.000008
C	-3.650399	2.844571	0.000003
C	-4.886867	-0.687259	0.000003
C	-3.650402	-2.844568	-0.000004
C	-0.000004	-0.714719	-0.000001
C	-1.219242	-2.846883	-0.000004
C	-0.000003	0.714721	-0.000001
C	1.223021	-1.420706	0.000000
C	1.223020	1.420703	-0.000002
C	-1.219236	2.846887	-0.000002
C	2.454224	-0.710478	-0.000001
C	1.219245	-2.846879	0.000000
C	2.454226	0.710474	0.000001
C	3.681628	-1.417156	0.000003
C	3.681625	1.417153	0.000001
C	1.219252	2.846878	-0.000001
C	4.886876	-0.687251	0.000002
C	3.650401	-2.844559	0.000002
C	4.886877	0.687250	0.000002
C	3.650404	2.844558	0.000000
C	-2.476119	3.527945	-0.000003
C	-0.000004	3.525709	-0.000005
C	2.476114	3.527939	-0.000001
C	2.476111	-3.527940	0.000002
C	-0.000009	-3.525710	-0.000001
C	-2.476125	-3.527945	-0.000004
H	-5.824713	1.229184	0.000015
H	-4.592333	3.379519	0.000012
H	-5.824713	-1.229182	0.000002
H	-4.592340	-3.379510	-0.000007
H	5.824710	-1.229197	0.000001
H	4.592328	-3.379520	0.000001
H	5.824711	1.229194	0.000003
H	4.592337	3.379506	0.000001
H	-2.474045	4.611042	-0.000011
H	0.000008	4.609553	-0.000010
H	2.474048	4.611035	-0.000004
H	2.474047	-4.611036	0.000005
H	0.000004	-4.609554	0.000001
H	-2.474043	-4.611041	-0.000006

190-31-8-C30H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1152.27981870 (a.u.)
E(HF/CC-PVTZ) = -1144.67265581
E(DLPNO-CCSD(T)/CC-PVTZ) = -1149.564507125121
T1 (CC-PVTZ)= 0.010205622
T2 (CC-PVTZ)= 0.037702
E(HF/CC-PVQZ) = -1144.73901219
E(DLPNO-CCSD(T)/CC-PVQZ) = -1149.882423675962
E(HF/TZ-AUG) = -1144.68011631
E(DLPNO-CCSD(T)/TZ-AUG) = -1149.64014523
E(HF/TZ-CORE) = -1144.68100783
E(DLPNO-CCSD(T)/TZ-CORE) = -1151.088893
E(HF/TZ-IT) = -1144.6726558
E(DLPNO-CCSD(T)/TZ-IT) = -1149.58204041
T1 (CC-PVQZ)= 0.010198070
T2 (CC-PVQZ)= 0.038780
E(HF/CBS) = -1144.75518144
E(DLPNO-CCSD(T)/CBS) = -1150.08216386
Enthalpic correction = 0.34735934 (a.u.)
Entropy = 134.74442 (cal/(mol*K))

C	-1.534396	2.855953	-0.000002
C	-1.554941	1.426311	0.000001
C	-0.298329	3.531769	0.000022
C	-2.756549	3.560596	-0.000040
C	-0.326780	0.717264	0.000008
C	-2.801233	0.733095	-0.000020
C	-2.801233	-0.733095	0.000019
C	-3.970918	1.481103	-0.000081
C	0.902393	2.851560	0.000033
C	0.895207	1.417447	0.000019
C	2.166638	3.531628	0.000050
C	2.128085	0.709242	0.000011
C	-0.326780	-0.717264	-0.000008
C	3.333851	2.847765	0.000046
C	3.358780	1.414617	0.000023
C	4.558663	0.690010	0.000011
C	2.128084	-0.709242	-0.000011
C	0.895207	-1.417447	-0.000019
C	-1.554941	-1.426311	-0.000001
C	-1.534395	-2.855953	0.000003
C	-3.970918	-1.481103	0.000080
C	0.902394	-2.851560	-0.000033
C	-0.298329	-3.531768	-0.000021
C	2.166639	-3.531627	-0.000050
C	-2.756548	-3.560596	0.000041
C	-3.948686	-2.879817	0.000088
C	3.358779	-1.414617	-0.000024
C	3.333852	-2.847764	-0.000046
C	4.558662	-0.690009	-0.000012
C	-3.948687	2.879817	-0.000088
H	-0.297420	4.615418	0.000027
H	-2.737566	4.643165	-0.000040
H	-4.930933	0.986673	-0.000138
H	2.163633	4.614662	0.000066
H	4.279161	3.376678	0.000058
H	5.496856	1.231261	0.000021
H	-4.930934	-0.986674	0.000133
H	-0.297420	-4.615418	-0.000024
H	2.163633	-4.614662	-0.000065
H	-2.737566	-4.643165	0.000041
H	-4.884441	-3.423788	0.000135
H	4.279162	-3.376677	-0.000058
H	5.496856	-1.231261	-0.000023

H	-4.884441	3.423787	-0.000133

190-39-6-C28H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1075.99003075 (a.u.)
E(HF/CC-PVTZ) = -1068.86297992
E(DLPNO-CCSD(T)/CC-PVTZ) = -1073.450949405553
T1 (CC-PVTZ)= 0.010372483
T2 (CC-PVTZ)= 0.037596
E(HF/CC-PVQZ) = -1068.92513536
E(DLPNO-CCSD(T)/CC-PVQZ) = -1073.748173334789
E(HF/TZ-AUG) = -1068.87001088
E(DLPNO-CCSD(T)/TZ-AUG) = -1073.52166708
E(HF/TZ-CORE) = -1068.870773
E(DLPNO-CCSD(T)/TZ-CORE) = -1074.87341727
E(HF/TZ-IT) = -1068.86297992
E(DLPNO-CCSD(T)/TZ-IT) = -1073.46744802
T1 (CC-PVQZ)= 0.010328291
T2 (CC-PVQZ)= 0.038741
E(HF/CBS) = -1068.94028095
E(DLPNO-CCSD(T)/CBS) = -1073.93485539
Enthalpic correction = 0.33371699 (a.u.)
Entropy = 134.28037 (cal/(mol*K))

C	-1.224350	-1.426050	-0.000005
C	-1.216788	-2.861538	-0.000008
C	0.000000	-3.539790	-0.000006
C	1.216787	-2.861538	0.000000
C	2.449207	-3.564066	0.000009
C	3.631843	-2.880825	0.000021
C	3.643630	-1.475584	0.000019
C	2.476463	-0.733264	0.000004
C	2.476463	0.733264	-0.000004
C	3.643630	1.475584	-0.000019
C	3.631842	2.880825	-0.000021
C	2.449207	3.564066	-0.000009
C	1.216787	2.861537	0.000000
C	0.000000	3.539790	0.000006
C	-1.216787	2.861537	0.000008
C	-1.224350	1.426051	0.000005
C	0.000000	0.723345	0.000002
C	1.224349	1.426051	0.000001
C	0.000000	-0.723345	-0.000002
C	1.224350	-1.426051	-0.000001
C	-2.449207	3.564066	0.000011
C	-3.631842	2.880825	0.000009
C	-3.643630	1.475584	0.000004
C	-2.476462	0.733264	0.000002
C	-2.476463	-0.733263	-0.000002
C	-3.643630	-1.475584	-0.000004
C	-3.631843	-2.880825	-0.000009
C	-2.449208	-3.564066	-0.000011
H	0.000000	-4.623203	-0.000007
H	2.431154	-4.646560	0.000009
H	4.572212	-3.416740	0.000032
H	4.602041	-0.978262	0.000032
H	4.602041	0.978263	-0.000032
H	4.572211	3.416740	-0.000032
H	2.431153	4.646560	-0.000009
H	0.000000	4.623203	0.000007
H	-2.431153	4.646559	0.000014
H	-4.572211	3.416740	0.000010
H	-4.602041	0.978263	0.000001
H	-4.602041	-0.978262	-0.000002
H	-4.572212	-3.416740	-0.000010
H	-2.431154	-4.646560	-0.000014

190-55-6-C30H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1152.27161237 (a.u.)
E(HF/CC-PVTZ) = -1144.66116154
E(DLPNO-CCSD(T)/CC-PVTZ) = -1149.554194389300
T1 (CC-PVTZ)= 0.010489452
T2 (CC-PVTZ)= 0.033136
E(HF/CC-PVQZ) = -1144.72766874
E(DLPNO-CCSD(T)/CC-PVQZ) = -1149.872237124584
E(HF/TZ-AUG) = -1144.66880275
E(DLPNO-CCSD(T)/TZ-AUG) = -1149.62994541
E(HF/TZ-CORE) = -1144.66952084
E(DLPNO-CCSD(T)/TZ-CORE) = -1151.07855874
E(HF/TZ-IT) = -1144.66116154
E(DLPNO-CCSD(T)/TZ-IT) = -1149.57208734
T1 (CC-PVQZ)= 0.010462436
T2 (CC-PVQZ)= 0.037268
E(HF/CBS) = -1144.74387474
E(DLPNO-CCSD(T)/CBS) = -1150.07199608
Enthalpic correction = 0.34723706 (a.u.)
Entropy = 133.82493 (cal/(mol*K))

C	1.430004	-2.469683	0.000000
C	0.674706	-3.696753	-0.000001
C	-0.674705	-3.696753	0.000000
C	0.701659	-1.229131	0.000000
C	2.804515	-2.450157	-0.000001
C	3.539076	-1.235508	0.000000
C	-1.430003	-2.469683	0.000000
C	-0.701659	-1.229131	0.000000
C	-2.804515	-2.450157	0.000001
C	-1.412484	0.000000	0.000000
C	1.412484	0.000000	-0.000001
C	-3.539076	-1.235508	0.000000
C	-2.826896	0.000000	0.000000
C	-4.941701	-1.206567	0.000000
C	-3.539076	1.235508	0.000000
C	-0.701659	1.229131	0.000000
C	0.701659	1.229131	-0.000001
C	2.826896	0.000000	0.000000
C	3.539076	1.235508	0.000000
C	4.941701	-1.206567	0.000000
C	1.430004	2.469683	0.000000
C	2.804515	2.450157	0.000000
C	0.674706	3.696753	-0.000001
C	4.941701	1.206567	0.000000
C	5.626665	0.000000	0.000001
C	-1.430004	2.469684	0.000000
C	-0.674705	3.696754	0.000000
C	-2.804515	2.450157	0.000001
C	-4.941701	1.206567	0.000000
C	-5.626665	0.000000	0.000000
H	1.222899	-4.630995	-0.000001
H	-1.222899	-4.630995	0.000000
H	3.350891	-3.386199	0.000000
H	-3.350890	-3.386200	-0.000001
H	-5.487154	-2.141984	0.000000
H	5.487153	-2.141984	0.000001
H	3.350890	3.386199	0.000001
H	1.222900	4.630995	-0.000001
H	5.487154	2.141983	0.000001

H	6.709141	0.000000	0.000002
H	-1.222900	4.630995	0.000001
H	-3.350891	3.386199	0.000000
H	-5.487154	2.141984	-0.000001
H	-6.709141	0.000000	-0.000001

190-71-6-C28H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1076.02261869 (a.u.)
E(HF/CC-PVTZ) = -1068.90859548
E(DLPNO-CCSD(T)/CC-PVTZ) = -1073.486348986193
T1 (CC-PVTZ)= 0.010065803
T2 (CC-PVTZ)= 0.036066
E(HF/CC-PVQZ) = -1068.97081284
E(DLPNO-CCSD(T)/CC-PVQZ) = -1073.783842907305
E(HF/TZ-AUG) = -1068.91569517
E(DLPNO-CCSD(T)/TZ-AUG) = -1073.55687901
E(HF/TZ-CORE) = -1068.91639716
E(DLPNO-CCSD(T)/TZ-CORE) = -1074.90895831
E(HF/TZ-IT) = -1068.90859548
E(DLPNO-CCSD(T)/TZ-IT) = -1073.50213059
T1 (CC-PVQZ)= 0.010071620
T2 (CC-PVQZ)= 0.037695
E(HF/CBS) = -1068.98597352
E(DLPNO-CCSD(T)/CBS) = -1073.97069189
Enthalpic correction = 0.33444950 (a.u.)
Entropy = 132.41812 (cal/(mol*K))

C	3.958383	0.218657	-0.000008
C	4.895711	-0.821448	-0.000010
C	2.568123	-0.090611	-0.000005
C	4.369312	1.586780	-0.000007
C	4.476265	-2.137030	-0.000005
C	3.120553	-2.445312	-0.000002
C	2.145050	-1.446634	-0.000004
C	0.717783	-1.740932	-0.000004
C	1.612771	0.969526	0.000001
C	0.217888	0.684497	0.000002
C	-0.217888	-0.684498	0.000001
C	-1.612771	-0.969526	0.000006
C	-0.717783	1.740931	0.000007
C	-2.568123	0.090611	0.000004
C	-3.958384	-0.218656	0.000004
C	-2.145050	1.446633	-0.000005
C	-3.120552	2.445312	-0.000028
C	-4.895711	0.821448	-0.000009
C	-4.369312	-1.586780	0.000014
C	-4.476264	2.137031	-0.000029
C	2.059774	2.312676	0.000008
C	3.459100	2.590051	0.000002
C	1.105825	3.343817	0.000025
C	-0.235989	3.064911	0.000025
C	0.235989	-3.064911	-0.000006
C	-1.105825	-3.343817	0.000001
C	-2.059774	-2.312676	0.000009
C	-3.459101	-2.590051	0.000016
H	5.951283	-0.580017	-0.000015
H	5.430283	1.804111	-0.000012
H	5.204204	-2.938016	-0.000004
H	2.833030	-3.485702	0.000007
H	-2.833028	3.485702	-0.000051
H	-5.951283	0.580018	-0.000008
H	-5.430283	-1.804111	0.000018
H	-5.204203	2.938017	-0.000046
H	3.778549	3.624975	0.000006
H	1.445447	4.372253	0.000039
H	-0.932560	3.889395	0.000047
H	0.932559	-3.889396	-0.000017
H	-1.445447	-4.372253	-0.000001
H	-3.778550	-3.624974	0.000022

190-88-5-C24H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -922.265862280 (a.u.)
E(HF/CC-PVTZ) = -916.17114379
E(DLPNO-CCSD(T)/CC-PVTZ) = -920.094449287150
T1 (CC-PVTZ)= 0.010308088
T2 (CC-PVTZ)= 0.036918
E(HF/CC-PVQZ) = -916.22455755
E(DLPNO-CCSD(T)/CC-PVQZ) = -920.349488762070
E(HF/TZ-AUG) = -916.17733451
E(DLPNO-CCSD(T)/TZ-AUG) = -920.154709953
E(HF/TZ-CORE) = -916.17785771
E(DLPNO-CCSD(T)/TZ-CORE) = -921.313796423
E(HF/TZ-IT) = -916.17114379
E(DLPNO-CCSD(T)/TZ-IT) = -920.108063982
T1 (CC-PVQZ)= 0.010323221
T2 (CC-PVQZ)= 0.037535
E(HF/CBS) = -916.237573031
E(DLPNO-CCSD(T)/CBS) = -920.509636522
Enthalpic correction = 0.28549821 (a.u.)
Entropy = 119.44453 (cal/(mol*K))

C	-4.575045	-0.799165	0.000018
C	-4.515688	0.563364	0.000013
C	-3.109396	0.980043	-0.000015
C	-2.361112	-0.233625	-0.000024
C	-3.211167	-1.344247	-0.000005
C	-2.612606	-2.598430	0.000014
C	-1.211352	-2.699271	0.000011
C	-2.421054	2.161484	-0.000007
C	-0.981988	2.150033	-0.000009
C	-0.223686	3.344007	0.000001
C	1.148611	3.317175	0.000006
C	-0.365350	-1.580289	-0.000006
C	-0.984588	-0.304093	-0.000019
C	-0.269963	0.921925	-0.000013
C	1.094722	-1.612371	-0.000005
C	3.916769	-1.613986	0.000003
C	3.214295	-2.802901	-0.000005
C	1.822008	-2.800767	-0.000009
C	1.815275	-0.378213	-0.000002
C	1.141148	0.884503	-0.000004
C	1.865263	2.097660	0.000005
C	3.290897	2.046193	0.000012
C	3.943439	0.855775	0.000010
C	3.236296	-0.388090	0.000004
H	-5.480247	-1.388134	0.000035
H	-5.362968	1.232253	0.000024
H	-3.203066	-3.506540	0.000035
H	-0.781093	-3.691155	0.000028
H	-2.926893	3.120365	0.000007
H	-0.744243	4.294047	0.000004
H	1.706527	4.245525	0.000012
H	4.999691	-1.616199	0.000007
H	3.745878	-3.745619	-0.000008
H	1.300501	-3.747477	-0.000018
H	3.845398	2.976568	0.000017
H	5.026160	0.826071	0.000015

191-07-1-C24H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -922.314620209 (a.u.)
E(HF/CC-PVTZ) = -916.22067201
E(DLPNO-CCSD(T)/CC-PVTZ) = -920.139764891806
T1 (CC-PVTZ)= 0.010023540
T2 (CC-PVTZ)= 0.033948
E(HF/CC-PVQZ) = -916.27399205
E(DLPNO-CCSD(T)/CC-PVQZ) = -920.394792685536
E(HF/TZ-AUG) = -916.22664815
E(DLPNO-CCSD(T)/TZ-AUG) = -920.199877711
E(HF/TZ-CORE) = -916.22736312
E(DLPNO-CCSD(T)/TZ-CORE) = -921.359414128
E(HF/TZ-IT) = -916.22067201
E(DLPNO-CCSD(T)/TZ-IT) = -920.153394365
T1 (CC-PVQZ)= 0.010006561
T2 (CC-PVQZ)= 0.037179
E(HF/CBS) = -916.286984694
E(DLPNO-CCSD(T)/CBS) = -920.554977474
Enthalpic correction = 0.28637185 (a.u.)
Entropy = 117.22555 (cal/(mol*K))

C	0.354411	-1.376792	0.000001
C	1.369562	-0.381473	0.000000
C	1.015139	0.995332	-0.000001
C	2.732968	-0.761216	0.000000
C	-1.015139	-0.995332	0.000000
C	0.707250	-2.747418	0.000002
C	-0.354410	1.376791	0.000000
C	2.025733	1.986187	-0.000001
C	3.724374	0.253358	-0.000001
C	3.057124	-2.142217	0.000000
C	-1.369562	0.381473	-0.000001
C	-2.025733	-1.986186	0.000000
C	-0.326676	-3.718629	0.000001
C	2.081609	-3.098690	0.000001
C	-0.707251	2.747417	0.000000
C	1.642766	3.352056	0.000000
C	3.383792	1.576413	-0.000001
C	-2.732968	0.761216	0.000000
C	-3.383791	-1.576413	-0.000001
C	-1.642766	-3.352056	0.000000
C	-2.081609	3.098691	0.000002
C	0.326676	3.718629	0.000000
C	-3.057123	2.142217	0.000001
C	-3.724374	-0.253358	-0.000001
H	4.766936	-0.040492	0.000000
H	4.101477	-2.429638	-0.000002
H	-0.053427	-4.766780	0.000001
H	2.348411	-4.148501	0.000001
H	2.418518	4.108030	0.000000
H	4.154871	2.337150	-0.000002
H	-4.154871	-2.337150	-0.000003
H	-2.418518	-4.108030	-0.000001
H	-2.348411	4.148501	0.000004
H	0.053425	4.766780	0.000002
H	-4.101476	2.429638	0.000003
H	-4.766937	0.040492	-0.000003

191-13-9-C30H16

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1153.45688383 (a.u.)
E(HF/CC-PVTZ) = -1145.81103926
E(DLPNO-CCSD(T)/CC-PVTZ) = -1150.734452715341
T1 (CC-PVTZ)= 0.010309066
T2 (CC-PVTZ)= 0.035302
E(HF/CC-PVQZ) = -1145.87805195
E(DLPNO-CCSD(T)/CC-PVQZ) = -1151.054034365925
E(HF/TZ-AUG) = -1145.81884063
E(DLPNO-CCSD(T)/TZ-AUG) = -1150.81037664
E(HF/TZ-CORE) = -1145.81941916
E(DLPNO-CCSD(T)/TZ-CORE) = -1152.25869489
E(HF/TZ-IT) = -1145.81103926
E(DLPNO-CCSD(T)/TZ-IT) = -1150.75140977
T1 (CC-PVQZ)= 0.010305432
T2 (CC-PVQZ)= 0.037614
E(HF/CBS) = -1145.89438112
E(DLPNO-CCSD(T)/CBS) = -1151.25467062
Enthalpic correction = 0.36903634 (a.u.)
Entropy = 142.71956 (cal/(mol*K))

C	6.761380	-0.323154	0.000007
C	6.128813	-1.578644	-0.000005
C	6.003203	0.818514	0.000012
C	4.757116	-1.666504	-0.000008
C	3.944770	-0.513443	0.000000
C	4.589754	0.757635	0.000007
C	2.501154	-0.566894	0.000001
C	3.816135	1.940546	0.000006
C	2.441660	1.909786	-0.000001
C	1.762831	0.643873	-0.000002
C	0.345818	0.614810	-0.000004
C	1.655764	3.115101	-0.000009
C	1.787189	-1.780878	0.000006
C	-0.406701	1.831169	-0.000010
C	0.306971	3.079474	-0.000015
C	-1.787188	1.780879	-0.000011
C	-0.345817	-0.614810	-0.000001
C	-2.501155	0.566894	-0.000003
C	-1.762832	-0.643872	-0.000002
C	-2.441658	-1.909785	-0.000003
C	-3.944769	0.513442	0.000002
C	0.406700	-1.831168	0.000003
C	-0.306970	-3.079473	0.000005
C	-1.655764	-3.115101	0.000001
C	-3.816136	-1.940546	-0.000008
C	-4.589753	-0.757637	-0.000005
C	-6.003204	-0.818515	-0.000006
C	-4.757117	1.666504	0.000017
C	-6.128813	1.578644	0.000017
C	-6.761380	0.323152	0.000004
H	7.841858	-0.261822	0.000012
H	6.724989	-2.481862	-0.000012
H	6.477477	1.792335	0.000019
H	4.301333	-2.645718	-0.000022
H	4.328156	2.895714	0.000010
H	2.180770	4.062503	-0.000011
H	2.322879	-2.719355	0.000014
H	-0.268028	3.997447	-0.000022
H	-2.322880	2.719355	-0.000022
H	0.268030	-3.997445	0.000010
H	-2.180771	-4.062502	0.000001
H	-4.328154	-2.895716	-0.000013
H	-6.477477	-1.792337	-0.000014
H	-4.301333	2.645718	0.000033
H	-6.724990	2.481861	0.000029
H	-7.841858	0.261822	0.000002

191-24-2-C22H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -846.038248982 (a.u.)
E(HF/CC-PVTZ) = -840.43186061
E(DLPNO-CCSD(T)/CC-PVTZ) = -844.041673371971
T1 (CC-PVTZ)= 0.010077927
T2 (CC-PVTZ)= 0.037339
E(HF/CC-PVQZ) = -840.4810409
E(DLPNO-CCSD(T)/CC-PVQZ) = -844.276159422479
E(HF/TZ-AUG) = -840.43747332
E(DLPNO-CCSD(T)/TZ-AUG) = -844.096724596
E(HF/TZ-CORE) = -840.43800536
E(DLPNO-CCSD(T)/TZ-CORE) = -845.159476758
E(HF/TZ-IT) = -840.43186061
E(DLPNO-CCSD(T)/TZ-IT) = -844.053842614
T1 (CC-PVQZ)= 0.010085307
T2 (CC-PVQZ)= 0.038554
E(HF/CBS) = -840.4930248
E(DLPNO-CCSD(T)/CBS) = -844.423366445
Enthalpic correction = 0.27296500 (a.u.)
Entropy = 115.53504 (cal/(mol*K))

C	0.731690	-1.584200	-0.000001
C	1.425239	-0.342740	0.000001
C	1.482431	-2.758850	-0.000005
C	-0.731689	-1.584200	0.000001
C	2.848740	-0.322024	0.000001
C	0.710789	0.892046	0.000001
C	3.553796	-1.532369	-0.000001
C	3.526340	0.935960	0.000003
C	2.873802	-2.733706	-0.000005
C	-1.425239	-0.342740	-0.000001
C	-1.482430	-2.758850	0.000006
C	-0.710789	0.892045	-0.000001
C	-2.848740	-0.322024	-0.000002
C	-1.412368	2.119553	-0.000002
C	1.412368	2.119552	0.000002
C	-0.684525	3.329314	-0.000001
C	-2.839039	2.104739	-0.000003
C	0.684525	3.329315	0.000001
C	2.839039	2.104739	0.000003
C	-3.526340	0.935961	-0.000004
C	-3.553796	-1.532369	0.000001
C	-2.873802	-2.733706	0.000005
H	0.987081	-3.718384	-0.000009
H	4.636493	-1.512622	-0.000001
H	4.609379	0.934731	0.000004
H	3.422488	-3.666678	-0.000009
H	-0.987081	-3.718384	0.000011
H	-1.230315	4.264859	-0.000001
H	-3.364757	3.051757	-0.000004
H	1.230316	4.264858	0.000002
H	3.364757	3.051757	0.000004
H	-4.609380	0.934730	-0.000005
H	-4.636493	-1.512623	-0.000001
H	-3.422489	-3.666678	0.000009

191-26-4-C22H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -846.028546895 (a.u.)
E(HF/CC-PVTZ) = -840.41897914
E(DLPNO-CCSD(T)/CC-PVTZ) = -844.030211514106
T1 (CC-PVTZ)= 0.010375387
T2 (CC-PVTZ)= 0.033083
E(HF/CC-PVQZ) = -840.46822728
E(DLPNO-CCSD(T)/CC-PVQZ) = -844.264862689897
E(HF/TZ-AUG) = -840.42467568
E(DLPNO-CCSD(T)/TZ-AUG) = -844.085473551
E(HF/TZ-CORE) = -840.42512472
E(DLPNO-CCSD(T)/TZ-CORE) = -845.148210317
E(HF/TZ-IT) = -840.41897914
E(DLPNO-CCSD(T)/TZ-IT) = -844.0427142
T1 (CC-PVQZ)= 0.010369359
T2 (CC-PVQZ)= 0.037370
E(HF/CBS) = -840.480227713
E(DLPNO-CCSD(T)/CBS) = -844.41215723
Enthalpic correction = 0.27277854 (a.u.)
Entropy = 114.77782 (cal/(mol*K))

C	-0.526789	0.469416	0.000000
C	0.526789	-0.469416	0.000000
C	1.869373	-0.026967	0.000002
C	0.229562	-1.874504	-0.000002
C	-1.869373	0.026967	-0.000001
C	-0.229562	1.874504	0.000001
C	2.157416	1.370562	0.000001
C	2.936619	-0.971946	0.000002
C	-1.086230	-2.290157	-0.000003
C	1.329349	-2.800082	0.000001
C	-2.157417	-1.370563	-0.000002
C	-2.936618	0.971946	0.000000
C	1.086231	2.290157	0.000003
C	-1.329348	2.800081	0.000000
C	3.506240	1.783701	-0.000002
C	2.611348	-2.372279	0.000003
C	4.248448	-0.512199	-0.000001
C	-3.506239	-1.783700	0.000000
C	-2.611348	2.372278	-0.000002
C	-4.248450	0.512199	0.000001
C	4.526926	0.857826	-0.000003
C	-4.526926	-0.857825	0.000002
H	-1.309193	-3.350826	-0.000007
H	1.104448	-3.859664	-0.000001
H	1.309193	3.350826	0.000006
H	-1.104451	3.859664	0.000001
H	3.728959	2.843467	0.000000
H	3.426708	-3.085421	0.000007
H	5.060428	-1.228815	0.000002
H	-3.728962	-2.843467	-0.000002
H	-3.426705	3.085423	-0.000004
H	-5.060428	1.228816	-0.000001
H	5.556377	1.192327	-0.000008
H	-5.556378	-1.192325	0.000005

191-68-4-C26H16

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1000.91254754 (a.u.)
E(HF/CC-PVTZ) = -994.23952914
E(DLPNO-CCSD(T)/CC-PVTZ) = -998.550068652148
T1 (CC-PVTZ)= 0.010000113
T2 (CC-PVTZ)= 0.035933
E(HF/CC-PVQZ) = -994.29824712
E(DLPNO-CCSD(T)/CC-PVQZ) = -998.828325742361
E(HF/TZ-AUG) = -994.24653648
E(DLPNO-CCSD(T)/TZ-AUG) = -998.616242916
E(HF/TZ-CORE) = -994.24687064
E(DLPNO-CCSD(T)/TZ-CORE) = -999.871030062

E(HF/TZ-IT) = -994.23952914
E(DLPNO-CCSD(T)/TZ-IT) = -998.564013124
T1 (CC-PVQZ)= 0.010037048
T2 (CC-PVQZ)= 0.037253
E(HF/CBS) = -994.312555095
E(DLPNO-CCSD(T)/CBS) = -999.002837933
Enthalpic correction = 0.34342298 (a.u.)
Entropy = 134.49189 (cal/(mol*K))

C	-2.473080	-0.687243	-0.232377
C	-2.473079	0.687244	0.232379
C	-1.242524	1.386131	0.304795
C	-3.653043	1.339293	0.628848
C	-3.653045	-1.339292	-0.628844
C	-1.242525	-1.386131	-0.304796
C	-3.637069	-2.631743	-1.104327
C	0.000000	0.694916	-0.000001
C	-1.250312	2.691806	0.838831
C	0.000000	-0.694916	-0.000001
C	1.242525	1.386130	-0.304797
C	1.242524	-1.386131	0.304796
C	-1.250314	-2.691804	-0.838835
C	2.473079	-0.687244	0.232379
C	1.250312	-2.691805	0.838832
C	-2.420022	-3.306503	-1.226699
C	-3.637067	2.631745	1.104328
C	-2.420020	3.306505	1.226696
C	2.473080	0.687243	-0.232377
C	3.653043	-1.339293	0.628847
C	3.653045	1.339292	-0.628844
C	1.250314	2.691804	-0.838835
C	2.420022	3.306503	-1.226698
C	3.637069	2.631743	-1.104326
C	3.637067	-2.631745	1.104328
C	2.420020	-3.306505	1.226697
H	-4.592316	0.806904	0.594868
H	-4.592318	-0.806904	-0.594860
H	-4.558923	-3.107256	-1.412815
H	-0.314345	3.202687	0.999687
H	-0.314346	-3.202685	-0.999695
H	0.314344	-3.202687	0.999689
H	-2.388843	-4.302023	-1.650080
H	-4.558920	3.107258	1.412819
H	-2.388840	4.302027	1.650074
H	4.592317	-0.806905	0.594866
H	4.592318	0.806903	-0.594860
H	0.314346	3.202685	-0.999693
H	2.388844	4.302023	-1.650079
H	4.558922	3.107256	-1.412815
H	4.558920	-3.107258	1.412818
H	2.388841	-4.302026	1.650076

192-51-8_C24H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -923.482230428 (a.u.)
E(HF/CC-PVTZ) = -917.34528194
E(DLPNO-CCSD(T)/CC-PVTZ) = -921.303079156538
T1 (CC-PVTZ)= 0.009965927
T2 (CC-PVTZ)= 0.034790
E(HF/CC-PVQZ) = -917.39922375
E(DLPNO-CCSD(T)/CC-PVQZ) = -921.559673171597
E(HF/TZ-AUG) = -917.35165739
E(DLPNO-CCSD(T)/TZ-AUG) = -921.363685699
E(HF/TZ-CORE) = -917.35199006
E(DLPNO-CCSD(T)/TZ-CORE) = -922.522308773
E(HF/TZ-IT) = -917.34528194
E(DLPNO-CCSD(T)/TZ-IT) = -921.31590526
T1 (CC-PVQZ)= 0.010001480
T2 (CC-PVQZ)= 0.037901
E(HF/CBS) = -917.412367903
E(DLPNO-CCSD(T)/CBS) = -921.720698663
Enthalpic correction = 0.30804814 (a.u.)
Entropy = 128.69560 (cal/(mol*K))

C	0.000000	0.720459	-0.018240
C	-0.000000	-0.720459	-0.018240
C	-1.229369	-1.433549	-0.029408
C	1.229369	-1.433549	-0.029408
C	1.229369	1.433549	-0.029408
C	-1.229369	1.433549	-0.029408
C	-2.494266	-0.705534	0.010200
C	-1.198529	-2.829025	-0.076028
C	2.494266	-0.705534	0.010200
C	1.198529	-2.829025	-0.076028
C	2.494266	0.705534	0.010200
C	1.198529	2.829025	-0.076028
C	-2.494266	0.705534	0.010200
C	-1.198529	2.829025	-0.076028
C	-3.729782	-1.378523	0.055610
C	0.000000	-3.517092	-0.103886
C	3.729782	-1.378523	0.055610
C	3.729782	1.378523	0.055610
C	0.000000	3.517092	-0.103886
C	-3.729782	1.378523	0.055610
C	-4.925510	-0.697986	0.096310
C	4.925510	-0.697986	0.096310
C	4.925510	0.697986	0.096310
C	-4.925510	0.697986	0.096310
H	-2.116843	-3.394078	-0.101317
H	2.116843	-3.394078	-0.101317
H	2.116843	3.394078	-0.101317
H	-2.116843	3.394078	-0.101317
H	-3.755500	-2.457027	0.068282
H	0.000000	-4.598502	-0.146956
H	3.755500	-2.457027	0.068282
H	3.755500	2.457027	0.068282
H	0.000000	4.598502	-0.146956
H	-3.755500	2.457027	0.068282
H	-5.858281	-1.245446	0.132794
H	5.858281	-1.245446	0.132794
H	5.858281	1.245446	0.132794
H	-5.858281	1.245446	0.132794

192-65-4_C24H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -923.480117696 (a.u.)
E(HF/CC-PVTZ) = -917.3428216
E(DLPNO-CCSD(T)/CC-PVTZ) = -921.299808708149
T1 (CC-PVTZ)= 0.010090085
T2 (CC-PVTZ)= 0.036289
E(HF/CC-PVQZ) = -917.39675643
E(DLPNO-CCSD(T)/CC-PVQZ) = -921.556329978501
E(HF/TZ-AUG) = -917.34916397
E(DLPNO-CCSD(T)/TZ-AUG) = -921.360325281
E(HF/TZ-CORE) = -917.34953173
E(DLPNO-CCSD(T)/TZ-CORE) = -922.519042671
E(HF/TZ-IT) = -917.3428216
E(DLPNO-CCSD(T)/TZ-IT) = -921.312823628
T1 (CC-PVQZ)= 0.010100613
T2 (CC-PVQZ)= 0.038802
E(HF/CBS) = -917.409898882
E(DLPNO-CCSD(T)/CBS) = -921.717305779

Enthalpic correction = 0.30780422 (a.u.)
Entropy = 128.65597 (cal/(mol*K))

C	1.448347	1.096465	-0.000004
C	0.188390	0.452520	-0.000001
C	-1.012345	1.231693	0.000000
C	0.108326	-0.981199	0.000005
C	0.354153	3.265075	-0.000006
C	-0.928086	2.652587	-0.000001
C	-2.099566	3.424816	0.000004
C	1.487601	2.520670	-0.000007
C	2.655567	0.318138	-0.000002
C	-1.206118	-1.629561	0.000004
C	1.277099	-1.705192	0.000009
C	2.549765	-1.099601	0.000005
C	3.725549	-1.888468	0.000008
C	3.951365	0.884466	-0.000007
C	5.075297	0.096698	-0.000005
C	4.964831	-1.306839	0.000003
C	-1.329514	-3.029864	0.000004
C	-2.382805	-0.849678	-0.000002
C	-2.559007	-3.651600	-0.000003
C	-3.721314	-2.880670	-0.000012
C	-3.625770	-1.506247	-0.000012
C	-2.292243	0.611340	0.000002
C	-3.423851	1.421807	0.000009
C	-3.331936	2.812344	0.000010
H	0.410070	4.346650	-0.000007
H	-2.017269	4.504493	0.000004
H	2.441480	3.025496	-0.000010
H	1.253887	-2.784780	0.000016
H	3.624101	-2.966957	0.000014
H	4.073062	1.957222	-0.000013
H	6.054217	0.558286	-0.000009
H	5.857147	-1.919153	0.000004
H	-0.444603	-3.647591	0.000009
H	-2.618283	-4.732144	-0.000002
H	-4.693776	-3.355418	-0.000021
H	-4.537871	-0.929455	-0.000023
H	-4.407840	0.978925	0.000017
H	-4.236735	3.406225	0.000016

192-97-2-C20H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -769.768380836 (a.u.)
E(HF/CC-PVTZ) = -764.65024638
E(DLPNO-CCSD(T)/CC-PVTZ) = -767.950291036292
T1 (CC-PVTZ)= 0.010064241
T2 (CC-PVTZ)= 0.033821
E(HF/CC-PVQZ) = -764.69530656
E(DLPNO-CCSD(T)/CC-PVQZ) = -768.164303120989
E(HF/TZ-AUG) = -764.65552539
E(DLPNO-CCSD(T)/TZ-AUG) = -768.0003189
E(HF/TZ-CORE) = -764.65584477
E(DLPNO-CCSD(T)/TZ-CORE) = -768.966403212
E(HF/TZ-IT) = -764.65024638
E(DLPNO-CCSD(T)/TZ-IT) = -767.960996526
T1 (CC-PVQZ)= 0.010090260
T2 (CC-PVQZ)= 0.038344
E(HF/CBS) = -764.706286501
E(DLPNO-CCSD(T)/CBS) = -768.29857229
Enthalpic correction = 0.25968623 (a.u.)
Entropy = 113.91785 (cal/(mol*K))

C	0.865053	0.715126	0.000005
C	0.865054	-0.715126	0.000005
C	-0.355044	-1.440197	-0.000018
C	2.104267	-1.416407	0.000017
C	-0.355045	1.440196	-0.000016
C	2.104266	1.416408	0.000015
C	-1.619176	-0.707409	-0.000009
C	-0.297873	-2.834902	-0.000043
C	3.328016	-0.676113	0.000041
C	2.106420	-2.815261	0.000001
C	-1.619176	0.707408	-0.000002
C	-0.297874	2.834901	-0.000046
C	3.328016	0.676114	0.000039
C	2.106418	2.815262	-0.000004
C	-2.855117	-1.379251	0.000004
C	0.914877	-3.513524	-0.000033
C	-2.855117	1.379250	0.000024
C	0.914875	3.513525	-0.000040
C	-4.051689	-0.697982	0.000024
C	-4.051689	0.697981	0.000036
H	-1.207300	-3.415969	-0.000074
H	4.260053	-1.227819	0.000056
H	3.053033	-3.341136	0.000010
H	-1.207302	3.415967	-0.000082
H	4.260052	1.227821	0.000054
H	3.053031	3.341137	0.000004
H	-2.878705	-2.458318	0.000006
H	0.920006	-4.595847	-0.000053
H	-2.878705	2.458316	0.000046
H	0.920004	4.595847	-0.000064
H	-4.985474	-1.244956	0.000034
H	-4.985475	1.244955	0.000058

193-09-9-C24H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -923.479472161 (a.u.)
E(HF/CC-PVTZ) = -917.34320835
E(DLPNO-CCSD(T)/CC-PVTZ) = -921.298638836814
T1 (CC-PVTZ)= 0.010130963
T2 (CC-PVTZ)= 0.037581
E(HF/CC-PVQZ) = -917.39709591
E(DLPNO-CCSD(T)/CC-PVQZ) = -921.555175973274
E(HF/TZ-AUG) = -917.34941736
E(DLPNO-CCSD(T)/TZ-AUG) = -921.358954296
E(HF/TZ-CORE) = -917.34992494
E(DLPNO-CCSD(T)/TZ-CORE) = -922.518002357
E(HF/TZ-IT) = -917.34320835
E(DLPNO-CCSD(T)/TZ-IT) = -921.311654483
T1 (CC-PVQZ)= 0.010139270
T2 (CC-PVQZ)= 0.038798
E(HF/CBS) = -917.410226843
E(DLPNO-CCSD(T)/CBS) = -921.716186327
Enthalpic correction = 0.30774632 (a.u.)
Entropy = 127.98396 (cal/(mol*K))

C	5.498350	-0.707991	0.000014
C	5.498350	0.707991	0.000010
C	4.318792	-1.399521	0.000011
C	4.318792	1.399521	0.000002
C	3.076847	0.713170	-0.000002
C	3.076847	-0.713171	0.000003
C	1.845915	1.382410	-0.000007
C	1.845915	-1.382410	0.000000
C	0.631078	-0.717061	-0.000007
C	0.631078	0.717061	-0.000009
C	-0.640976	1.444920	-0.000009
C	-0.640976	-1.444920	-0.000009
C	-1.858268	-0.716852	0.000002

C	-1.858268	0.716852	0.000002
C	-3.097881	1.415798	0.000009
C	-3.097881	-1.415797	0.000009
C	-0.701155	-2.837861	-0.000021
C	-0.701153	2.837861	-0.000017
C	-1.915297	3.516082	-0.000011
C	-3.103985	2.815880	0.000003
C	-4.321681	0.675990	0.000021
C	-3.103987	-2.815879	0.000001
C	-1.915299	-3.516082	-0.000015
C	-4.321681	-0.675989	0.000021
H	6.440512	-1.240648	0.000020
H	6.440512	1.240648	0.000013
H	4.315801	-2.482822	0.000014
H	4.315801	2.482821	0.000000
H	1.873206	2.462318	-0.000007
H	1.873206	-2.462319	0.000007
H	0.207266	-3.420656	-0.000037
H	0.207268	3.420655	-0.000028
H	-1.921448	4.598368	-0.000018
H	-4.052268	3.338672	0.000008
H	-5.253509	1.228000	0.000029
H	-4.052270	-3.338671	0.000007
H	-1.921450	-4.598368	-0.000024
H	-5.253509	-1.227998	0.000029

193-43-1-C22H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -845.970561353 (a.u.)
E(HF/CC-PVTZ) = -840.36929063
E(DLPNO-CCSD(T)/CC-PVTZ) = -843.978709182787
T1 (CC-PVTZ)= 0.010240204
T2 (CC-PVTZ)= 0.031737
E(HF/CC-PVQZ) = -840.41839428
E(DLPNO-CCSD(T)/CC-PVQZ) = -844.212940710235
E(HF/TZ-AUG) = -840.37488345
E(DLPNO-CCSD(T)/TZ-AUG) = -844.033123149
E(HF/TZ-CORE) = -840.3755266
E(DLPNO-CCSD(T)/TZ-CORE) = -845.09627681
E(HF/TZ-IT) = -840.36929063
E(DLPNO-CCSD(T)/TZ-IT) = -843.990752395
T1 (CC-PVQZ)= 0.010250447
T2 (CC-PVQZ)= 0.037572
E(HF/CBS) = -840.430359505
E(DLPNO-CCSD(T)/CBS) = -844.359999251
Enthalpic correction = 0.27171632 (a.u.)
Entropy = 119.25979 (cal/(mol*K))

C	-0.678391	0.000000	0.000006
C	-1.432174	1.185363	0.000000
C	0.678391	0.000000	0.000006
C	-1.432174	-1.185364	0.000006
C	-0.717855	2.372324	-0.000008
C	-2.838864	0.718093	0.000005
C	0.717854	2.372325	-0.000008
C	1.432174	1.185364	0.000001
C	2.838864	0.718094	0.000007
C	1.432174	-1.185364	0.000006
C	0.717855	-2.372324	0.000011
C	-0.717855	-2.372324	0.000010
C	2.838864	-0.718093	-0.000006
C	4.036024	-1.408892	-0.000014
C	4.036025	1.408892	0.000010
C	-2.838864	-0.718094	-0.000004
C	-4.036024	-1.408892	-0.000011
C	-4.036024	1.408892	0.000007
C	5.237248	0.694448	0.000001
C	5.237248	-0.694448	-0.000011
C	-5.237248	-0.694448	-0.000009
C	-5.237248	0.694448	0.000000
H	-1.222619	3.330500	-0.000011
H	1.222618	3.330501	-0.000010
H	1.222618	-3.330501	0.000008
H	-1.222618	-3.330501	0.000008
H	4.047374	-2.491626	-0.000019
H	4.047374	2.491626	0.000015
H	-4.047374	-2.491626	-0.000015
H	-4.047374	2.491626	0.000010
H	6.177546	1.230247	0.000002
H	6.177546	-1.230247	-0.000017
H	-6.177545	-1.230247	-0.000013
H	-6.177545	1.230248	0.000000

194-69-4-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.205434811 (a.u.)
E(HF/CC-PVTZ) = -841.55562944
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.202931827809
T1 (CC-PVTZ)= 0.010106562
T2 (CC-PVTZ)= 0.034886
E(HF/CC-PVQZ) = -841.6054246
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.438983394128
E(HF/TZ-AUG) = -841.56154249
E(DLPNO-CCSD(T)/TZ-AUG) = -845.25853337
E(HF/TZ-CORE) = -841.56182759
E(DLPNO-CCSD(T)/TZ-CORE) = -846.320721379
E(HF/TZ-IT) = -841.55562944
E(DLPNO-CCSD(T)/TZ-IT) = -845.214635406
T1 (CC-PVQZ)= 0.010127151
T2 (CC-PVQZ)= 0.037707
E(HF/CBS) = -841.617558327
E(DLPNO-CCSD(T)/CBS) = -845.587033958
Enthalpic correction = 0.29494327 (a.u.)
Entropy = 122.47369 (cal/(mol*K))

C	5.119536	0.471413	-0.406185
C	3.858726	1.021363	-0.401349
C	2.722351	0.252020	-0.072660
C	5.309054	-0.878374	-0.071659
C	4.223735	-1.654183	0.253435
C	2.921477	-1.114874	0.254328
C	-3.419804	-2.432299	-0.580768
C	-2.260372	-1.696260	-0.493695
C	-2.264352	-0.347449	-0.070483
C	-4.655578	-1.856404	-0.254752
C	-4.707478	-0.525903	0.080422
C	-3.537722	0.258206	0.141494
C	0.533981	-1.406218	0.548321
C	1.794068	-1.904233	0.613223
C	0.269822	-0.060409	0.141052
C	1.381160	0.796910	-0.058653
C	1.154512	2.190498	-0.178465
C	-0.097660	2.708520	-0.052617
C	-1.230829	1.869356	0.069709
C	-1.068764	0.466371	0.047114
C	-2.525219	2.445182	0.230800
C	-3.629056	1.667434	0.330756
H	5.970605	1.084575	-0.672965
H	3.747022	2.059347	-0.677606
H	6.304526	-1.302832	-0.073901
H	4.352483	-2.698051	0.512704
H	-3.375565	-3.458550	-0.921952

H	-1.336020	-2.152391	-0.808373
H	-5.562372	-2.444564	-0.308132
H	-5.659257	-0.046028	0.273433
H	-0.286239	-2.021811	0.878566
H	1.959550	-2.917586	0.958273
H	1.989847	2.862737	-0.302268
H	-0.248226	3.780954	-0.062949
H	-2.600306	3.523612	0.296162
H	-4.605586	2.106588	0.492811

195-06-2-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.200598538 (a.u.)
E(HF/CC-PVTZ) = -841.54986726
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.197321995312
T1 (CC-PVTZ)= 0.010206935
T2 (CC-PVTZ)= 0.035882
E(HF/CC-PVQZ) = -841.59964044
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.433322064143
E(HF/TZ-AUG) = -841.55572201
E(DLPNO-CCSD(T)/TZ-AUG) = -845.252817987
E(HF/TZ-CORE) = -841.55607469
E(DLPNO-CCSD(T)/TZ-CORE) = -846.31522745
E(HF/TZ-IT) = -841.54986726
E(DLPNO-CCSD(T)/TZ-IT) = -845.209144787
T1 (CC-PVQZ)= 0.010222494
T2 (CC-PVQZ)= 0.037608
E(HF/CBS) = -841.611768811
E(DLPNO-CCSD(T)/CBS) = -845.581345732
Enthalpic correction = 0.29462211 (a.u.)
Entropy = 122.44377 (cal/(mol*K))

C	-3.174259	0.419234	0.137985
C	-4.589681	0.316631	0.209962
C	-5.218272	-0.865955	-0.057102
C	-1.105163	1.701278	0.254918
C	-2.489338	1.619732	0.338523
C	0.872819	3.071011	0.059169
C	-0.452387	2.972149	0.299626
C	-4.466507	-2.012961	-0.418130
C	-2.412779	-0.742171	-0.209301
C	-0.321544	0.512021	0.028270
C	1.690311	1.906709	-0.105946
C	-3.104360	-1.950617	-0.495129
C	-1.015911	-0.660000	-0.257634
C	1.130985	0.620663	0.006684
C	3.077426	2.068374	-0.370369
C	2.033917	-0.504013	0.093508
C	3.899654	0.994749	-0.489188
C	3.413847	-0.312366	-0.222284
C	1.660683	-1.783612	0.572078
C	2.553618	-2.826852	0.622730
C	4.300529	-1.410389	-0.197771
C	3.880542	-2.654417	0.197314
H	-5.161793	1.196898	0.476851
H	-6.296967	-0.933348	0.000692
H	-3.055262	2.525508	0.523908
H	1.355546	4.039698	0.020019
H	-1.054518	3.855829	0.470425
H	-4.981031	-2.940792	-0.632109
H	-2.527853	-2.826255	-0.768050
H	-0.480029	-1.540302	-0.574412
H	3.461134	3.073089	-0.497783
H	4.947342	1.121727	-0.731911
H	0.667746	-1.935708	0.961481
H	2.233006	-3.784420	1.012543
H	5.335110	-1.241287	-0.470658
H	4.572791	-3.485817	0.221534

195-19-7-C18H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -693.490929111 (a.u.)
E(HF/CC-PVTZ) = -688.85914535
E(DLPNO-CCSD(T)/CC-PVTZ) = -691.850482234505
T1 (CC-PVTZ)= 0.010091127
T2 (CC-PVTZ)= 0.034671
E(HF/CC-PVQZ) = -688.90005289
E(DLPNO-CCSD(T)/CC-PVQZ) = -692.044049304295
E(HF/TZ-AUG) = -688.86401479
E(DLPNO-CCSD(T)/TZ-AUG) = -691.895790488
E(HF/TZ-CORE) = -688.86423179
E(DLPNO-CCSD(T)/TZ-CORE) = -692.765091353
E(HF/TZ-IT) = -688.85914535
E(DLPNO-CCSD(T)/TZ-IT) = -691.859939904
T1 (CC-PVQZ)= 0.010122032
T2 (CC-PVQZ)= 0.037044
E(HF/CBS) = -688.910020945
E(DLPNO-CCSD(T)/CBS) = -692.165417557
Enthalpic correction = 0.24678290 (a.u.)
Entropy = 108.84367 (cal/(mol*K))

C	0.000000	0.397149	-0.000002
C	1.280902	-0.277038	-0.055448
C	-1.280902	-0.277038	0.055446
C	0.000000	1.808109	0.000000
C	2.470595	0.472674	0.187110
C	1.445809	-1.628671	-0.439234
C	-2.470595	0.472674	-0.187109
C	-1.445808	-1.628671	0.439233
C	-1.213548	2.528879	-0.191045
C	1.213547	2.528879	0.191045
C	2.395577	1.884301	0.345851
C	3.722775	-0.176427	0.191561
C	2.682461	-2.229935	-0.463583
C	-2.395577	1.884301	-0.345851
C	-3.722775	-0.176428	-0.191559
C	-2.682460	-2.229936	0.463583
C	3.833154	-1.510977	-0.107815
C	-3.833153	-1.510978	0.107817
H	0.592762	-2.193500	-0.776572
H	-0.592760	-2.193500	0.776569
H	-1.164575	3.609924	-0.234249
H	1.164574	3.609924	0.234250
H	3.308840	2.435546	0.532456
H	4.606161	0.412273	0.407193
H	2.767194	-3.262035	-0.778575
H	-3.308841	2.435545	-0.532455
H	-4.606162	0.412272	-0.407189
H	-2.767192	-3.262036	0.778575
H	4.801112	-1.994809	-0.110944
H	-4.801112	-1.994809	0.110947

196-78-1-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.204403272 (a.u.)
E(HF/CC-PVTZ) = -841.55311747

E(DLPNO-CCSD(T)/CC-PVTZ) = -845.202888539491
T1 (CC-PVTZ)= 0.010033550
T2 (CC-PVTZ)= 0.034271
E(HF/CC-PVQZ) = -841.6029418
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.438862828183
E(HF/TZ-AUG) = -841.55908836
E(DLPNO-CCSD(T)/TZ-AUG) = -845.258554121
E(HF/TZ-CORE) = -841.55931623
E(DLPNO-CCSD(T)/TZ-CORE) = -846.320619105
E(HF/TZ-IT) = -841.55311747
E(DLPNO-CCSD(T)/TZ-IT) = -845.214548139
T1 (CC-PVQZ)= 0.010066431
T2 (CC-PVQZ)= 0.037074
E(HF/CBS) = -841.615082635
E(DLPNO-CCSD(T)/CBS) = -845.586842822
Enthalpic correction = 0.29515699 (a.u.)
Entropy = 122.77266 (cal/(mol*K))

C	-3.664928	-0.129428	0.470188
C	-4.332534	-1.333248	0.500416
C	-2.294447	-0.054238	0.163816
C	-3.640781	-2.514487	0.222467
C	-2.293175	-2.469020	-0.056292
C	-1.583758	-1.252570	-0.080689
C	4.111389	0.900364	0.809085
C	2.748280	0.991014	0.660350
C	1.991948	-0.059633	0.086679
C	4.802455	-0.247961	0.389000
C	4.095336	-1.313841	-0.105283
C	2.690567	-1.260652	-0.229459
C	0.414334	2.462092	-0.474812
C	-0.301579	3.636743	-0.536244
C	-0.194170	1.235500	-0.136215
C	-1.672290	3.629132	-0.271574
C	-2.305982	2.434050	-0.014842
C	-1.601568	1.217678	0.032590
C	-0.138352	-1.215786	-0.254865
C	0.558316	-0.011219	-0.089710
C	0.591781	-2.400381	-0.555134
C	1.949051	-2.408684	-0.605735
H	-4.212920	0.772504	0.698201
H	-5.387008	-1.361685	0.742033
H	-4.155672	-3.466128	0.242813
H	-1.773961	-3.399102	-0.228634
H	4.653005	1.716034	1.270518
H	2.241955	1.864225	1.039036
H	5.878306	-0.303199	0.491852
H	4.602657	-2.230481	-0.380584
H	1.458026	2.476823	-0.742815
H	0.196823	4.556847	-0.812449
H	-2.243401	4.547453	-0.311956
H	-3.378246	2.434959	0.110284
H	0.058164	-3.310009	-0.782979
H	2.482923	-3.310775	-0.877735

19740-34-2-C12H20

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -469.577101765 (a.u.)
E(HF/CC-PVTZ) = -466.23006971
E(DLPNO-CCSD(T)/CC-PVTZ) = -468.480343243825
T1 (CC-PVTZ)= 0.008638882
T2 (CC-PVTZ)= 0.027526
E(HF/CC-PVQZ) = -466.25816613
E(DLPNO-CCSD(T)/CC-PVQZ) = -468.616346020716
E(HF/TZ-AUG) = -466.23214293
E(DLPNO-CCSD(T)/TZ-AUG) = -468.515601452
E(HF/TZ-CORE) = -466.23326966
E(DLPNO-CCSD(T)/TZ-CORE) = -469.086575263
E(HF/TZ-IT) = -466.23006971
E(DLPNO-CCSD(T)/TZ-IT) = -468.483459185
T1 (CC-PVQZ)= 0.008820121
T2 (CC-PVQZ)= 0.031838
E(HF/CBS) = -466.265012464
E(DLPNO-CCSD(T)/CBS) = -468.701934831
Enthalpic correction = 0.30065954 (a.u.)
Entropy = 94.30911 (cal/(mol*K))

C	1.393641	-1.251955	0.000000
C	0.509898	-1.242812	1.256626
C	0.509900	-1.242805	-1.256631
C	2.281274	0.000001	0.000001
C	-0.397322	-0.000001	1.248541
C	-1.323505	-0.000001	0.000000
C	0.509898	1.242805	1.256631
C	-0.397321	0.000000	-1.248541
C	-2.251340	-1.224466	-0.000001
C	-2.251339	1.224466	0.000000
C	0.509898	1.242811	-1.256626
C	1.393640	1.251955	0.000001
H	2.020679	-2.147798	-0.000005
H	-0.078443	-2.159525	1.315316
H	1.140932	-1.221673	2.150112
H	1.140941	-1.221661	-2.150113
H	-0.078433	-2.159523	-1.315329
H	2.931117	0.000001	0.880327
H	2.931119	0.000001	-0.880324
H	-1.023574	-0.000005	2.146631
H	1.140937	1.221663	2.150113
H	-0.078437	2.159522	1.315327
H	-1.023573	0.000003	-2.146632
H	-2.896262	-1.207475	0.881878
H	-2.896267	-1.207469	-0.881876
H	-1.722658	-2.173833	-0.000005
H	-1.722654	2.173833	0.000007
H	-2.896259	1.207477	-0.881880
H	-2.896267	1.207469	0.881874
H	1.140933	1.221673	-2.150111
H	-0.078443	2.159524	-1.315317
H	2.020677	2.147799	0.000006

197-61-5-C26H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -999.697423059 (a.u.)
E(HF/CC-PVTZ) = -993.07346254
E(DLPNO-CCSD(T)/CC-PVTZ) = -997.341922264158
T1 (CC-PVTZ)= 0.010311386
T2 (CC-PVTZ)= 0.038985
E(HF/CC-PVQZ) = -993.13156317
E(DLPNO-CCSD(T)/CC-PVQZ) = -997.618886040129
E(HF/TZ-AUG) = -993.0803453
E(DLPNO-CCSD(T)/TZ-AUG) = -997.407532737
E(HF/TZ-CORE) = -993.08077391
E(DLPNO-CCSD(T)/TZ-CORE) = -998.662592472
E(HF/TZ-IT) = -993.07346254
E(DLPNO-CCSD(T)/TZ-IT) = -997.356430043
T1 (CC-PVQZ)= 0.010318567
T2 (CC-PVQZ)= 0.037782
E(HF/CBS) = -993.145720714
E(DLPNO-CCSD(T)/CBS) = -997.792754529
Enthalpic correction = 0.31991449 (a.u.)
Entropy = 132.34773 (cal/(mol*K))

```
 C     5.017044     1.565730     0.000004
 C     5.554697     0.282723    -0.000001
 C     3.636706     1.765483     0.000005
 C     4.719410    -0.834463    -0.000005
 C     2.792151     0.663567     0.000001
 C     3.348920    -0.647646    -0.000003
 C     1.327653     0.534601    -0.000003
 C     2.240137    -1.609581    -0.000002
 C     0.283334     2.862957    -0.000004
 C     0.249689     1.438345    -0.000003
 C    -0.881101     3.589732    -0.000003
 C     1.038921    -0.844883    -0.000001
 C     2.163718    -2.975188     0.000002
 C    -2.163719     2.975188     0.000000
 C    -1.038922     0.844883     0.000000
 C    -0.249690    -1.438344     0.000002
 C     0.881100    -3.589732     0.000005
 C    -2.240137     1.609581     0.000003
 C    -1.327653    -0.534600     0.000002
 C    -0.283335    -2.862956     0.000005
 C    -3.348920     0.647645     0.000005
 C    -2.792151    -0.663566    -0.000003
 C    -4.719410     0.834462     0.000008
 C    -3.636704    -1.765483    -0.000009
 C    -5.554697    -0.282724     0.000002
 C    -5.017043    -1.565730    -0.000006
 H     5.678273     2.422549     0.000006
 H     6.628760     0.150739    -0.000002
 H     3.245545     2.772633     0.000009
 H     5.141772    -1.831574    -0.000007
 H     1.230930     3.380433    -0.000007
 H    -0.825803     4.670848    -0.000005
 H     3.051928    -3.594368     0.000002
 H    -3.051928     3.594367     0.000002
 H     0.825801    -4.670847     0.000008
 H    -1.230930    -3.380432     0.000008
 H    -5.141772     1.831573     0.000012
 H    -3.245544    -2.772632    -0.000015
 H    -6.628759    -0.150740     0.000004
 H    -5.678271    -2.422549    -0.000010
```

198-55-0_C20H12

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -769.756879350
(a.u.)
E(HF/CC-PVTZ) = -764.635428
E(DLPNO-CCSD(T)/CC-PVTZ) = -767.938103721751
T1 (CC-PVTZ)= 0.010152737
T2 (CC-PVTZ)= 0.038327
E(HF/CC-PVQZ) = -764.68043178
E(DLPNO-CCSD(T)/CC-PVQZ) = -768.151897167506
E(HF/TZ-AUG) = -764.64061096
E(DLPNO-CCSD(T)/TZ-AUG) = -767.988087875
E(HF/TZ-CORE) = -764.64102512
E(DLPNO-CCSD(T)/TZ-CORE) = -768.954044767
E(HF/TZ-IT) = -764.635428
E(DLPNO-CCSD(T)/TZ-IT) = -767.948995414
T1 (CC-PVQZ)= 0.010149700
T2 (CC-PVQZ)= 0.039356
E(HF/CBS) = -764.691397978
E(DLPNO-CCSD(T)/CBS) = -768.286034202
Enthalpic correction = 0.25956875 (a.u.)
Entropy = 112.36236 (cal/(mol*K))

 C        0.000000       -1.433310
0.000000
 C       -0.000012       -0.735295
1.244121
 C        0.000012       -0.735295       -
1.244121
 C        0.000000       -2.862524
0.000000
 C        0.000012        0.735295
1.244121
 C       -0.000042       -1.471598
2.417063
 C       -0.000012        0.735295       -
1.244121
 C        0.000042       -1.471598       -
2.417063
 C        0.000026       -3.559812       -
1.228186
 C       -0.000026       -3.559812
1.228186
 C        0.000000        1.433310
0.000000
 C        0.000042        1.471598
2.417063
 C       -0.000050       -2.872443
2.412576
 C       -0.000042        1.471598       -
2.417063
 C        0.000050       -2.872443       -
2.412576
 C        0.000000        2.862524
0.000000
 C        0.000050        2.872443
2.412576
 C       -0.000050        2.872443       -
2.412576
 C       -0.000026        3.559812       -
1.228186
 C        0.000026        3.559812
1.228186
 H       -0.000064       -0.969061
3.372583
 H        0.000064       -0.969061       -
3.372583
 H        0.000027       -4.642472       -
1.214187
 H       -0.000027       -4.642472
1.214187
 H        0.000064        0.969061
3.372583
 H       -0.000075       -3.405868
3.354346
 H       -0.000064        0.969061       -
3.372583
 H        0.000075       -3.405868       -
3.354346
 H        0.000075        3.405868
3.354346
 H       -0.000075        3.405868       -
3.354346
 H       -0.000027        4.642472       -
1.214187
 H        0.000027        4.642472
1.214187
```

201-06-9-C16H10

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -616.016228058
(a.u.)
```

E(HF/CC-PVTZ) = -611.91837868
E(DLPNO-CCSD(T)/CC-PVTZ) = -614.562879794839
T1 (CC-PVTZ)= 0.010369419
T2 (CC-PVTZ)= 0.037517
E(HF/CC-PVQZ) = -611.95465185
E(DLPNO-CCSD(T)/CC-PVQZ) = -614.734573942368
E(HF/TZ-AUG) = -611.9227739
E(DLPNO-CCSD(T)/TZ-AUG) = -614.60279168
E(HF/TZ-CORE) = -611.92289534
E(DLPNO-CCSD(T)/TZ-CORE) = -615.375731286
E(HF/TZ-IT) = -611.91837868
E(DLPNO-CCSD(T)/TZ-IT) = -614.571369994
T1 (CC-PVQZ)= 0.010405668
T2 (CC-PVQZ)= 0.038054
E(HF/CBS) = -611.963490635
E(DLPNO-CCSD(T)/CBS) = -614.842233441
Enthalpic correction = 0.21091188 (a.u.)
Entropy = 100.60427 (cal/(mol*K))

C	2.205896	1.437537	-0.000003
C	3.529356	1.049841	0.000000
C	1.168079	0.493288	-0.000002
C	1.509114	-0.896742	0.000000
C	-0.234983	0.863649	-0.000005
C	-0.787806	2.165834	0.000000
C	-1.147433	-0.177353	-0.000008
C	-2.160961	2.340974	0.000004
C	-3.063971	1.255953	0.000003
C	-2.547892	-0.023030	-0.000003
C	-3.108708	-1.380756	0.000003
C	-2.094177	-2.285410	0.000000
C	-0.817093	-1.566897	-0.000004
C	0.495988	-1.918840	0.000001
C	2.869869	-1.259898	0.000003
C	3.865478	-0.309318	0.000003
H	1.962601	2.491302	-0.000005
H	4.310305	1.799168	0.000000
H	-0.147814	3.037576	0.000003
H	-2.558407	3.347923	0.000008
H	-4.130627	1.442680	0.000008
H	-4.163269	-1.613444	0.000008
H	-2.200638	-3.359687	0.000002
H	0.814225	-2.955070	0.000005
H	3.124226	-2.312926	0.000004
H	4.904866	-0.610509	0.000006

202-03-9-C16H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -616.005128852 (a.u.)
E(HF/CC-PVTZ) = -611.90368214
E(DLPNO-CCSD(T)/CC-PVTZ) = -614.551083668557
T1 (CC-PVTZ)= 0.010671359
T2 (CC-PVTZ)= 0.033852
E(HF/CC-PVQZ) = -611.93999148
E(DLPNO-CCSD(T)/CC-PVQZ) = -614.722799853642
E(HF/TZ-AUG) = -611.90815568
E(DLPNO-CCSD(T)/TZ-AUG) = -614.591173439
E(HF/TZ-CORE) = -611.90818925
E(DLPNO-CCSD(T)/TZ-CORE) = -615.36395413
E(HF/TZ-IT) = -611.90368214
E(DLPNO-CCSD(T)/TZ-IT) = -614.55983165
T1 (CC-PVQZ)= 0.010707927
T2 (CC-PVQZ)= 0.037514
E(HF/CBS) = -611.948839079
E(DLPNO-CCSD(T)/CBS) = -614.830457853
Enthalpic correction = 0.21062994 (a.u.)
Entropy = 100.77568 (cal/(mol*K))

C	-3.702515	0.753314	0.000003
C	-3.852227	-0.657337	0.000002
C	-2.754193	-1.465877	0.000000
C	-2.460845	1.320570	0.000001
C	-1.288859	0.518495	-0.000004
C	-1.435349	-0.926758	-0.000002
C	-0.316773	-1.774539	-0.000001
C	0.013309	1.035876	-0.000005
C	1.086972	0.146242	-0.000005
C	0.981142	-1.249807	-0.000002
C	2.214131	-1.970704	0.000002
C	3.406778	-1.290923	0.000004
C	3.479477	0.135570	0.000001
C	2.316696	0.859597	-0.000004
C	0.597144	2.383024	0.000005
C	1.955453	2.280092	-0.000001
H	-4.584481	1.380929	0.000005
H	-4.845081	-1.087864	0.000004
H	-2.868011	-2.543131	0.000000
H	-2.352677	2.397296	0.000002
H	-0.474292	-2.846835	0.000000
H	2.204641	-3.053627	0.000003
H	4.332886	-1.851396	0.000008
H	4.450882	0.615060	0.000006
H	0.038787	3.306787	0.000009
H	2.655295	3.101770	-0.000001

202-33-5-C20H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -769.722906391 (a.u.)
E(HF/CC-PVTZ) = -764.60513028
E(DLPNO-CCSD(T)/CC-PVTZ) = -767.907175480412
T1 (CC-PVTZ)= 0.010468863
T2 (CC-PVTZ)= 0.037194
E(HF/CC-PVQZ) = -764.65029843
E(DLPNO-CCSD(T)/CC-PVQZ) = -768.121348482372
E(HF/TZ-AUG) = -764.61059748
E(DLPNO-CCSD(T)/TZ-AUG) = -767.957439821
E(HF/TZ-CORE) = -764.61075281
E(DLPNO-CCSD(T)/TZ-CORE) = -768.923184277
E(HF/TZ-IT) = -764.60513027
E(DLPNO-CCSD(T)/TZ-IT) = -767.918060345
T1 (CC-PVQZ)= 0.010491967
T2 (CC-PVQZ)= 0.038269
E(HF/CBS) = -764.66130468
E(DLPNO-CCSD(T)/CBS) = -768.255682598
Enthalpic correction = 0.25883271 (a.u.)
Entropy = 114.85198 (cal/(mol*K))

C	-2.252886	2.331513	-0.000006
C	-3.528330	1.853364	-0.000007
C	-3.481869	0.387229	-0.000004
C	-2.581302	-2.295060	0.000008
C	-3.920878	-1.981165	0.000010
C	-4.395112	-0.637186	0.000005
C	-2.106265	0.046559	-0.000006
C	-1.316433	1.199573	-0.000007
C	-0.207010	-1.387468	0.000001
C	-1.607950	-1.254259	0.000001
C	0.632916	-0.273080	-0.000003
C	0.071707	1.064955	-0.000004
C	0.946111	2.197057	0.000002
C	2.288340	2.048812	0.000010
C	2.088255	-0.411111	-0.000003

C	2.899453	0.752158	0.000007
C	4.300258	0.629163	0.000011
C	4.906074	-0.606678	0.000003
C	4.112535	-1.758485	-0.000011
C	2.736974	-1.658588	-0.000013
H	-1.976310	3.374770	-0.000007
H	-4.428631	2.448867	-0.000008
H	-2.265737	-3.331133	0.000013
H	-4.648846	-2.782334	0.000017
H	-5.462415	-0.452195	0.000008
H	0.214301	-2.382378	0.000007
H	0.504867	3.184847	0.000003
H	2.935995	2.917141	0.000018
H	4.899123	1.531824	0.000020
H	5.985088	-0.687909	0.000006
H	4.577835	-2.735676	-0.000020
H	2.157204	-2.569646	-0.000026

20244-28-4-C14H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -540.970243266 (a.u.)
E(HF/CC-PVTZ) = -537.31882922
E(DLPNO-CCSD(T)/CC-PVTZ) = -539.691955536710
T1 (CC-PVTZ)= 0.010125260
T2 (CC-PVTZ)= 0.059182
E(HF/CC-PVQZ) = -537.35121676
E(DLPNO-CCSD(T)/CC-PVQZ) = -539.844586415263
E(HF/TZ-AUG) = -537.32275481
E(DLPNO-CCSD(T)/TZ-AUG) = -539.728081078
E(HF/TZ-CORE) = -537.32280874
E(DLPNO-CCSD(T)/TZ-CORE) = -540.402899817
E(HF/TZ-IT) = -537.31882922
E(DLPNO-CCSD(T)/TZ-IT) = -539.698330906
T1 (CC-PVQZ)= 0.010185694
T2 (CC-PVQZ)= 0.058305
E(HF/CBS) = -537.359108723
E(DLPNO-CCSD(T)/CBS) = -539.940223517
Enthalpic correction = 0.22075730 (a.u.)
Entropy = 100.47830 (cal/(mol*K))

C	-2.833031	0.977570	0.000016
C	-3.537132	-0.339247	-0.000016
C	-2.900340	-1.501913	-0.000018
C	-1.410967	-1.635255	0.000009
C	-0.662643	-0.324905	0.000007
C	0.767551	-0.343744	0.000004
C	1.512202	-1.548783	0.000008
C	2.884839	-1.538942	0.000003
C	3.591310	-0.321682	-0.000006
C	2.903275	0.863827	-0.000009
C	1.490338	0.885931	-0.000004
C	0.768248	2.102893	-0.000005
C	-0.595091	2.093322	0.000001
C	-1.328086	0.880502	0.000008
H	-3.154679	1.566551	0.868612
H	-3.154685	1.566599	-0.868545
H	-4.621346	-0.316826	-0.000037
H	-3.467496	-2.426424	-0.000041
H	-1.104765	-2.232209	-0.868324
H	-1.104794	-2.232191	0.868365
H	0.994456	-2.496974	0.000016
H	3.429294	-2.474601	0.000007
H	4.673591	-0.325738	-0.000010
H	3.435373	1.807596	-0.000015
H	1.314950	3.037979	-0.000011
H	-1.142736	3.028788	0.000001

203-12-3-C18H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -692.270211032 (a.u.)
E(HF/CC-PVTZ) = -687.68437951
E(DLPNO-CCSD(T)/CC-PVTZ) = -690.640477127840
T1 (CC-PVTZ)= 0.010297637
T2 (CC-PVTZ)= 0.044675
E(HF/CC-PVQZ) = -687.72466332
E(DLPNO-CCSD(T)/CC-PVQZ) = -690.832312262094
E(HF/TZ-AUG) = -687.68913465
E(DLPNO-CCSD(T)/TZ-AUG) = -690.685267646
E(HF/TZ-CORE) = -687.68947181
E(DLPNO-CCSD(T)/TZ-CORE) = -691.554873409
E(HF/TZ-IT) = -687.68437951
E(DLPNO-CCSD(T)/TZ-IT) = -690.650337726
T1 (CC-PVQZ)= 0.010313343
T2 (CC-PVQZ)= 0.044062
E(HF/CBS) = -687.734479389
E(DLPNO-CCSD(T)/CBS) = -690.952719838
Enthalpic correction = 0.22416499 (a.u.)
Entropy = 104.01988 (cal/(mol*K))

C	-1.131276	-0.102023	-0.000045
C	-0.752441	-1.470603	-0.000024
C	-2.407923	0.435954	-0.000012
C	0.000000	0.712515	-0.000053
C	-1.791529	-2.374628	0.000020
C	0.752441	-1.470604	-0.000041
C	-3.124523	-1.876812	0.000037
C	-3.446945	-0.528583	0.000026
C	-2.455071	1.878862	0.000000
C	-1.319765	2.665075	0.000002
C	0.000000	2.086514	-0.000015
C	1.319765	2.665075	0.000022
C	1.131276	-0.102023	-0.000045
C	2.455071	1.878862	0.000028
C	2.407923	0.435954	-0.000003
C	3.446946	-0.528584	0.000027
C	3.124523	-1.876812	0.000019
C	1.791528	-2.374628	-0.000012
H	-1.629543	-3.445220	0.000037
H	-3.931656	-2.598417	0.000066
H	-4.487109	-0.226678	0.000051
H	-3.422190	2.367312	0.000024
H	-1.433271	3.742471	0.000027
H	1.433271	3.742471	0.000048
H	3.422190	2.367312	0.000057
H	4.487109	-0.226679	0.000059
H	3.931655	-2.598417	0.000045
H	1.629543	-3.445220	0.000003

203-64-5-C15H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -577.902551280 (a.u.)
E(HF/CC-PVTZ) = -574.04878
E(DLPNO-CCSD(T)/CC-PVTZ) = -576.539850372249
T1 (CC-PVTZ)= 0.010127646
T2 (CC-PVTZ)= 0.038095
E(HF/CC-PVQZ) = -574.08272535

E(DLPNO-CCSD(T)/CC-PVQZ) = -576.701041568471
E(HF/TZ-AUG) = -574.0528117
E(DLPNO-CCSD(T)/TZ-AUG) = -576.577520915
E(HF/TZ-CORE) = -574.05300819
E(DLPNO-CCSD(T)/TZ-CORE) = -577.301753581
E(HF/TZ-IT) = -574.04878
E(DLPNO-CCSD(T)/TZ-IT) = -576.547493604
T1 (CC-PVQZ)= 0.010159379
T2 (CC-PVQZ)= 0.037595
E(HF/CBS) = -574.090996909
E(DLPNO-CCSD(T)/CBS) = -576.802168204
Enthalpic correction = 0.20476705 (a.u.)
Entropy = 96.49755 (cal/(mol*K))

C	-3.373986	-0.327483	-0.000018
C	-2.568241	-1.491868	-0.000006
C	-1.199270	-1.340009	0.000017
C	-0.701901	-0.031712	0.000033
C	-1.452899	1.141944	0.000013
C	0.701901	-0.031712	0.000033
C	1.199270	-1.340010	0.000018
C	1.452899	1.141943	0.000012
C	0.000000	-2.293056	-0.000006
C	2.568240	-1.491868	-0.000006
C	3.373986	-0.327483	-0.000018
C	2.851596	0.957298	-0.000011
C	0.685772	2.362001	-0.000003
C	-0.685772	2.362001	-0.000003
C	-2.851596	0.957299	-0.000011
H	-4.449840	-0.449752	-0.000040
H	-3.040859	-2.466244	-0.000027
H	0.000000	-2.944628	-0.877889
H	0.000000	-2.944670	0.877846
H	3.040859	-2.466243	-0.000027
H	4.449840	-0.449752	-0.000040
H	3.519738	1.809784	-0.000028
H	1.212299	3.309007	-0.000015
H	-1.212299	3.309007	-0.000015
H	-3.519738	1.809784	-0.000027

20532-03-0-C28H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1078.37827840 (a.u.)
E(HF/CC-PVTZ) = -1071.18420916
E(DLPNO-CCSD(T)/CC-PVTZ) = -1075.830995850662
T1 (CC-PVTZ)= 0.010067364
T2 (CC-PVTZ)= 0.039403
E(HF/CC-PVQZ) = -1071.24753615
E(DLPNO-CCSD(T)/CC-PVQZ) = -1076.131235423780
E(HF/TZ-AUG) = -1071.1917726
E(DLPNO-CCSD(T)/TZ-AUG) = -1075.90226826
E(HF/TZ-CORE) = -1071.19210804
E(DLPNO-CCSD(T)/TZ-CORE) = -1077.25356869
E(HF/TZ-IT) = -1071.18420916
E(DLPNO-CCSD(T)/TZ-IT) = -1075.84564369
T1 (CC-PVQZ)= 0.010087355
T2 (CC-PVQZ)= 0.040951
E(HF/CBS) = -1071.26296722
E(DLPNO-CCSD(T)/CBS) = -1076.31954864
Enthalpic correction = 0.37766175 (a.u.)
Entropy = 150.15728 (cal/(mol*K))

C	2.855079	-1.325401	0.698407
C	3.529162	-2.319250	1.435202
C	3.600322	-0.358056	-0.022012
C	1.428948	-1.277039	0.679032
C	4.902313	-2.366736	1.468032
C	5.644502	-1.411710	0.759199
C	5.005833	-0.431859	0.032650
C	2.886344	0.652280	-0.779312
C	0.743521	-0.330679	-0.012526
C	1.464785	0.658361	-0.776339
C	-0.743521	-0.330679	0.012526
C	0.779785	1.628617	-1.535888
C	3.552827	1.635772	-1.536593
C	2.861016	2.578792	-2.261352
C	1.460441	2.574416	-2.264706
C	-3.529161	-2.319250	-1.435202
C	-2.855078	-1.325402	-0.698407
C	-4.902312	-2.366736	-1.468032
C	-1.428948	-1.277039	-0.679032
C	-3.600322	-0.358056	0.022012
C	-1.464785	0.658361	0.776339
C	-2.886344	0.652280	0.779312
C	-0.779785	1.628617	1.535888
C	-3.552827	1.635772	1.536593
C	-5.005832	-0.431860	-0.032650
C	-5.644502	-1.411711	-0.759199
C	-1.460441	2.574416	2.264706
C	-2.861016	2.578792	2.261351
H	2.941933	-3.048713	1.979621
H	0.883345	-2.016691	1.252257
H	5.409344	-3.134633	2.037593
H	6.726113	-1.443440	0.782399
H	5.605602	0.289640	-0.502444
H	-0.300714	1.620337	-1.539430
H	4.632449	1.655558	-1.557437
H	3.402118	3.321508	-2.833237
H	0.915765	3.311395	-2.840303
H	-2.941932	-3.048713	-1.979621
H	-5.409344	-3.134633	-2.037593
H	-0.883344	-2.016691	-1.252257
H	0.300714	1.620338	1.539430
H	-4.632449	1.655558	1.557437
H	-5.605602	0.289640	0.502444
H	-6.726113	-1.443440	-0.782399
H	-0.915766	3.311395	2.840303
H	-3.402118	3.321507	2.833237

205-99-2_C20H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -769.746996978 (a.u.)
E(HF/CC-PVTZ) = -764.63345885
E(DLPNO-CCSD(T)/CC-PVTZ) = -767.930286424604
T1 (CC-PVTZ)= 0.010107856
T2 (CC-PVTZ)= 0.036559
E(HF/CC-PVQZ) = -764.67849377
E(DLPNO-CCSD(T)/CC-PVQZ) = -768.144305821502
E(HF/TZ-AUG) = -764.63871728
E(DLPNO-CCSD(T)/TZ-AUG) = -767.980175739
E(HF/TZ-CORE) = -764.63909649
E(DLPNO-CCSD(T)/TZ-CORE) = -768.946307863
E(HF/TZ-IT) = -764.63345885
E(DLPNO-CCSD(T)/TZ-IT) = -767.940918222
T1 (CC-PVQZ)= 0.010131874
T2 (CC-PVQZ)= 0.038786
E(HF/CBS) = -764.689467556
E(DLPNO-CCSD(T)/CBS) = -768.278592604
Enthalpic correction = 0.25917013 (a.u.)
Entropy = 114.08733 (cal/(mol*K))

C	0.158795	0.579743	0.000009
C	0.422347	-0.825534	0.000007
C	1.360820	1.316800	0.000005
C	-1.110178	1.147426	0.000006
C	1.885490	-0.968492	0.000006
C	-0.626897	-1.687430	0.000000
C	2.456413	0.333838	0.000001
C	1.290429	2.693285	-0.000002
C	-2.232920	0.229654	0.000003
C	-1.154303	2.559202	-0.000001
C	2.700141	-2.089207	0.000005
C	-1.970579	-1.176283	-0.000001
C	3.832936	0.492041	-0.000005
C	0.016982	3.297213	-0.000005
C	-3.568780	0.662276	0.000004
C	4.083382	-1.918248	-0.000002
C	-3.060997	-2.068521	-0.000006
C	4.642778	-0.642573	-0.000007
C	-4.614267	-0.235817	-0.000001
C	-4.359381	-1.613161	-0.000007
H	-0.487973	-2.762145	-0.000006
H	2.179737	3.310645	-0.000008
H	-2.101585	3.080628	-0.000005
H	2.273451	-3.084443	0.000008
H	4.277447	1.479373	-0.000007
H	-0.046982	4.377862	-0.000012
H	-3.782178	1.722415	0.000009
H	4.730514	-2.785700	-0.000003
H	-2.858267	-3.132669	-0.000010
H	5.719398	-0.531668	-0.000011
H	-5.634735	0.124640	0.000000
H	-5.182079	-2.316219	-0.000011

206-44-0-C16H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -616.027897935 (a.u.)
E(HF/CC-PVTZ) = -611.93119297
E(DLPNO-CCSD(T)/CC-PVTZ) = -614.573496050808
T1 (CC-PVTZ)= 0.010165082
T2 (CC-PVTZ)= 0.032094
E(HF/CC-PVQZ) = -611.96735464
E(DLPNO-CCSD(T)/CC-PVQZ) = -614.745025119904
E(HF/TZ-AUG) = -611.93545061
E(DLPNO-CCSD(T)/TZ-AUG) = -614.613104584
E(HF/TZ-CORE) = -611.93571281
E(DLPNO-CCSD(T)/TZ-CORE) = -615.386375253
E(HF/TZ-IT) = -611.93119297
E(DLPNO-CCSD(T)/TZ-IT) = -614.581945566
T1 (CC-PVQZ)= 0.010193514
T2 (CC-PVQZ)= 0.037635
E(HF/CBS) = -611.976166256
E(DLPNO-CCSD(T)/CBS) = -614.852618351
Enthalpic correction = 0.21104821 (a.u.)
Entropy = 100.59459 (cal/(mol*K))

C	0.738037	-2.387980	0.000005
C	2.156250	-2.419832	0.000007
C	2.923420	-1.274446	0.000004
C	0.105533	-1.168433	-0.000003
C	-1.294635	-0.711847	-0.000008
C	0.901899	0.000000	-0.000006
C	2.298739	0.000000	-0.000002
C	0.105533	1.168433	-0.000005
C	2.923421	1.274446	-0.000001
C	2.156251	2.419832	-0.000002
C	0.738037	2.387980	-0.000004
C	-1.294635	0.711847	0.000003
C	-2.490808	-1.409446	-0.000011
C	-2.490808	1.409446	0.000011
C	-3.689356	0.696032	0.000008
C	-3.689356	-0.696032	-0.000002
H	0.184226	-3.318436	0.000007
H	2.650484	-3.383022	0.000011
H	4.004073	-1.345781	0.000006
H	4.004074	1.345780	0.000001
H	2.650485	3.383021	0.000001
H	0.184227	3.318436	0.000000
H	-2.500920	-2.492244	-0.000016
H	-2.500920	2.492245	0.000014
H	-4.630434	1.230561	0.000013
H	-4.630434	-1.230561	-0.000002

207-08-9-C20H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -769.743187692 (a.u.)
E(HF/CC-PVTZ) = -764.62920281
E(DLPNO-CCSD(T)/CC-PVTZ) = -767.925691270510
T1 (CC-PVTZ)= 0.010236002
T2 (CC-PVTZ)= 0.031729
E(HF/CC-PVQZ) = -764.67419097
E(DLPNO-CCSD(T)/CC-PVQZ) = -768.139727687096
E(HF/TZ-AUG) = -764.63436176
E(DLPNO-CCSD(T)/TZ-AUG) = -767.975421949
E(HF/TZ-CORE) = -764.63484889
E(DLPNO-CCSD(T)/TZ-CORE) = -768.941858418
E(HF/TZ-IT) = -764.62920281
E(DLPNO-CCSD(T)/TZ-IT) = -767.936431827
T1 (CC-PVQZ)= 0.010248212
T2 (CC-PVQZ)= 0.037645
E(HF/CBS) = -764.685153362
E(DLPNO-CCSD(T)/CBS) = -768.274049617
Enthalpic correction = 0.25904236 (a.u.)
Entropy = 114.02002 (cal/(mol*K))

C	-1.858200	2.390426	-0.000008
C	-3.275184	2.420229	-0.000004
C	-4.041374	1.273768	-0.000001
C	-1.224345	1.170915	-0.000007
C	0.176643	0.722701	0.000003
C	-2.017802	0.000000	-0.000006
C	-3.416802	0.000000	-0.000001
C	-1.224346	-1.170914	-0.000003
C	-4.041374	-1.273769	0.000008
C	-3.275183	-2.420229	0.000012
C	-1.858200	-2.390426	0.000008
C	0.176643	-0.722701	-0.000010
C	1.353051	1.415558	0.000009
C	1.353051	-1.415557	-0.000015
C	2.588172	-0.715486	-0.000007
C	2.588172	0.715486	0.000004
C	3.827350	-1.394410	-0.000008
C	3.827350	1.394410	0.000011
C	5.013433	-0.704313	-0.000001
C	5.013433	0.704313	0.000009
H	-1.304580	3.320843	-0.000004
H	-3.770961	3.382661	-0.000002
H	-5.122054	1.344195	0.000002
H	-5.122054	-1.344195	0.000012
H	-3.770961	-3.382661	0.000018
H	-1.304578	-3.320842	0.000011
H	1.365278	2.499136	0.000013

H	1.365278	-2.499136	-0.000018
H	3.825504	-2.477797	-0.000016
H	3.825504	2.477797	0.000019
H	5.953354	-1.240892	-0.000003
H	5.953354	1.240892	0.000016

208-96-8_C12H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -462.296422801 (a.u.)
E(HF/CC-PVTZ) = -459.2154566
E(DLPNO-CCSD(T)/CC-PVTZ) = -461.205850723124
T1 (CC-PVTZ)= 0.010518816
T2 (CC-PVTZ)= 0.039173
E(HF/CC-PVQZ) = -459.24286049
E(DLPNO-CCSD(T)/CC-PVQZ) = -461.334949218530
E(HF/TZ-AUG) = -459.21887546
E(DLPNO-CCSD(T)/TZ-AUG) = -461.235474121
E(HF/TZ-CORE) = -459.21885569
E(DLPNO-CCSD(T)/TZ-CORE) = -461.815420653
E(HF/TZ-IT) = -459.2154566
E(DLPNO-CCSD(T)/TZ-IT) = -461.212160098
T1 (CC-PVQZ)= 0.010550705
T2 (CC-PVQZ)= 0.037533
E(HF/CBS) = -459.249538073
E(DLPNO-CCSD(T)/CBS) = -461.415836378
Enthalpic correction = 0.16276274 (a.u.)
Entropy = 87.22782 (cal/(mol*K))

C	0.000000	0.139538	-0.000043
C	1.158156	0.947612	-0.000018
C	-1.158156	0.947611	-0.000018
C	0.000000	-1.250882	-0.000024
C	0.679756	2.337781	-0.000004
C	2.381318	0.319766	0.000019
C	-0.679758	2.337781	0.000011
C	-2.381318	0.319765	0.000016
C	-1.277681	-1.873294	-0.000003
C	1.277682	-1.873294	-0.000002
C	2.419415	-1.100421	0.000017
C	-2.419414	-1.100422	0.000015
H	1.313425	3.211958	0.000004
H	3.310287	0.876781	0.000044
H	-1.313427	3.211958	0.000029
H	-3.310287	0.876780	0.000045
H	-1.354298	-2.953646	0.000004
H	1.354299	-2.953645	0.000006
H	3.385082	-1.589716	0.000038
H	-3.385080	-1.589718	0.000035

212-74-8-C24H16

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -924.645332769 (a.u.)
E(HF/CC-PVTZ) = -918.46760633
E(DLPNO-CCSD(T)/CC-PVTZ) = -922.463640087608
T1 (CC-PVTZ)= 0.009857866
T2 (CC-PVTZ)= 0.038846
E(HF/CC-PVQZ) = -918.52215372
E(DLPNO-CCSD(T)/CC-PVQZ) = -922.721141984995
E(HF/TZ-AUG) = -918.47408021
E(DLPNO-CCSD(T)/TZ-AUG) = -922.525370788
E(HF/TZ-CORE) = -918.47448551
E(DLPNO-CCSD(T)/TZ-CORE) = -923.683260094
E(HF/TZ-IT) = -918.46760633
E(DLPNO-CCSD(T)/TZ-IT) = -922.475669679
T1 (CC-PVQZ)= 0.009910137
T2 (CC-PVQZ)= 0.041145
E(HF/CBS) = -918.535445436
E(DLPNO-CCSD(T)/CBS) = -922.882535639
Enthalpic correction = 0.32941007 (a.u.)
Entropy = 132.99618 (cal/(mol*K))

C	-0.488200	1.564656	0.497037
C	-1.050471	2.447529	1.420520
C	-0.262465	3.122238	2.341959
C	1.112923	2.929049	2.341863
C	1.684427	2.063289	1.420408
C	0.900569	1.369518	0.496999
C	1.564656	0.488201	-0.497041
C	2.447533	1.050472	-1.420521
C	3.122244	0.262465	-2.341959
C	2.929052	-1.112924	-2.341863
C	2.063288	-1.684427	-1.420411
C	1.369515	-0.900567	-0.497004
C	0.488200	-1.564652	0.497039
C	1.050474	-2.447526	1.420520
C	0.262470	-3.122237	2.341960
C	-1.112919	-2.929049	2.341865
C	-1.684426	-2.063290	1.420411
C	-0.900569	-1.369516	0.497002
C	-1.564657	-0.488200	-0.497038
C	-1.369518	0.900569	-0.497002
C	-2.063292	1.684426	-1.420411
C	-2.929055	1.112920	-2.341862
C	-3.122246	-0.262468	-2.341955
C	-2.447533	-1.050473	-1.420517
H	-2.122767	2.595852	1.412833
H	-0.720661	3.794405	3.055868
H	1.738664	3.448938	3.055712
H	2.756073	1.910332	1.412661
H	2.595857	2.122767	-1.412834
H	3.794414	0.720660	-3.055865
H	3.448944	-1.738665	-3.055710
H	1.910329	-2.756072	-1.412666
H	2.122769	-2.595850	1.412829
H	0.720667	-3.794402	3.055869
H	-1.738659	-3.448940	3.055714
H	-2.756071	-1.910336	1.412665
H	-1.910335	2.756071	-1.412666
H	-3.448946	1.738660	-3.055711
H	-3.794416	-0.720665	-3.055860
H	-2.595857	-2.122768	-1.412827

213-46-7-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.214574225 (a.u.)
E(HF/CC-PVTZ) = -841.56810627
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.211842239123
T1 (CC-PVTZ)= 0.010112109
T2 (CC-PVTZ)= 0.035019
E(HF/CC-PVQZ) = -841.61791489
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.447948961719
E(HF/TZ-AUG) = -841.57407796
E(DLPNO-CCSD(T)/TZ-AUG) = -845.267231474
E(HF/TZ-CORE) = -841.57426882
E(DLPNO-CCSD(T)/TZ-CORE) = -846.329507377
E(HF/TZ-IT) = -841.56810627

E(DLPNO-CCSD(T)/TZ-IT) = -845.2234432
T1 (CC-PVQZ)= 0.010129643
T2 (CC-PVQZ)= 0.037646
E(HF/CBS) = -841.630051897
E(DLPNO-CCSD(T)/CBS) = -845.596033232
Enthalpic correction = 0.29465040 (a.u.)
Entropy = 125.11958 (cal/(mol*K))

C	2.874659	-0.461038	0.000002
C	3.641409	-1.645683	0.000022
C	5.016385	-1.609637	0.000027
C	3.570622	0.776365	-0.000012
C	1.427315	-0.457298	-0.000003
C	4.980306	0.788866	-0.000008
C	2.824748	1.987853	-0.000029
C	5.696929	-0.382212	0.000011
C	1.468479	1.983054	-0.000024
C	0.720492	0.766294	-0.000007
C	-0.720491	0.766294	0.000002
C	0.681088	-1.660794	-0.000009
C	-1.427315	-0.457298	-0.000005
C	-0.681088	-1.660794	-0.000014
C	-2.874659	-0.461038	-0.000003
C	-1.468479	1.983054	0.000022
C	-2.824748	1.987853	0.000027
C	-3.570622	0.776365	0.000012
C	-4.980306	0.788866	0.000013
C	-3.641409	-1.645683	-0.000014
C	-5.696929	-0.382212	0.000000
C	-5.016385	-1.609638	-0.000013
H	3.151130	-2.607694	0.000039
H	5.576654	-2.535689	0.000044
H	5.489969	1.744743	-0.000019
H	3.364956	2.926714	-0.000046
H	6.778923	-0.362153	0.000014
H	0.951551	2.929806	-0.000042
H	1.194437	-2.610345	-0.000016
H	-1.194437	-2.610345	-0.000023
H	-0.951551	2.929806	0.000042
H	-3.364956	2.926714	0.000045
H	-5.489969	1.744742	0.000024
H	-3.151129	-2.607694	-0.000025
H	-6.778923	-0.362153	0.000001
H	-5.576654	-2.535689	-0.000023

214-17-5-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.209199348 (a.u.)
E(HF/CC-PVTZ) = -841.561634
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.205504148398
T1 (CC-PVTZ)= 0.010217508
T2 (CC-PVTZ)= 0.035809
E(HF/CC-PVQZ) = -841.6114246
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.441654962068
E(HF/TZ-AUG) = -841.56752925
E(DLPNO-CCSD(T)/TZ-AUG) = -845.260859039
E(HF/TZ-CORE) = -841.56780672
E(DLPNO-CCSD(T)/TZ-CORE) = -846.323251835
E(HF/TZ-IT) = -841.561634
E(DLPNO-CCSD(T)/TZ-IT) = -845.217227376
T1 (CC-PVQZ)= 0.010230597
T2 (CC-PVQZ)= 0.037673
E(HF/CBS) = -841.623557216
E(DLPNO-CCSD(T)/CBS) = -845.589780166
Enthalpic correction = 0.29446829 (a.u.)
Entropy = 124.29067 (cal/(mol*K))

C	0.763128	-0.074757	-0.000009
C	-0.654141	-0.403175	-0.000012
C	-1.614090	0.624813	-0.000008
C	-1.096474	-1.755145	-0.000022
C	1.157765	1.305893	-0.000014
C	1.765803	-1.037657	0.000001
C	-3.019742	0.298353	0.000003
C	-1.169560	1.987177	-0.000018
C	-2.417314	-2.075049	-0.000024
C	2.504952	1.645617	-0.000010
C	0.143614	2.310806	-0.000022
C	3.125070	-0.704526	0.000005
C	-3.416678	-1.067691	-0.000009
C	-4.039963	1.276683	0.000028
C	3.509742	0.675925	-0.000001
C	4.144397	-1.695667	0.000016
C	-4.787895	-1.400760	-0.000003
C	-5.368738	0.926930	0.000035
C	4.893204	1.002752	0.000004
C	5.463765	-1.344488	0.000021
C	-5.751680	-0.424842	0.000017
C	5.843102	0.022277	0.000015
H	-0.370594	-2.553997	-0.000033
H	1.515683	-2.088790	0.000008
H	-1.898873	2.782564	-0.000029
H	-2.726841	-3.112985	-0.000036
H	2.781846	2.693672	-0.000014
H	0.449972	3.349667	-0.000033
H	-3.784322	2.325445	0.000048
H	3.853262	-2.739133	0.000021
H	-5.065789	-2.447765	-0.000014
H	-6.126114	1.700159	0.000056
H	5.179633	2.047422	0.000000
H	6.229641	-2.109230	0.000029
H	-6.800692	-0.690714	0.000022
H	6.893586	0.282879	0.000019

2143-69-30_C2H2

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -77.2982597803 (a.u.)
E(HF/CC-PVTZ) = -76.79393029
E(DLPNO-CCSD(T)/CC-PVTZ) = -77.116318693769
T1 (CC-PVTZ)= 0.016868366
T2 (CC-PVTZ)= 0.104258
E(HF/CC-PVQZ) = -76.79884987
E(DLPNO-CCSD(T)/CC-PVQZ) = -77.137183229169
E(HF/TZ-AUG) = -76.79491119
E(DLPNO-CCSD(T)/TZ-AUG) = -77.1212157834
E(HF/TZ-CORE) = -76.79455245
E(DLPNO-CCSD(T)/TZ-CORE) = -77.2171126684
E(HF/TZ-IT) = -76.79393029
E(DLPNO-CCSD(T)/TZ-IT) = -77.1169011108
T1 (CC-PVQZ)= 0.017077889
T2 (CC-PVQZ)= 0.101293
E(HF/CBS) = -76.8000486379
E(DLPNO-CCSD(T)/CBS) = -77.1500175051
Enthalpic correction = 0.02711116 (a.u.)
Entropy = 53.18741 (cal/(mol*K))

C	0.000000	0.000000	-0.474479
C	0.000000	0.000000	0.816375
H	0.000000	0.937318	-1.025688
H	0.000000	-0.937318	-1.025688

214-63-1-C24H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -923.456232643 (a.u.)
E(HF/CC-PVTZ) = -917.31252211
E(DLPNO-CCSD(T)/CC-PVTZ) = -921.272989957490
T1 (CC-PVTZ)= 0.010428881
T2 (CC-PVTZ)= 0.032584
E(HF/CC-PVQZ) = -917.36645937
E(DLPNO-CCSD(T)/CC-PVQZ) = -921.529322312369
E(HF/TZ-AUG) = -917.3188076
E(DLPNO-CCSD(T)/TZ-AUG) = -921.333373572
E(HF/TZ-CORE) = -917.31924309
E(DLPNO-CCSD(T)/TZ-CORE) = -922.492299133
E(HF/TZ-IT) = -917.31252211
E(DLPNO-CCSD(T)/TZ-IT) = -921.28640911
T1 (CC-PVQZ)= 0.010419148
T2 (CC-PVQZ)= 0.038261
E(HF/CBS) = -917.379602414
E(DLPNO-CCSD(T)/CBS) = -921.690159074
Enthalpic correction = 0.30746987 (a.u.)
Entropy = 129.38607 (cal/(mol*K))

C	-4.501949	2.040332	-0.217497
C	-4.920326	0.737562	-0.115479
C	-3.134319	2.349058	-0.205405
C	-2.176794	1.350120	-0.099877
C	-0.778801	1.654784	-0.058887
C	0.190913	0.705191	0.034102
C	-0.190913	-0.705191	0.034102
C	0.778801	-1.654784	-0.058887
C	2.176794	-1.350120	-0.099877
C	3.134319	-2.349058	-0.205405
C	4.501949	-2.040332	-0.217496
C	4.920326	-0.737562	-0.115479
C	-2.589472	-0.010568	-0.007444
C	-3.980299	-0.317763	-0.003398
C	-4.382233	-1.663556	0.116380
C	-3.440303	-2.656830	0.239454
C	-2.075354	-2.352830	0.229934
C	-1.621580	-1.047358	0.087588
C	1.621580	1.047358	0.087588
C	2.589472	0.010568	-0.007444
C	3.980299	0.317763	-0.003397
C	4.382233	1.663556	0.116380
C	3.440303	2.656830	0.239454
C	2.075354	2.352830	0.229934
H	-5.228463	2.838190	-0.302159
H	-5.975811	0.496046	-0.116888
H	-2.814213	3.381470	-0.273328
H	-0.512228	2.700968	-0.119801
H	0.512228	-2.700968	-0.119801
H	2.814213	-3.381470	-0.273328
H	5.228463	-2.838190	-0.302158
H	5.975811	-0.496046	-0.116888
H	-5.438876	-1.900040	0.120172
H	-3.751075	-3.687937	0.348579
H	-1.370204	-3.162950	0.346597
H	5.438876	1.900040	0.120172
H	3.751075	3.687937	0.348579
H	1.370204	3.162950	0.346597

215-58-7-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.210850424 (a.u.)
E(HF/CC-PVTZ) = -841.56330642
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.208669265877
T1 (CC-PVTZ)= 0.010057011
T2 (CC-PVTZ)= 0.037939
E(HF/CC-PVQZ) = -841.61305482
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.444692114670
E(HF/TZ-AUG) = -841.56916079
E(DLPNO-CCSD(T)/TZ-AUG) = -845.264041041
E(HF/TZ-CORE) = -841.56947579
E(DLPNO-CCSD(T)/TZ-CORE) = -846.326312497
E(HF/TZ-IT) = -841.56330642
E(DLPNO-CCSD(T)/TZ-IT) = -845.220225986
T1 (CC-PVQZ)= 0.010074813
T2 (CC-PVQZ)= 0.038952
E(HF/CBS) = -841.625177153
E(DLPNO-CCSD(T)/CBS) = -845.59274445
Enthalpic correction = 0.29456947 (a.u.)
Entropy = 127.68074 (cal/(mol*K))

C	-0.247173	0.716593	-0.000004
C	-0.247173	-0.716593	-0.000003
C	1.025281	-1.442258	-0.000003
C	-1.462809	-1.381748	-0.000001
C	1.025281	1.442258	-0.000004
C	-1.462809	1.381748	-0.000002
C	2.246519	-0.732387	0.000003
C	1.065994	-2.847500	-0.000008
C	-2.693738	-0.712976	0.000000
C	2.246519	0.732387	0.000004
C	1.065994	2.847500	-0.000010
C	-2.693738	0.712976	0.000000
C	3.447441	-1.463682	0.000006
C	2.255923	-3.541980	-0.000005
C	-3.935681	-1.399529	0.000002
C	3.447441	1.463682	0.000010
C	2.255923	3.541980	-0.000006
C	-3.935681	1.399529	0.000002
C	3.461456	-2.841544	0.000003
C	-5.115186	-0.708060	0.000004
C	3.461456	2.841543	0.000005
C	-5.115186	0.708060	0.000004
H	-1.492680	-2.461223	0.000002
H	-1.492680	2.461223	0.000000
H	0.146450	-3.412101	-0.000015
H	0.146451	3.412101	-0.000020
H	4.393417	-0.944997	0.000011
H	2.250316	-4.624131	-0.000009
H	-3.932652	-2.482846	0.000003
H	4.393417	0.944997	0.000018
H	2.250316	4.624130	-0.000011
H	-3.932652	2.482846	0.000002
H	4.404352	-3.372594	0.000005
H	-6.057367	-1.240694	0.000006
H	4.404352	3.372594	0.000010
H	-6.057367	1.240694	0.000006

217-59-4-C18H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -693.499839976 (a.u.)
E(HF/CC-PVTZ) = -688.87055419
E(DLPNO-CCSD(T)/CC-PVTZ) = -691.860231965588
T1 (CC-PVTZ)= 0.009946784
T2 (CC-PVTZ)= 0.037351

E(HF/CC-PVQZ) = -688.9114685
E(DLPNO-CCSD(T)/CC-PVQZ) = -692.053741404193
E(HF/TZ-AUG) = -688.8754647
E(DLPNO-CCSD(T)/TZ-AUG) = -691.905319591
E(HF/TZ-CORE) = -688.87560585
E(DLPNO-CCSD(T)/TZ-CORE) = -692.774645038
E(HF/TZ-IT) = -688.87055419
E(DLPNO-CCSD(T)/TZ-IT) = -691.869470917
T1 (CC-PVQZ)= 0.009985651
T2 (CC-PVQZ)= 0.038390
E(HF/CBS) = -688.921438205
E(DLPNO-CCSD(T)/CBS) = -692.175064311
Enthalpic correction = 0.24654798 (a.u.)
Entropy = 112.82617 (cal/(mol*K))

C	-0.495483	1.349113	-0.000001
C	0.940938	1.086411	0.000000
C	1.416111	-0.245452	0.000000
C	1.880212	2.134496	0.000000
C	-1.411323	0.271668	0.000001
C	-1.002972	2.661797	-0.000003
C	0.470389	-1.358065	0.000000
C	2.806680	-0.462317	0.000001
C	3.236029	1.895454	0.000001
C	-0.920634	-1.103650	0.000001
C	-2.788631	0.561050	0.000002
C	-2.355620	2.918150	-0.000002
C	0.908425	-2.695534	-0.000001
C	3.705015	0.580925	0.000001
C	-1.803717	-2.199491	0.000001
C	-3.259541	1.854729	0.000001
C	0.023517	-3.750192	-0.000001
C	-1.349400	-3.499089	0.000000
H	1.542568	3.159263	0.000002
H	-0.324444	3.500682	-0.000006
H	3.193920	-1.469383	0.000002
H	3.931249	2.724793	0.000001
H	-3.507259	-0.243757	0.000003
H	-2.712280	3.939878	-0.000003
H	1.964721	-2.915478	-0.000003
H	4.768187	0.378934	0.000001
H	-2.869480	-2.031315	0.000001
H	-4.325381	2.042131	0.000003
H	0.394145	-4.766937	-0.000002
H	-2.055908	-4.318833	0.000000

218-01-9-C18H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -693.499923051
(a.u.)
E(HF/CC-PVTZ) = -688.87124548
E(DLPNO-CCSD(T)/CC-PVTZ) = -691.859227885055
T1 (CC-PVTZ)= 0.010097953
T2 (CC-PVTZ)= 0.035003
E(HF/CC-PVQZ) = -688.91217177
E(DLPNO-CCSD(T)/CC-PVQZ) = -692.052937502732
E(HF/TZ-AUG) = -688.87616505
E(DLPNO-CCSD(T)/TZ-AUG) = -691.904362969
E(HF/TZ-CORE) = -688.8762976
E(DLPNO-CCSD(T)/TZ-CORE) = -692.773788712
E(HF/TZ-IT) = -688.87124548
E(DLPNO-CCSD(T)/TZ-IT) = -691.868583562
T1 (CC-PVQZ)= 0.010130019
T2 (CC-PVQZ)= 0.037661
E(HF/CBS) = -688.922144394
E(DLPNO-CCSD(T)/CBS) = -692.174400663
Enthalpic correction = 0.24656855 (a.u.)
Entropy = 110.71705 (cal/(mol*K))

C	-0.427438	0.561053	0.000004
C	0.427438	-0.561053	-0.000003
C	-1.861513	0.374849	-0.000001
C	0.150756	1.863821	0.000016
C	1.861513	-0.374849	0.000001
C	-0.150757	-1.863821	-0.000014
C	-2.390809	-0.943992	0.000004
C	-2.778323	1.448897	-0.000013
C	1.495517	2.047824	0.000008
C	2.390809	0.943992	-0.000003
C	2.778323	-1.448897	0.000010
C	-1.495517	-2.047824	-0.000006
C	-3.787519	-1.140021	0.000010
C	-4.136149	1.233134	-0.000009
C	3.787518	1.140021	-0.000010
C	4.136149	-1.233133	0.000006
C	-4.650731	-0.073193	0.000006
C	4.650731	0.073193	-0.000007
H	-0.490995	2.731594	0.000039
H	0.490995	-2.731594	-0.000036
H	-2.419253	2.467028	-0.000032
H	1.908655	3.049090	0.000014
H	2.419254	-2.467028	0.000028
H	-1.908656	-3.049090	-0.000010
H	-4.167682	-2.154385	0.000017
H	-4.812784	2.077917	-0.000019
H	4.167681	2.154385	-0.000015
H	4.812784	-2.077917	0.000015
H	-5.720850	-0.234347	0.000012
H	5.720850	0.234348	-0.000014

219-08-9-C17H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -655.351397622
(a.u.)
E(HF/CC-PVTZ) = -650.96773796
E(DLPNO-CCSD(T)/CC-PVTZ) = -653.804472925618
T1 (CC-PVTZ)= 0.010190233
T2 (CC-PVTZ)= 0.036299
E(HF/CC-PVQZ) = -651.00649033
E(DLPNO-CCSD(T)/CC-PVQZ) = -653.987894588836
E(HF/TZ-AUG) = -650.97241627
E(DLPNO-CCSD(T)/TZ-AUG) = -653.847534706
E(HF/TZ-CORE) = -650.97250147
E(DLPNO-CCSD(T)/TZ-CORE) = -654.667880268
E(HF/TZ-IT) = -650.96773796
E(DLPNO-CCSD(T)/TZ-IT) = -653.812981732
T1 (CC-PVQZ)= 0.010235518
T2 (CC-PVQZ)= 0.037718
E(HF/CBS) = -651.015933229
E(DLPNO-CCSD(T)/CBS) = -654.102906972
Enthalpic correction = 0.23925735 (a.u.)
Entropy = 107.66978 (cal/(mol*K))

C	-3.141377	1.401579	-0.000005
C	-4.323602	0.764691	0.000005
C	-4.116900	-0.725959	-0.000001
C	-2.054183	0.422182	-0.000001
C	-2.617760	-0.851360	0.000000
C	-1.806127	-1.981824	0.000000
C	-0.433547	-1.827251	0.000000
C	-0.654901	0.602257	0.000000
C	0.174950	-0.555057	0.000000
C	1.284093	2.056814	0.000000
C	-0.060768	1.900961	0.000000

C	2.160271	0.928647	0.000001
C	1.617064	-0.383826	0.000000
C	2.518019	-1.467227	0.000000
C	3.880559	-1.270465	0.000000
C	4.410222	0.027464	0.000000
C	3.558082	1.105470	0.000001
H	-3.009203	2.473479	-0.000008
H	-5.297303	1.231737	0.000009
H	-4.570387	-1.201369	0.876727
H	-4.570393	-1.201372	-0.876723
H	-2.238510	-2.975016	-0.000001
H	0.182666	-2.713817	0.000000
H	1.722431	3.047344	0.000001
H	-0.705966	2.769118	-0.000001
H	2.142615	-2.479908	-0.000001
H	4.545633	-2.124435	-0.000001
H	5.482064	0.176923	0.000001
H	3.951795	2.114738	0.000001

222-93-5-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.207148449 (a.u.)
E(HF/CC-PVTZ) = -841.56053503
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.202829288339
T1 (CC-PVTZ)= 0.010246528
T2 (CC-PVTZ)= 0.037905
E(HF/CC-PVQZ) = -841.61026086
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.439001556741
E(HF/TZ-AUG) = -841.56625878
E(DLPNO-CCSD(T)/TZ-AUG) = -845.258016698
E(HF/TZ-CORE) = -841.56672278
E(DLPNO-CCSD(T)/TZ-CORE) = -846.320783006
E(HF/TZ-IT) = -841.56053503
E(DLPNO-CCSD(T)/TZ-IT) = -845.214564921
T1 (CC-PVQZ)= 0.010271139
T2 (CC-PVQZ)= 0.038705
E(HF/CBS) = -841.622377693
E(DLPNO-CCSD(T)/CBS) = -845.587173899
Enthalpic correction = 0.29433502 (a.u.)
Entropy = 124.02804 (cal/(mol*K))

C	0.732655	0.269954	0.000001
C	1.427138	1.526688	-0.000005
C	0.673282	2.752758	-0.000003
C	2.811601	1.550172	-0.000008
C	-0.732655	0.269954	0.000000
C	1.484120	-0.891470	0.000007
C	-1.427138	1.526688	0.000005
C	-1.484120	-0.891470	-0.000007
C	-0.673282	2.752758	0.000004
C	-2.811601	1.550172	0.000008
C	3.574411	0.374297	-0.000005
C	2.888379	-0.880307	0.000005
C	4.993004	0.380321	-0.000008
C	3.652484	-2.075688	0.000011
C	5.697602	-0.791736	-0.000003
C	5.019525	-2.034107	0.000008
C	-2.888379	-0.880307	-0.000005
C	-3.574411	0.374297	0.000004
C	-3.652484	-2.075688	-0.000011
C	-4.993004	0.380321	0.000007
C	-5.019525	-2.034108	-0.000008
C	-5.697602	-0.791736	0.000002
H	1.223554	3.685688	-0.000006
H	3.321183	2.506972	-0.000012
H	0.996263	-1.856483	0.000017
H	-0.996263	-1.856483	-0.000016
H	-1.223554	3.685688	0.000007
H	-3.321183	2.506972	0.000012
H	5.509178	1.332676	-0.000016
H	3.131869	-3.025721	0.000019
H	6.779795	-0.775103	-0.000006
H	5.590869	-2.953314	0.000012
H	-3.131869	-3.025721	-0.000018
H	-5.509178	1.332676	0.000015
H	-5.590869	-2.953314	-0.000013
H	-6.779795	-0.775103	0.000004

224-41-9-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.213803157 (a.u.)
E(HF/CC-PVTZ) = -841.56820902
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.210661468341
T1 (CC-PVTZ)= 0.010133701
T2 (CC-PVTZ)= 0.036342
E(HF/CC-PVQZ) = -841.61795099
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.446798280645
E(HF/TZ-AUG) = -841.57400596
E(DLPNO-CCSD(T)/TZ-AUG) = -845.265835927
E(HF/TZ-CORE) = -841.57438566
E(DLPNO-CCSD(T)/TZ-CORE) = -846.328462785
E(HF/TZ-IT) = -841.56820902
E(DLPNO-CCSD(T)/TZ-IT) = -845.222233062
T1 (CC-PVQZ)= 0.010160173
T2 (CC-PVQZ)= 0.037723
E(HF/CBS) = -841.630071756
E(DLPNO-CCSD(T)/CBS) = -845.594936904
Enthalpic correction = 0.29453295 (a.u.)
Entropy = 124.39529 (cal/(mol*K))

C	2.608649	-1.872923	-0.000003
C	2.502432	-0.470379	-0.000001
C	3.702599	0.286923	0.000003
C	1.225062	0.228049	-0.000003
C	3.834948	-2.502232	0.000001
C	5.015566	-1.750064	0.000007
C	4.943379	-0.375839	0.000008
C	3.641918	1.719303	0.000001
C	2.459202	2.371750	-0.000005
C	1.218497	1.656007	-0.000006
C	0.000000	2.329041	-0.000007
C	0.000000	-0.437060	0.000001
C	-1.218496	1.656007	-0.000005
C	-1.225061	0.228049	-0.000003
C	-2.459202	2.371750	0.000000
C	-2.502432	-0.470379	-0.000002
C	-3.641917	1.719303	0.000008
C	-3.702599	0.286923	0.000006
C	-4.943379	-0.375838	0.000011
C	-2.608650	-1.872923	-0.000011
C	-5.015566	-1.750063	0.000005
C	-3.834949	-2.502232	-0.000007
H	1.716207	-2.481709	-0.000011
H	3.883076	-3.583463	-0.000001
H	5.976862	-2.247024	0.000011
H	5.848687	0.219062	0.000011
H	4.574560	2.270091	0.000003
H	2.425815	3.454340	-0.000008
H	0.000000	3.413040	-0.000007
H	0.000000	-1.514681	0.000011
H	-2.425815	3.454341	-0.000001
H	-4.574560	2.270092	0.000014

H	-5.848686	0.219063	0.000018
H	-1.716208	-2.481709	-0.000024
H	-5.976863	-2.247024	0.000008
H	-3.883077	-3.583462	-0.000015

226-88-0-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.202089707 (a.u.)
E(HF/CC-PVTZ) = -841.55323782
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.197568599539
T1 (CC-PVTZ)= 0.010346796
T2 (CC-PVTZ)= 0.036775
E(HF/CC-PVQZ) = -841.60298425
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.433653557061
E(HF/TZ-AUG) = -841.5589788
E(DLPNO-CCSD(T)/TZ-AUG) = -845.252563801
E(HF/TZ-CORE) = -841.55942333
E(DLPNO-CCSD(T)/TZ-CORE) = -846.315370954
E(HF/TZ-IT) = -841.55323782
E(DLPNO-CCSD(T)/TZ-IT) = -845.209418941
T1 (CC-PVQZ)= 0.010363344
T2 (CC-PVQZ)= 0.038451
E(HF/CBS) = -841.615106103
E(DLPNO-CCSD(T)/CBS) = -845.581752173
Enthalpic correction = 0.29417061 (a.u.)
Entropy = 123.87372 (cal/(mol*K))

C	3.568428	0.569375	0.000008
C	3.307710	-0.850063	-0.000008
C	4.924402	1.012486	0.000013
C	2.498063	1.455541	0.000015
C	4.417493	-1.746151	-0.000018
C	1.992221	-1.298550	-0.000012
C	5.696440	-1.278948	-0.000013
C	5.953635	0.121125	0.000003
C	1.172126	1.006922	0.000009
C	0.910849	-0.409895	-0.000002
C	0.071789	1.885634	0.000011
C	-0.427510	-0.857359	-0.000004
C	-1.230780	1.429873	0.000005
C	-1.499333	0.009723	0.000003
C	-2.332222	2.352380	-0.000006
C	-2.889751	-0.442416	0.000004
C	-3.609303	1.922022	-0.000019
C	-3.929967	0.519374	-0.000013
C	-5.268559	0.095553	-0.000018
C	-3.247326	-1.799733	0.000025
C	-5.591515	-1.244684	-0.000002
C	-4.569565	-2.197486	0.000022
H	5.118492	2.078180	0.000026
H	2.692875	2.521864	0.000026
H	4.220131	-2.811252	-0.000031
H	1.797098	-2.364896	-0.000023
H	6.528469	-1.971142	-0.000022
H	6.977384	0.472368	0.000007
H	0.256359	2.953728	0.000013
H	-0.589246	-1.926291	-0.000016
H	-2.107321	3.411889	-0.000007
H	-4.428432	2.630722	-0.000032
H	-6.050470	0.845300	-0.000033
H	-2.479338	-2.559641	0.000048
H	-6.627617	-1.556988	-0.000006
H	-4.812332	-3.252184	0.000040

232-54-2-C13H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -501.635433005 (a.u.)
E(HF/CC-PVTZ) = -498.26916666
E(DLPNO-CCSD(T)/CC-PVTZ) = -500.450780814906
T1 (CC-PVTZ)= 0.010236038
T2 (CC-PVTZ)= 0.038354
E(HF/CC-PVQZ) = -498.29902832
E(DLPNO-CCSD(T)/CC-PVQZ) = -500.591691137713
E(HF/TZ-AUG) = -498.27279977
E(DLPNO-CCSD(T)/TZ-AUG) = -500.483602024
E(HF/TZ-CORE) = -498.27282537
E(DLPNO-CCSD(T)/TZ-CORE) = -501.111059626
E(HF/TZ-IT) = -498.26916666
E(DLPNO-CCSD(T)/TZ-IT) = -500.457098897
T1 (CC-PVQZ)= 0.010293476
T2 (CC-PVQZ)= 0.037758
E(HF/CBS) = -498.306304795
E(DLPNO-CCSD(T)/CBS) = -500.680003123
Enthalpic correction = 0.19115353 (a.u.)
Entropy = 93.72284 (cal/(mol*K))

C	0.503375	-0.398346	-0.000001
C	1.129851	0.889918	0.000001
C	1.321644	-1.554615	-0.000003
C	2.543029	0.957725	0.000003
C	2.687710	-1.448862	0.000000
C	3.306376	-0.180441	0.000003
C	-1.660242	0.723572	-0.000001
C	-1.041194	1.989556	0.000000
C	-0.904087	-0.440007	-0.000002
C	0.328043	2.059630	0.000001
C	-3.076852	0.358482	-0.000009
C	-3.195748	-0.978256	0.000018
C	-1.833967	-1.622993	-0.000007
H	0.853054	-2.530535	-0.000007
H	3.015474	1.932750	0.000003
H	3.299718	-2.341775	0.000000
H	4.386415	-0.111083	0.000005
H	-1.639279	2.892212	-0.000002
H	0.824392	3.022483	0.000001
H	-3.890012	1.070818	-0.000014
H	-4.118899	-1.538528	0.000031
H	-1.689252	-2.264256	-0.876466
H	-1.689238	-2.264265	0.876443

235-92-7-C17H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -655.351079789 (a.u.)
E(HF/CC-PVTZ) = -650.96647279
E(DLPNO-CCSD(T)/CC-PVTZ) = -653.804675142692
T1 (CC-PVTZ)= 0.010157063
T2 (CC-PVTZ)= 0.037978
E(HF/CC-PVQZ) = -651.00525875
E(DLPNO-CCSD(T)/CC-PVQZ) = -653.988110274998
E(HF/TZ-AUG) = -650.97123207
E(DLPNO-CCSD(T)/TZ-AUG) = -653.847919149
E(HF/TZ-CORE) = -650.97123745
E(DLPNO-CCSD(T)/TZ-CORE) = -654.668084317
E(HF/TZ-IT) = -650.96647279
E(DLPNO-CCSD(T)/TZ-IT) = -653.813204275

T1 (CC-PVQZ)= 0.010208546
T2 (CC-PVQZ)= 0.039168
E(HF/CBS) = -651.014709834
E(DLPNO-CCSD(T)/CBS) = -654.10311616
Enthalpic correction = 0.23922769 (a.u.)
Entropy = 107.70305 (cal/(mol*K))

C	1.255851	2.781500	0.000001
C	-1.077840	2.823697	-0.000006
C	0.004691	3.617318	0.000005
C	-0.653295	1.421697	-0.000002
C	0.717860	1.377141	0.000001
C	0.688248	-1.068499	0.000000
C	1.430770	0.147684	0.000001
C	2.840408	0.101593	0.000002
C	3.511356	-1.097524	0.000000
C	2.787377	-2.297793	-0.000003
C	1.410654	-2.277500	-0.000003
C	-1.439571	0.227238	-0.000002
C	-0.765738	-1.026584	0.000001
C	-1.554661	-2.193830	0.000004
C	-2.930160	-2.136458	0.000004
C	-3.585762	-0.898560	0.000000
C	-2.847362	0.261221	-0.000003
H	1.880513	2.986064	0.876548
H	1.880518	2.986068	-0.876541
H	-2.103802	3.160664	-0.000010
H	0.007089	4.696996	0.000009
H	3.394449	1.031354	0.000003
H	4.593523	-1.116668	0.000001
H	3.310856	-3.244988	-0.000006
H	0.882314	-3.219442	-0.000007
H	-1.079851	-3.163799	0.000008
H	-3.505736	-3.053044	0.000007
H	-4.667189	-0.856429	-0.000001
H	-3.349645	1.219174	-0.000005

238-84-6_C17H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -655.365724336
(a.u.)
E(HF/CC-PVTZ) = -650.98387387
E(DLPNO-CCSD(T)/CC-PVTZ) = -653.817823118899
T1 (CC-PVTZ)= 0.010035757
T2 (CC-PVTZ)= 0.034982
E(HF/CC-PVQZ) = -651.0225961
E(DLPNO-CCSD(T)/CC-PVQZ) = -654.001132103619
E(HF/TZ-AUG) = -650.98851544
E(DLPNO-CCSD(T)/TZ-AUG) = -653.860677167
E(HF/TZ-CORE) = -650.98864941
E(DLPNO-CCSD(T)/TZ-CORE) = -654.681309798
E(HF/TZ-IT) = -650.98387387
E(DLPNO-CCSD(T)/TZ-IT) = -653.826252136
T1 (CC-PVQZ)= 0.010069473
T2 (CC-PVQZ)= 0.037857
E(HF/CBS) = -651.032031655
E(DLPNO-CCSD(T)/CBS) = -654.116076912
Enthalpic correction = 0.23969337 (a.u.)
Entropy = 107.17491 (cal/(mol*K))

C	-0.236599	-0.401623	0.000001
C	0.484311	0.782340	0.000003
C	-1.646468	-0.397591	0.000001
C	0.702027	-1.583106	-0.000011
C	1.914321	0.470010	0.000001
C	-0.172198	2.030086	0.000001
C	-2.310285	0.870602	0.000001
C	-2.428896	-1.577417	0.000002
C	2.062645	-0.928025	0.000003
C	3.031243	1.297423	-0.000004
C	-1.541380	2.063128	0.000000
C	-3.723884	0.897557	0.000001
C	-3.798188	-1.512311	0.000002
C	3.321370	-1.500350	0.000007
C	4.295521	0.716365	-0.000002
C	-4.453375	-0.263378	0.000001
C	4.441386	-0.668853	0.000005
H	0.557915	-2.221166	0.877590
H	0.557931	-2.221089	-0.877676
H	0.398941	2.949649	0.000000
H	-1.931778	-2.538925	0.000003
H	2.924887	2.374902	-0.000006
H	-2.064073	3.011868	-0.000004
H	-4.224954	1.858111	0.000001
H	-4.383399	-2.422933	0.000003
H	3.441894	-2.577021	0.000015
H	5.175649	1.346482	-0.000006
H	-5.534973	-0.225705	-0.000001
H	5.432658	-1.103312	0.000009

243-17-4_C17H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -655.365638966
(a.u.)
E(HF/CC-PVTZ) = -650.98459056
E(DLPNO-CCSD(T)/CC-PVTZ) = -653.817098183536
T1 (CC-PVTZ)= 0.010053258
T2 (CC-PVTZ)= 0.034679
E(HF/CC-PVQZ) = -651.02324676
E(DLPNO-CCSD(T)/CC-PVQZ) = -654.000506524286
E(HF/TZ-AUG) = -650.98907017
E(DLPNO-CCSD(T)/TZ-AUG) = -653.859809431
E(HF/TZ-CORE) = -650.98937689
E(DLPNO-CCSD(T)/TZ-CORE) = -654.680748234
E(HF/TZ-IT) = -650.98459056
E(DLPNO-CCSD(T)/TZ-IT) = -653.825531876
T1 (CC-PVQZ)= 0.010085195
T2 (CC-PVQZ)= 0.037808
E(HF/CBS) = -651.032666225
E(DLPNO-CCSD(T)/CBS) = -654.11555593
Enthalpic correction = 0.23965261 (a.u.)
Entropy = 107.27055 (cal/(mol*K))

C	0.405706	-0.246893	0.000006
C	1.856924	-0.435006	0.000004
C	0.137672	1.154319	0.000004
C	-0.619882	-1.156311	0.000006
C	2.478563	0.824759	0.000000
C	2.620958	-1.597563	0.000002
C	1.439823	1.922117	0.000012
C	-1.145065	1.617062	-0.000001
C	-1.960793	-0.704440	0.000003
C	3.859391	0.924981	-0.000007
C	4.006594	-1.491189	-0.000005
C	-2.229266	0.701386	-0.000002
C	-3.053796	-1.604333	0.000003
C	4.622530	-0.240683	-0.000010
C	-3.574444	1.137009	-0.000007
C	-4.345744	-1.147678	-0.000002
C	-4.609461	0.237885	-0.000007
H	-0.424371	-2.222049	0.000007
H	2.147342	-2.571184	0.000005
H	1.531238	2.568485	-0.877897
H	1.531235	2.568446	0.877952

H	-1.358145	2.680124	-0.000006
H	4.344381	1.893713	-0.000012
H	4.614407	-2.386810	-0.000006
H	-2.849292	-2.668250	0.000006
H	5.702905	-0.175628	-0.000017
H	-3.775009	2.201741	-0.000012
H	-5.169552	-1.849735	-0.000002
H	-5.633395	0.588617	-0.000011

256-61-1-C15H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -579.037500380 (a.u.)
E(HF/CC-PVTZ) = -575.11950155
E(DLPNO-CCSD(T)/CC-PVTZ) = -577.665746091927
T1 (CC-PVTZ)= 0.010848964
T2 (CC-PVTZ)= 0.037877
E(HF/CC-PVQZ) = -575.15408649
E(DLPNO-CCSD(T)/CC-PVQZ) = -577.827829732908
E(HF/TZ-AUG) = -575.12383964
E(DLPNO-CCSD(T)/TZ-AUG) = -577.704400325
E(HF/TZ-CORE) = -575.1237266
E(DLPNO-CCSD(T)/TZ-CORE) = -578.427278574
E(HF/TZ-IT) = -575.11950154
E(DLPNO-CCSD(T)/TZ-IT) = -577.673585854
T1 (CC-PVQZ)= 0.010867700
T2 (CC-PVQZ)= 0.037792
E(HF/CBS) = -575.1625139
E(DLPNO-CCSD(T)/CBS) = -577.929296735
Enthalpic correction = 0.22625227 (a.u.)
Entropy = 100.68876 (cal/(mol*K))

C	-1.128544	-1.149260	0.331072
C	0.106065	-1.538580	-0.100682
C	1.285823	-0.724028	0.006887
C	1.285823	0.724029	0.006887
C	0.106065	1.538580	-0.100683
C	-1.128544	1.149261	0.331071
C	-2.392597	1.582197	-0.188768
C	-3.436265	0.723211	-0.381398
C	-3.436265	-0.723212	-0.381398
C	-2.392596	-1.582198	-0.188768
C	-1.181731	0.000000	1.276667
C	2.538545	1.380270	-0.098228
C	3.728384	0.702567	-0.145920
C	3.728384	-0.702567	-0.145920
C	2.538545	-1.380270	-0.098228
H	0.204216	-2.456520	-0.671799
H	0.204217	2.456519	-0.671801
H	-2.500770	2.609143	-0.520897
H	-4.354246	1.162136	-0.755786
H	-4.354245	-1.162137	-0.755788
H	-2.500767	-2.609143	-0.520898
H	-0.323199	0.000001	1.944582
H	-2.101334	0.000001	1.856279
H	2.537204	2.463112	-0.124564
H	4.662590	1.246777	-0.195161
H	4.662591	-1.246777	-0.195160
H	2.537204	-2.463112	-0.124564

257-55-6-C14H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -540.841334596 (a.u.)
E(HF/CC-PVTZ) = -537.1831908
E(DLPNO-CCSD(T)/CC-PVTZ) = -539.561405009828
T1 (CC-PVTZ)= 0.011322926
T2 (CC-PVTZ)= 0.055628
E(HF/CC-PVQZ) = -537.2159181
E(DLPNO-CCSD(T)/CC-PVQZ) = -539.713056200122
E(HF/TZ-AUG) = -537.18740516
E(DLPNO-CCSD(T)/TZ-AUG) = -539.597827812
E(HF/TZ-CORE) = -537.18740241
E(DLPNO-CCSD(T)/TZ-CORE) = -540.272301383
E(HF/TZ-IT) = -537.1831908
E(DLPNO-CCSD(T)/TZ-IT) = -539.567732158
T1 (CC-PVQZ)= 0.011356711
T2 (CC-PVQZ)= 0.055437
E(HF/CBS) = -537.223892853
E(DLPNO-CCSD(T)/CBS) = -539.807813252
Enthalpic correction = 0.21830539 (a.u.)
Entropy = 104.69570 (cal/(mol*K))

C	0.059087	-0.494430	0.414199
C	-0.199787	0.948919	0.174330
C	-1.371955	1.538925	0.481072
C	0.883074	1.761889	-0.350006
C	-0.543991	-1.484814	-0.240948
C	1.083811	-0.775916	1.447897
C	-2.806165	-0.769298	-0.991370
C	-3.237725	-0.102839	0.238216
C	-1.624593	-1.350433	-1.221101
C	-2.612531	0.890621	0.885683
C	2.087984	1.430013	-0.862828
C	2.847087	0.196203	-0.968074
C	3.020914	-0.810262	-0.090896
C	2.381647	-0.964135	1.202197
H	-1.413654	2.624853	0.429950
H	0.618017	2.810360	-0.447689
H	-0.207231	-2.500397	-0.046841
H	0.720656	-0.864133	2.467878
H	-3.566629	-0.847388	-1.764197
H	-4.221831	-0.390819	0.598478
H	-1.485751	-1.869016	-2.165797
H	-3.137895	1.349293	1.719495
H	2.605093	2.259100	-1.339216
H	3.483095	0.164606	-1.848300
H	3.782476	-1.544517	-0.335364
H	3.022512	-1.278600	2.021379

259-06-3-C17H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -655.344342735 (a.u.)
E(HF/CC-PVTZ) = -650.9603472
E(DLPNO-CCSD(T)/CC-PVTZ) = -653.795814443945
T1 (CC-PVTZ)= 0.010505409
T2 (CC-PVTZ)= 0.036136
E(HF/CC-PVQZ) = -650.99903074
E(DLPNO-CCSD(T)/CC-PVQZ) = -653.979202252601
E(HF/TZ-AUG) = -650.96480301
E(DLPNO-CCSD(T)/TZ-AUG) = -653.838618583
E(HF/TZ-CORE) = -650.96514422
E(DLPNO-CCSD(T)/TZ-CORE) = -654.659439005
E(HF/TZ-IT) = -650.9603472
E(DLPNO-CCSD(T)/TZ-IT) = -653.804494988
T1 (CC-PVQZ)= 0.010533415
T2 (CC-PVQZ)= 0.037650
E(HF/CBS) = -651.008456867

```
E(DLPNO-CCSD(T)/CBS) = -654.094223387
Enthalpic correction = 0.23908196 (a.u.)
Entropy = 107.26570 (cal/(mol*K))

 C     4.061656     1.181297     0.000002
 C     4.885031     0.122113    -0.000004
 C     4.112179    -1.173233     0.000002
 C     2.672700     0.736543     0.000000
 C     2.678230    -0.701054     0.000000
 C     1.517367    -1.401012     0.000000
 C     1.501168     1.435589     0.000000
 C     0.260221     0.734907     0.000000
 C     0.266218    -0.708789     0.000000
 C    -0.948097    -1.389691     0.000000
 C    -0.963773     1.402894     0.000000
 C    -2.179264     0.718860     0.000000
 C    -2.172044    -0.718929     0.000000
 C    -3.417690    -1.407382     0.000000
 C    -4.597892    -0.723435     0.000000
 C    -4.605411     0.696780     0.000000
 C    -3.433108     1.393724     0.000000
 H     4.365681     2.218678     0.000004
 H     5.964736     0.163566    -0.000007
 H     4.345231    -1.786908     0.876695
 H     4.345231    -1.786915    -0.876685
 H     1.510456    -2.485173     0.000000
 H     1.492795     2.519084     0.000000
 H    -0.943186    -2.473930     0.000000
 H    -0.970465     2.487037     0.000000
 H    -3.409683    -2.490711     0.000000
 H    -5.537709    -1.260337     0.000000
 H    -5.551022     1.223474     0.000000
 H    -3.437018     2.477043     0.000000
```

259-79-0-C12H8

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -462.236260041
(a.u.)
E(HF/CC-PVTZ) = -459.15625315
E(DLPNO-CCSD(T)/CC-PVTZ) = -461.146670980263
T1 (CC-PVTZ)= 0.010443130
T2 (CC-PVTZ)= 0.049833
E(HF/CC-PVQZ) = -459.18347362
E(DLPNO-CCSD(T)/CC-PVQZ) = -461.275350902114
E(HF/TZ-AUG) = -459.1594531
E(DLPNO-CCSD(T)/TZ-AUG) = -461.175522662
E(HF/TZ-CORE) = -459.15975644
E(DLPNO-CCSD(T)/TZ-CORE) = -461.75604535
E(HF/TZ-IT) = -459.15625315
E(DLPNO-CCSD(T)/TZ-IT) = -461.152904224
T1 (CC-PVQZ)= 0.010439590
T2 (CC-PVQZ)= 0.049637
E(HF/CBS) = -459.190106509
E(DLPNO-CCSD(T)/CBS) = -461.356021769
Enthalpic correction = 0.16198502 (a.u.)
Entropy = 90.07561 (cal/(mol*K))

 C    -0.754522     0.710919    -0.000002
 C     0.754522     0.710919     0.000002
 C    -0.754522    -0.710919    -0.000001
 C    -1.910731     1.439855    -0.000001
 C     0.754522    -0.710919     0.000002
 C     1.910731     1.439855     0.000001
 C    -1.910731    -1.439855     0.000001
 C    -3.112717     0.691853    -0.000001
 C     1.910731    -1.439855    -0.000001
 C     3.112717     0.691853     0.000000
 C    -3.112717    -0.691853     0.000001
 C     3.112717    -0.691853    -0.000001
 H    -1.931518     2.521598    -0.000002
 H     1.931518     2.521598     0.000002
 H    -1.931517    -2.521598     0.000003
 H    -4.058827     1.217638    -0.000001
 H     1.931518    -2.521598    -0.000003
 H     4.058827     1.217638     0.000000
 H    -4.058827    -1.217639     0.000002
 H     4.058827    -1.217638    -0.000003
```

26460-76-4-C15H22

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Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -584.998855865
(a.u.)
E(HF/CC-PVTZ) = -580.85625389
E(DLPNO-CCSD(T)/CC-PVTZ) = -583.643729245220
T1 (CC-PVTZ)= 0.009025956
T2 (CC-PVTZ)= 0.033069
E(HF/CC-PVQZ) = -580.89084425
E(DLPNO-CCSD(T)/CC-PVQZ) = -583.811185214520
E(HF/TZ-AUG) = -580.85894806
E(DLPNO-CCSD(T)/TZ-AUG) = -583.688236548
E(HF/TZ-CORE) = -580.86030646
E(DLPNO-CCSD(T)/TZ-CORE) = -584.400645787
E(HF/TZ-IT) = -580.85625389
E(DLPNO-CCSD(T)/TZ-IT) = -583.64819702
T1 (CC-PVQZ)= 0.009148729
T2 (CC-PVQZ)= 0.036100
E(HF/CBS) = -580.89927298
E(DLPNO-CCSD(T)/CBS) = -583.91656993
Enthalpic correction = 0.34326484 (a.u.)
Entropy = 98.73246 (cal/(mol*K))

 C    -1.939813    -0.817738     1.364121
 C    -0.406910    -0.756606     1.120970
 C     0.335942     0.610834     1.282265
 C     0.216284    -1.754074     0.088755
 C    -2.415585    -0.134226     0.037041
 C    -1.864401    -0.964013    -1.177265
 C    -1.766236     1.291006    -0.029184
 C    -0.187021     1.320562    -0.040613
 C     0.318567     0.405359    -1.244012
 C     0.264541     2.767263    -0.201601
 C     1.852448     0.446705     1.286836
 C    -0.300982    -1.052028    -1.224478
 C     1.737064    -1.799344     0.152759
 C     1.846941     0.288953    -1.225876
 C     2.314637    -0.379429     0.075563
 H    -2.258527    -0.258649     2.246837
 H    -2.317421    -1.838220     1.458854
 H    -0.711792    -0.295944     0.258093
 H     0.005426     1.160822     2.167561
 H    -0.204776    -2.757729     0.185049
 H    -3.503496    -0.041652    -0.052230
 H    -2.285018    -1.973654    -1.154757
 H    -2.210696    -0.491419    -2.099918
 H    -2.110557     1.784055    -0.942262
 H    -2.120240     1.894629     0.812415
 H    -0.008222     0.887893    -2.169733
 H    -0.136861     3.377243     0.611573
 H     1.348600     2.869542    -0.183267
 H    -0.093859     3.191219    -1.142832
 H     2.157478    -0.052225     2.210777
 H     2.341893     1.424490     1.276037
 H     0.002861    -1.567885    -2.143704
 H     2.052447    -2.281452     1.082288
```

H	2.127874	-2.400053	-0.675064
H	2.175280	-0.305982	-2.083592
H	2.310587	1.271658	-1.333149
H	3.406166	-0.436037	0.079333

268-40-6-C13H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -501.636361958 (a.u.)
E(HF/CC-PVTZ) = -498.27132351
E(DLPNO-CCSD(T)/CC-PVTZ) = -500.451090869372
T1 (CC-PVTZ)= 0.010337145
T2 (CC-PVTZ)= 0.035022
E(HF/CC-PVQZ) = -498.3011453
E(DLPNO-CCSD(T)/CC-PVQZ) = -500.591964119733
E(HF/TZ-AUG) = -498.27483815
E(DLPNO-CCSD(T)/TZ-AUG) = -500.483684563
E(HF/TZ-CORE) = -498.27499698
E(DLPNO-CCSD(T)/TZ-CORE) = -501.111415282
E(HF/TZ-IT) = -498.27132351
E(DLPNO-CCSD(T)/TZ-IT) = -500.45741238
T1 (CC-PVQZ)= 0.010381434
T2 (CC-PVQZ)= 0.037728
E(HF/CBS) = -498.30841206
E(DLPNO-CCSD(T)/CBS) = -500.680268431
Enthalpic correction = 0.19121816 (a.u.)
Entropy = 93.70569 (cal/(mol*K))

C	-0.964966	0.721789	0.000001
C	-0.954649	-0.709388	0.000000
C	-2.212454	1.390461	0.000002
C	-2.188809	-1.398497	-0.000002
C	-3.391227	0.690839	0.000002
C	-3.380062	-0.718957	0.000000
C	1.444068	0.733139	0.000000
C	1.453470	-0.694662	-0.000001
C	0.262861	1.428282	0.000002
C	0.287542	-1.399033	-0.000002
C	2.831782	1.186576	-0.000013
C	3.659292	0.130688	0.000014
C	2.887263	-1.164608	-0.000003
H	-2.219565	2.473880	0.000003
H	-2.177812	-2.481971	-0.000004
H	-4.335850	1.219359	0.000004
H	-4.315756	-1.262974	0.000000
H	0.249706	2.511854	-0.000001
H	0.283788	-2.483301	-0.000004
H	3.130702	2.225454	-0.000020
H	4.738810	0.174198	0.000021
H	3.120662	-1.778137	-0.876725
H	3.120652	-1.778129	0.876728

2717-39-7-C14H16

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -543.392167816 (a.u.)
E(HF/CC-PVTZ) = -539.63930985
E(DLPNO-CCSD(T)/CC-PVTZ) = -542.102727896857
T1 (CC-PVTZ)= 0.009557100
T2 (CC-PVTZ)= 0.033046
E(HF/CC-PVQZ) = -539.67195559
E(DLPNO-CCSD(T)/CC-PVQZ) = -542.257695290078
E(HF/TZ-AUG) = -539.64282656
E(DLPNO-CCSD(T)/TZ-AUG) = -542.140352799
E(HF/TZ-CORE) = -539.6432165
E(DLPNO-CCSD(T)/TZ-CORE) = -542.812907125
E(HF/TZ-IT) = -539.63930985
E(DLPNO-CCSD(T)/TZ-IT) = -542.108907534
T1 (CC-PVQZ)= 0.009665729
T2 (CC-PVQZ)= 0.036511
E(HF/CBS) = -539.679910469
E(DLPNO-CCSD(T)/CBS) = -542.354911916
Enthalpic correction = 0.26502404 (a.u.)
Entropy = 111.41794 (cal/(mol*K))

C	-1.418153	1.254092	0.125847
C	-0.692254	2.417433	0.088608
C	-0.726730	0.000000	0.000002
C	-2.898667	1.404122	0.387429
C	0.692262	2.417433	-0.088571
C	1.418155	1.254089	-0.125844
C	0.726728	0.000000	-0.000001
C	2.898659	1.404108	-0.387483
C	1.418155	-1.254089	0.125843
C	-1.418153	-1.254092	-0.125845
C	-0.692254	-2.417433	-0.088606
C	-2.898666	-1.404123	-0.387432
C	0.692263	-2.417433	0.088575
C	2.898660	-1.404107	0.387480
H	-1.207924	3.364322	0.190741
H	-3.224235	0.802631	1.235784
H	-3.520891	1.135334	-0.464643
H	-3.110064	2.445494	0.627269
H	1.207933	3.364323	-0.190697
H	3.224198	0.802572	-1.235817
H	3.520915	1.135366	0.464582
H	3.110047	2.445468	-0.627385
H	-1.207923	-3.364323	-0.190738
H	-3.520893	-1.135345	0.464641
H	-3.110061	-2.445492	-0.627283
H	-3.224233	-0.802622	-1.235782
H	1.207934	-3.364323	0.190702
H	3.520914	-1.135370	-0.464587
H	3.110048	-2.445465	0.627388
H	3.224201	-0.802565	1.235810

27208-37-3-C18H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -692.278611349 (a.u.)
E(HF/CC-PVTZ) = -687.69033169
E(DLPNO-CCSD(T)/CC-PVTZ) = -690.647092933931
T1 (CC-PVTZ)= 0.010492387
T2 (CC-PVTZ)= 0.038000
E(HF/CC-PVQZ) = -687.73075923
E(DLPNO-CCSD(T)/CC-PVQZ) = -690.839181198363
E(HF/TZ-AUG) = -687.69515372
E(DLPNO-CCSD(T)/TZ-AUG) = -690.691983251
E(HF/TZ-CORE) = -687.69538322
E(DLPNO-CCSD(T)/TZ-CORE) = -691.561528829
E(HF/TZ-IT) = -687.69033169
E(DLPNO-CCSD(T)/TZ-IT) = -690.657117782
T1 (CC-PVQZ)= 0.010516020
T2 (CC-PVQZ)= 0.038215
E(HF/CBS) = -687.740610322
E(DLPNO-CCSD(T)/CBS) = -690.95970363
Enthalpic correction = 0.22405089 (a.u.)
Entropy = 103.12897 (cal/(mol*K))

C	1.333995	-0.321577	-0.000031
C	0.245377	0.522421	-0.000023
C	-1.043039	-0.056938	-0.000015
C	0.470445	1.923450	-0.000006
C	1.248943	-1.747188	-0.000015
C	2.661289	0.105953	-0.000009
C	-1.169665	-1.478725	-0.000006
C	-2.171248	0.794567	-0.000003
C	-0.695764	2.757215	0.000002
C	1.805887	2.367789	0.000009
C	0.008326	-2.317324	-0.000001
C	2.642849	-2.209298	0.000011
C	3.468425	-1.124139	0.000014
C	2.892259	1.482675	0.000013
C	-2.465151	-2.009443	0.000006
C	-1.946105	2.216675	0.000001
C	-3.441610	0.208256	0.000009
C	-3.578284	-1.175429	0.000012
H	-0.572618	3.833561	0.000010
H	1.999430	3.433642	0.000024
H	-0.130330	-3.392530	0.000017
H	2.957259	-3.241878	0.000023
H	4.547958	-1.158947	0.000032
H	3.898584	1.883456	0.000032
H	-2.598401	-3.084470	0.000013
H	-2.812776	2.866609	0.000007
H	-4.322152	0.839156	0.000016
H	-4.568519	-1.612241	0.000022

275-51-4-C10H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -386.014824791 (a.u.)
E(HF/CC-PVTZ) = -383.4061874
E(DLPNO-CCSD(T)/CC-PVTZ) = -385.094718234015
T1 (CC-PVTZ)= 0.011615531
T2 (CC-PVTZ)= 0.061790
E(HF/CC-PVQZ) = -383.42951308
E(DLPNO-CCSD(T)/CC-PVQZ) = -385.203464262002
E(HF/TZ-AUG) = -383.40943888
E(DLPNO-CCSD(T)/TZ-AUG) = -385.120090232
E(HF/TZ-CORE) = -383.40903528
E(DLPNO-CCSD(T)/TZ-CORE) = -385.602475273
E(HF/TZ-IT) = -383.4061874
E(DLPNO-CCSD(T)/TZ-IT) = -385.099841083
T1 (CC-PVQZ)= 0.011622724
T2 (CC-PVQZ)= 0.061137
E(HF/CBS) = -383.435196914
E(DLPNO-CCSD(T)/CBS) = -385.271481864
Enthalpic correction = 0.14932479 (a.u.)
Entropy = 84.17360 (cal/(mol*K))

C	0.550231	-0.747461	0.000000
C	0.550231	0.747458	0.000000
C	1.894040	1.146060	-0.000009
C	-0.550008	1.588488	0.000004
C	1.894026	-1.146067	0.000012
C	-0.550023	-1.588491	-0.000004
C	2.698683	0.000000	-0.000002
C	-1.902519	1.260615	0.000006
C	-1.902521	-1.260612	-0.000006
C	-2.491632	0.000008	0.000000
H	2.237968	2.169030	-0.000017
H	-0.321518	2.650286	0.000002
H	2.237957	-2.169035	0.000021
H	-0.321530	-2.650287	-0.000002
H	3.779249	-0.000007	-0.000003
H	-2.589306	2.098879	0.000011
H	-2.589319	-2.098867	-0.000011
H	-3.576548	0.000007	-0.000001

2781-85-30_C3H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -116.673239591 (a.u.)
E(HF/CC-PVTZ) = -115.86553347
E(DLPNO-CCSD(T)/CC-PVTZ) = -116.396883402293
T1 (CC-PVTZ)= 0.009503005
T2 (CC-PVTZ)= 0.054516
E(HF/CC-PVQZ) = -115.87301155
E(DLPNO-CCSD(T)/CC-PVQZ) = -116.430451231789
E(HF/TZ-AUG) = -115.86640772
E(DLPNO-CCSD(T)/TZ-AUG) = -116.404121695
E(HF/TZ-CORE) = -115.86657998
E(DLPNO-CCSD(T)/TZ-CORE) = -116.549162938
E(HF/TZ-IT) = -115.86553347
E(DLPNO-CCSD(T)/TZ-IT) = -116.397900039
T1 (CC-PVQZ)= 0.009750321
T2 (CC-PVQZ)= 0.053775
E(HF/CBS) = -115.874833755
E(DLPNO-CCSD(T)/CBS) = -116.451311902
Enthalpic correction = 0.05839771 (a.u.)
Entropy = 58.14923 (cal/(mol*K))

C	0.000000	0.000000	0.860907
C	0.000000	0.643385	-0.499648
C	0.000000	-0.643385	-0.499648
H	-0.911469	0.000000	1.456709
H	0.911469	0.000000	1.456709
H	0.000000	1.571751	-1.041542
H	0.000000	-1.571751	-1.041542

28375-86-2-C15H22

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -585.171326595 (a.u.)
E(HF/CC-PVTZ) = -581.05490273
E(DLPNO-CCSD(T)/CC-PVTZ) = -583.812352475545
T1 (CC-PVTZ)= 0.008828323
T2 (CC-PVTZ)= 0.028026
E(HF/CC-PVQZ) = -581.08942147
E(DLPNO-CCSD(T)/CC-PVQZ) = -583.980550987295
E(HF/TZ-AUG) = -581.05741507
E(DLPNO-CCSD(T)/TZ-AUG) = -583.856330422
E(HF/TZ-CORE) = -581.05886721
E(DLPNO-CCSD(T)/TZ-CORE) = -584.570359098
E(HF/TZ-IT) = -581.05490273
E(DLPNO-CCSD(T)/TZ-IT) = -583.81641979
T1 (CC-PVQZ)= 0.008963179
T2 (CC-PVQZ)= 0.032176
E(HF/CBS) = -581.097832749
E(DLPNO-CCSD(T)/CBS) = -584.08651237
Enthalpic correction = 0.34438846 (a.u.)
Entropy = 97.68371 (cal/(mol*K))

C	-1.433849	0.823930	-1.435244
C	0.018607	0.338638	-1.438318
C	0.112350	-1.076390	-0.833316
C	0.905469	1.286539	-0.606652

C	-1.967690	0.856639	0.003015
C	-1.101574	1.816691	0.828355
C	-1.902414	-0.545163	0.639936
C	-0.442121	-1.029775	0.605876
C	-2.884174	-1.540322	0.025395
C	0.446795	-0.081485	1.436406
C	1.565753	-1.561117	-0.829491
C	0.351368	1.333356	0.831274
C	2.357461	0.799553	-0.605730
C	1.899252	-0.566491	1.437425
C	2.432812	-0.607381	0.000577
H	-1.492526	1.826268	-1.870337
H	-2.048036	0.174320	-2.063265
H	0.393676	0.311643	-2.466911
H	-0.489178	-1.761952	-1.435895
H	0.855904	2.291182	-1.039912
H	-3.005111	1.204213	0.003488
H	-1.478438	1.873628	1.854093
H	-1.157185	2.826358	0.410003
H	-2.179611	-0.434541	1.695282
H	-0.389569	-2.035128	1.039190
H	-2.692066	-1.719819	-1.032446
H	-2.826326	-2.503875	0.536945
H	-3.909998	-1.175877	0.115366
H	0.070277	-0.055108	2.464355
H	1.619858	-2.573386	-0.417233
H	1.941588	-1.613052	-1.856045
H	0.964086	2.017582	1.427774
H	2.747955	0.789580	-1.628014
H	2.982175	1.490211	-0.030924
H	2.514950	0.100639	2.048555
H	1.959784	-1.561571	1.888838
H	3.469527	-0.954637	0.000034

287-23-00_C4H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -157.285814306 (a.u.)
E(HF/CC-PVTZ) = -156.15019975
E(DLPNO-CCSD(T)/CC-PVTZ) = -156.912671805778
T1 (CC-PVTZ)= 0.007796183
T2 (CC-PVTZ)= 0.031145
E(HF/CC-PVQZ) = -156.15991898
E(DLPNO-CCSD(T)/CC-PVQZ) = -156.958791140051
E(HF/TZ-AUG) = -156.15101707
E(DLPNO-CCSD(T)/TZ-AUG) = -156.923212212
E(HF/TZ-CORE) = -156.15129588
E(DLPNO-CCSD(T)/TZ-CORE) = -157.114612094
E(HF/TZ-IT) = -156.15019975
E(DLPNO-CCSD(T)/TZ-IT) = -156.913557496
T1 (CC-PVQZ)= 0.008158677
T2 (CC-PVQZ)= 0.028043
E(HF/CBS) = -156.162287292
E(DLPNO-CCSD(T)/CBS) = -156.98772169
Enthalpic correction = 0.11214796 (a.u.)
Entropy = 66.03686 (cal/(mol*K))

C	-0.816957	0.708421	0.124830
C	-0.708421	-0.816957	-0.124830
C	0.708421	0.816957	-0.124830
C	0.816957	-0.708421	0.124831
H	-1.479822	1.283228	-0.521747
H	-1.069392	0.927316	1.163483
H	-1.283228	-1.479822	0.521746
H	-0.927316	-1.069392	-1.163483
H	1.479822	-1.283228	-0.521746
H	1.069392	-0.927315	1.163483
H	1.283228	1.479822	0.521746
H	0.927316	1.069392	-1.163483

30545-28-9-C15H22

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -585.175762766 (a.u.)
E(HF/CC-PVTZ) = -581.06005863
E(DLPNO-CCSD(T)/CC-PVTZ) = -583.817357437835
T1 (CC-PVTZ)= 0.008838115
T2 (CC-PVTZ)= 0.031341
E(HF/CC-PVQZ) = -581.0945875
E(DLPNO-CCSD(T)/CC-PVQZ) = -583.985534885062
E(HF/TZ-AUG) = -581.06255783
E(DLPNO-CCSD(T)/TZ-AUG) = -583.861254736
E(HF/TZ-CORE) = -581.06402663
E(DLPNO-CCSD(T)/TZ-CORE) = -584.575459864
E(HF/TZ-IT) = -581.06005863
E(DLPNO-CCSD(T)/TZ-IT) = -583.821433646
T1 (CC-PVQZ)= 0.008979654
T2 (CC-PVQZ)= 0.032012
E(HF/CBS) = -581.103001247
E(DLPNO-CCSD(T)/CBS) = -584.091475972
Enthalpic correction = 0.34372565 (a.u.)
Entropy = 97.46386 (cal/(mol*K))

C	1.507961	1.348391	0.501700
C	-0.021814	1.351927	0.502964
C	-0.562040	1.113126	-0.920460
C	-0.562058	0.240706	1.424172
C	2.051571	0.000124	0.000142
C	1.507982	-1.108518	0.916845
C	1.507955	-0.239664	-1.418194
C	3.575650	-0.000154	-0.000276
C	-0.021828	-0.240327	-1.422079
C	-0.562029	-1.353786	-0.503561
C	-2.093636	1.112452	-0.919997
C	-0.021785	-1.111520	0.919267
C	-2.093716	0.240526	1.423168
C	-2.093608	-1.353084	-0.503381
C	-2.611813	-0.000109	-0.000171
H	1.883601	1.541425	1.511936
H	1.883650	2.154726	-0.136776
H	-0.383359	2.320805	0.863451
H	-0.195904	1.908382	-1.578375
H	-0.195998	0.412768	2.441882
H	1.883629	-2.079845	0.578696
H	1.883649	-0.958893	1.934410
H	1.883530	-1.195834	-1.797210
H	1.883558	0.538653	-2.090562
H	3.967114	-0.956480	-0.356180
H	3.967952	0.169777	1.005532
H	3.967446	0.785878	-0.650742
H	-0.383417	-0.412650	-2.441358
H	-0.195911	-2.321138	-0.863482
H	-2.466920	0.962685	-1.937727
H	-2.467013	2.083849	-0.581584
H	-0.383340	-1.908023	1.578234
H	-2.467001	1.196906	1.802072
H	-2.467000	-0.538033	2.095510
H	-2.467031	-2.159374	0.135393
H	-2.466890	-1.546051	-1.513809
H	-3.705101	-0.000069	-0.000139

316-51-8-C20H16

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -772.170758502 (a.u.)
E(HF/CC-PVTZ) = -766.96799766
E(DLPNO-CCSD(T)/CC-PVTZ) = -770.341699274814
T1 (CC-PVTZ)= 0.009985666
T2 (CC-PVTZ)= 0.036610
E(HF/CC-PVQZ) = -767.01360679
E(DLPNO-CCSD(T)/CC-PVQZ) = -770.558553990521
E(HF/TZ-AUG) = -766.97305239
E(DLPNO-CCSD(T)/TZ-AUG) = -770.392769297
E(HF/TZ-CORE) = -766.9736035
E(DLPNO-CCSD(T)/TZ-CORE) = -771.357547485
E(HF/TZ-IT) = -766.96799766
E(DLPNO-CCSD(T)/TZ-IT) = -770.35166648
T1 (CC-PVQZ)= 0.010037827
T2 (CC-PVQZ)= 0.037810
E(HF/CBS) = -767.024720495
E(DLPNO-CCSD(T)/CBS) = -770.694630691
Enthalpic correction = 0.30297206 (a.u.)
Entropy = 128.75814 (cal/(mol*K))

C	2.435214	0.574898	0.000001
C	1.959261	-0.774050	0.000000
C	3.836501	0.810782	0.000000
C	1.495556	1.609986	0.000001
C	2.916363	-1.824315	0.000000
C	0.580486	-1.016898	0.000001
C	4.253250	-1.554882	0.000000
C	4.740345	-0.216277	0.000000
C	6.222306	0.029585	-0.000002
C	0.129081	1.362382	0.000001
C	-0.353326	0.009705	0.000001
C	-0.813223	2.443951	0.000000
C	-1.791328	-0.223348	0.000001
C	-2.143896	2.216821	0.000000
C	-2.674360	0.882961	0.000000
C	-4.064011	0.667240	-0.000001
C	-2.360257	-1.508848	0.000001
C	-4.608590	-0.600287	0.000000
C	-3.724706	-1.692953	0.000000
C	-6.095060	-0.822929	-0.000002
H	4.184734	1.837535	0.000000
H	1.842539	2.637080	0.000000
H	2.564256	-2.848967	0.000000
H	0.255789	-2.048340	0.000000
H	4.967449	-2.369918	0.000000
H	6.448460	1.095525	0.000003
H	6.694504	-0.417324	-0.878819
H	6.694507	-0.417332	0.878810
H	-0.427234	3.456052	0.000000
H	-2.842847	3.044400	-0.000001
H	-4.718259	1.531881	-0.000001
H	-1.722200	-2.380951	0.000002
H	-4.125875	-2.699681	0.000001
H	-6.407958	-1.391677	0.879106
H	-6.407958	-1.391668	-0.879116
H	-6.637538	0.122236	0.000003

3355-34-80_C6H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -230.953075184 (a.u.)
E(HF/CC-PVTZ) = -229.34776805
E(DLPNO-CCSD(T)/CC-PVTZ) = -230.421552593484
T1 (CC-PVTZ)= 0.016193644
T2 (CC-PVTZ)= 0.227860
E(HF/CC-PVQZ) = -229.36224532
E(DLPNO-CCSD(T)/CC-PVQZ) = -230.485280290675
E(HF/TZ-AUG) = -229.35046721
E(DLPNO-CCSD(T)/TZ-AUG) = -230.435794577
E(HF/TZ-CORE) = -229.34949312
E(DLPNO-CCSD(T)/TZ-CORE) = -230.725432452
E(HF/TZ-IT) = -229.34776805
E(DLPNO-CCSD(T)/TZ-IT) = -230.427573413
T1 (CC-PVQZ)= 0.016341025
T2 (CC-PVQZ)= 0.220237
E(HF/CBS) = -229.365773037
E(DLPNO-CCSD(T)/CBS) = -230.524747509
Enthalpic correction = 0.07487225 (a.u.)
Entropy = 67.85122 (cal/(mol*K))

C	0.000000	1.189686	-0.738692
C	0.000000	1.189686	0.738692
C	0.000000	0.000000	-1.350647
C	0.000000	0.000000	1.350647
C	0.000000	-1.189686	-0.738692
C	0.000000	-1.189686	0.738692
H	0.000000	2.170076	-1.192175
H	0.000000	2.170076	1.192175
H	0.000000	-2.170076	-1.192175
H	0.000000	-2.170076	1.192175

3355-34-82_C6H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -230.953075184 (a.u.)
E(HF/CC-PVTZ) = -229.34776805
E(DLPNO-CCSD(T)/CC-PVTZ) = -230.421552593484
T1 (CC-PVTZ)= 0.016193644
T2 (CC-PVTZ)= 0.227860
E(HF/CC-PVQZ) = -229.36224532
E(DLPNO-CCSD(T)/CC-PVQZ) = -230.485280290675
E(HF/TZ-AUG) = -229.35046721
E(DLPNO-CCSD(T)/TZ-AUG) = -230.435794577
E(HF/TZ-CORE) = -229.34949312
E(DLPNO-CCSD(T)/TZ-CORE) = -230.725432452
E(HF/TZ-IT) = -229.34776805
E(DLPNO-CCSD(T)/TZ-IT) = -230.427572862
T1 (CC-PVQZ)= 0.016341025
T2 (CC-PVQZ)= 0.220237
E(HF/CBS) = -229.365773037
E(DLPNO-CCSD(T)/CBS) = -230.524747509
Enthalpic correction = 0.07487225 (a.u.)
Entropy = 67.85122 (cal/(mol*K))

C	0.000000	1.189686	-0.738692
C	0.000000	1.189686	0.738692
C	0.000000	0.000000	-1.350647
C	0.000000	0.000000	1.350647
C	0.000000	-1.189686	-0.738692
C	0.000000	-1.189686	0.738692
H	0.000000	2.170076	-1.192175
H	0.000000	2.170076	1.192175
H	0.000000	-2.170076	-1.192175
H	0.000000	-2.170076	1.192175

35117-21-6-C26H26

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1006.86783657 (a.u.)
E(HF/CC-PVTZ) = -999.9366748
E(DLPNO-CCSD(T)/CC-PVTZ) = -1004.491707741606
T1 (CC-PVTZ)= 0.009422557
T2 (CC-PVTZ)= 0.036174
E(HF/CC-PVQZ) = -999.99603296
E(DLPNO-CCSD(T)/CC-PVQZ) = -1004.775466382621
E(HF/TZ-AUG) = -999.94297483
E(DLPNO-CCSD(T)/TZ-AUG) = -1004.56524257
E(HF/TZ-CORE) = -999.94378494
E(DLPNO-CCSD(T)/TZ-CORE) = -1005.8099383
E(HF/TZ-IT) = -999.9366748
E(DLPNO-CCSD(T)/TZ-IT) = -1004.50370129
T1 (CC-PVQZ)= 0.009517655
T2 (CC-PVQZ)= 0.037724
E(HF/CBS) = -1000.01049693
E(DLPNO-CCSD(T)/CBS) = -1004.95368205
Enthalpic correction = 0.45466576 (a.u.)
Entropy = 143.68390 (cal/(mol*K))

C	3.241502	0.881217	0.145223
C	3.357724	-0.245969	0.957560
C	3.081333	0.662965	-1.223581
C	2.967136	2.242013	0.733961
C	3.021337	-1.500980	0.470682
C	2.581627	-1.668191	-0.842884
C	2.767300	-0.596291	-1.714905
C	1.662534	-2.811512	-1.193361
C	0.575726	1.295380	0.816488
C	0.357799	0.125316	1.543136
C	0.028823	1.331265	-0.478062
C	1.499549	2.357225	1.349338
C	-0.125266	-1.043502	0.963889
C	-0.108507	-1.107655	-0.440079
C	-0.877351	-2.054786	1.781864
C	-0.164414	0.109110	-1.109219
C	0.130304	-2.374465	-1.216512
C	-0.586518	2.562704	-1.079535
C	-3.517353	-1.267676	-0.128372
C	-2.876720	-0.665825	0.953189
C	-3.812060	-0.529076	-1.269245
C	-2.589204	0.695900	0.867661
C	-2.309778	-1.475469	2.098820
C	-2.749069	1.418089	-0.314082
C	-3.397174	0.793545	-1.378794
C	-2.033200	2.741448	-0.480223
H	3.551822	-0.125560	2.017092
H	3.052684	1.512567	-1.895575
H	3.071561	2.995358	-0.047997
H	3.679629	2.493780	1.522111
H	2.955121	-2.333412	1.161241
H	2.503749	-0.703996	-2.760665
H	1.902332	-3.241608	-2.167968
H	1.783217	-3.603271	-0.452625
H	0.566128	0.130718	2.608519
H	1.572990	2.250446	2.432593
H	1.134889	3.366559	1.152243
H	-0.380733	-2.285510	2.727438
H	-0.988048	-2.990448	1.234809
H	-0.383792	0.104168	-2.170773
H	-0.164894	-2.206866	-2.252963
H	-0.462252	-3.213753	-0.851166
H	-0.665644	2.445624	-2.162047
H	-0.016408	3.473444	-0.888987
H	-3.762610	-2.322680	-0.090774
H	-4.323916	-1.002035	-2.098039
H	-2.098749	1.174867	1.702980
H	-2.972318	-2.303044	2.361440
H	-2.226869	-0.834100	2.977843
H	-3.547647	1.330842	-2.307977
H	-1.938045	3.220744	0.495801
H	-2.598675	3.418484	-1.124287

3526-04-3-C16H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -615.943147350 (a.u.)
E(HF/CC-PVTZ) = -611.81945027
E(DLPNO-CCSD(T)/CC-PVTZ) = -614.484509099269
T1 (CC-PVTZ)= 0.012550943
T2 (CC-PVTZ)= 0.032602
E(HF/CC-PVQZ) = -611.85575593
E(DLPNO-CCSD(T)/CC-PVQZ) = -614.656049622348
E(HF/TZ-AUG) = -611.82429254
E(DLPNO-CCSD(T)/TZ-AUG) = -614.525486602
E(HF/TZ-CORE) = -611.824004
E(DLPNO-CCSD(T)/TZ-CORE) = -615.296842572
E(HF/TZ-IT) = -611.81945027
E(DLPNO-CCSD(T)/TZ-IT) = -614.492152129
T1 (CC-PVQZ)= 0.012394960
T2 (CC-PVQZ)= 0.037374
E(HF/CBS) = -611.864602632
E(DLPNO-CCSD(T)/CBS) = -614.763581225
Enthalpic correction = 0.20993521 (a.u.)
Entropy = 101.88257 (cal/(mol*K))

C	0.677746	-0.000001	-0.000023
C	1.155086	1.351823	-0.000006
C	0.000000	2.183070	-0.000011
C	-1.155080	1.351840	-0.000009
C	-2.523539	1.652899	0.000004
C	-3.538782	0.709863	0.000013
C	-3.538785	-0.709863	0.000018
C	-2.523540	-1.652897	0.000009
C	-1.155085	-1.351825	-0.000010
C	-0.677747	0.000000	-0.000024
C	0.000000	-2.183072	-0.000017
C	1.155081	-1.351841	-0.000009
C	2.523539	-1.652898	0.000009
C	3.538782	-0.709860	0.000016
C	3.538785	0.709864	0.000012
C	2.523539	1.652897	0.000006
H	0.000014	3.262378	-0.000001
H	-2.823343	2.695121	0.000007
H	-4.538901	1.130451	0.000021
H	-4.538905	-1.130448	0.000032
H	-2.823336	-2.695121	0.000016
H	-0.000016	-3.262379	-0.000024
H	2.823345	-2.695118	0.000017
H	4.538900	-1.130450	0.000027
H	4.538905	1.130450	0.000019
H	2.823332	2.695121	0.000011

3697-27-6-C20H16

Charge of molecule: 0
Multiplicity: 1

E (B3LYP-D3/def2tzvp, G09)= -772.156640987
(a.u.)
E(HF/CC-PVTZ) = -766.94490791
E(DLPNO-CCSD(T)/CC-PVTZ) = -770.330199186126
T1 (CC-PVTZ)= 0.009925426
T2 (CC-PVTZ)= 0.033912
E(HF/CC-PVQZ) = -766.99061666
E(DLPNO-CCSD(T)/CC-PVQZ) = -770.546929958381
E(HF/TZ-AUG) = -766.95024621
E(DLPNO-CCSD(T)/TZ-AUG) = -770.382138695
E(HF/TZ-CORE) = -766.95050654
E(DLPNO-CCSD(T)/TZ-CORE) = -771.345804617
E(HF/TZ-IT) = -766.94490791
E(DLPNO-CCSD(T)/TZ-IT) = -770.340261904
T1 (CC-PVQZ)= 0.009982426
T2 (CC-PVQZ)= 0.037131
E(HF/CBS) = -767.00175464
E(DLPNO-CCSD(T)/CBS) = -770.682867792
Enthalpic correction = 0.30403283 (a.u.)
Entropy = 123.44319 (cal/(mol*K))

C	-3.951759	-1.285794	0.079573
C	-4.742025	-0.225378	-0.286484
C	-4.137495	0.999673	-0.603352
C	-2.776275	1.160290	-0.484674
C	-1.935773	0.112716	-0.042332
C	-0.495246	0.240009	0.096185
C	0.179334	1.513004	0.210253
C	1.543737	1.589367	0.054768
C	2.331004	0.398614	-0.090450
C	3.733526	0.453060	-0.260775
C	4.494589	-0.688557	-0.322818
C	3.878897	-1.942754	-0.216822
C	2.517726	-2.026156	-0.050225
C	1.707194	-0.872006	0.014950
C	0.272706	-0.941819	0.139643
C	-0.383250	-2.193836	0.328784
C	-1.732904	-2.290190	0.405437
C	-2.550881	-1.153386	0.171685
C	2.261978	2.914427	0.071171
C	-0.571505	2.748521	0.662327
H	-4.390687	-2.256792	0.274547
H	-5.815165	-0.340746	-0.365178
H	-4.742383	1.824115	-0.958417
H	-2.347212	2.100501	-0.784986
H	4.223922	1.411516	-0.338504
H	5.566627	-0.618730	-0.454682
H	4.472343	-2.846152	-0.271628
H	2.067084	-3.004976	0.008835
H	0.208512	-3.087549	0.451600
H	-2.207143	-3.246348	0.588884
H	1.578832	3.756235	0.032347
H	2.923123	3.001292	-0.792656
H	2.885734	3.026246	0.963075
H	-1.492931	2.482111	1.171837
H	-0.828761	3.428472	-0.154261
H	0.036620	3.311985	1.368119

38399-10-9-C14H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -540.973294919
(a.u.)
E(HF/CC-PVTZ) = -537.31927769
E(DLPNO-CCSD(T)/CC-PVTZ) = -539.694381582654
T1 (CC-PVTZ)= 0.010053552
T2 (CC-PVTZ)= 0.039410
E(HF/CC-PVQZ) = -537.35155044
E(DLPNO-CCSD(T)/CC-PVQZ) = -539.846720609503
E(HF/TZ-AUG) = -537.32312709
E(DLPNO-CCSD(T)/TZ-AUG) = -539.730329841
E(HF/TZ-CORE) = -537.32321217
E(DLPNO-CCSD(T)/TZ-CORE) = -540.405234281
E(HF/TZ-IT) = -537.31927769
E(DLPNO-CCSD(T)/TZ-IT) = -539.700923612
T1 (CC-PVQZ)= 0.010111918
T2 (CC-PVQZ)= 0.040549
E(HF/CBS) = -537.359414432
E(DLPNO-CCSD(T)/CBS) = -539.942200533
Enthalpic correction = 0.22097077 (a.u.)
Entropy = 99.50448 (cal/(mol*K))

C	-2.776019	0.962373	-0.165650
C	-3.526699	-0.118825	0.052349
C	-2.880393	-1.429206	0.393532
C	-1.496660	-1.558377	-0.246099
C	-0.660798	-0.308281	-0.092803
C	0.759569	-0.348739	-0.040592
C	1.501718	-1.557832	-0.084887
C	2.871358	-1.557352	-0.034400
C	3.584795	-0.346113	0.065911
C	2.904623	0.841929	0.104938
C	1.492187	0.877973	0.046983
C	0.787435	2.103141	0.059946
C	-0.575761	2.119050	-0.013765
C	-1.316402	0.915362	-0.088458
H	-3.235453	1.923192	-0.367451
H	-4.607815	-0.052802	0.040111
H	-3.509182	-2.265514	0.082270
H	-2.791852	-1.504354	1.486144
H	-0.989831	-2.424503	0.175274
H	-1.615704	-1.760192	-1.318778
H	0.981233	-2.500883	-0.164723
H	3.410951	-2.495107	-0.070582
H	4.666098	-0.359015	0.109554
H	3.441991	1.779929	0.176858
H	1.347612	3.028087	0.121276
H	-1.111765	3.060544	-0.011984

38765-94-5-C16H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -617.161021411
(a.u.)
E(HF/CC-PVTZ) = -612.98509316
E(DLPNO-CCSD(T)/CC-PVTZ) = -615.695996768634
T1 (CC-PVTZ)= 0.010448009
T2 (CC-PVTZ)= 0.044842
E(HF/CC-PVQZ) = -613.02185568
E(DLPNO-CCSD(T)/CC-PVQZ) = -615.868935341492
E(HF/TZ-AUG) = -612.98993972
E(DLPNO-CCSD(T)/TZ-AUG) = -615.738136065
E(HF/TZ-CORE) = -612.98958173
E(DLPNO-CCSD(T)/TZ-CORE) = -616.508032062
E(HF/TZ-IT) = -612.98509316
E(DLPNO-CCSD(T)/TZ-IT) = -615.705068811
T1 (CC-PVQZ)= 0.010463925
T2 (CC-PVQZ)= 0.044081
E(HF/CBS) = -613.030813707
E(DLPNO-CCSD(T)/CBS) = -615.977265082
Enthalpic correction = 0.23262557 (a.u.)
Entropy = 101.53815 (cal/(mol*K))

C	-0.771476	0.000000	0.833384
C	0.771479	0.000000	0.833384
C	1.154697	-1.247882	0.073642

C	1.154697	1.247882	0.073642
C	-1.154698	-1.247877	0.073643
C	-1.154698	1.247876	0.073643
C	0.000000	-1.941654	-0.285622
C	-2.481955	-1.575758	-0.191180
C	2.481957	-1.575763	-0.191178
C	2.481956	1.575763	-0.191178
C	0.000000	1.941654	-0.285622
C	-2.481955	1.575758	-0.191180
C	-3.559427	-0.703717	-0.116820
C	-3.559428	0.703717	-0.116820
C	3.559425	0.703719	-0.116821
C	3.559425	-0.703719	-0.116821
H	-1.221328	0.000000	1.828518
H	1.221339	0.000000	1.828513
H	-0.000004	-2.864927	-0.851234
H	-2.691851	-2.594357	-0.501193
H	2.691860	-2.594362	-0.501184
H	2.691859	2.594362	-0.501185
H	-0.000004	2.864927	-0.851233
H	-2.691851	2.594357	-0.501193
H	-4.539245	-1.155971	-0.224588
H	-4.539246	1.155971	-0.224588
H	4.539243	1.155971	-0.224595
H	4.539243	-1.155971	-0.224595

4218-50-22_C2H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -78.5057637816 (a.u.)
E(HF/CC-PVTZ) = -77.95394163
E(DLPNO-CCSD(T)/CC-PVTZ) = -78.316495111259
T1 (CC-PVTZ)= 0.012235232
T2 (CC-PVTZ)= 0.108789
E(HF/CC-PVQZ) = -77.95924208
E(DLPNO-CCSD(T)/CC-PVQZ) = -78.339198579518
E(HF/TZ-AUG) = -77.95518832
E(DLPNO-CCSD(T)/TZ-AUG) = -78.322489279
E(HF/TZ-CORE) = -77.95445632
E(DLPNO-CCSD(T)/TZ-CORE) = -78.4167142274
E(HF/TZ-IT) = -77.95394163
E(DLPNO-CCSD(T)/TZ-IT) = -78.3168188416
T1 (CC-PVQZ)= 0.012530517
T2 (CC-PVQZ)= 0.102401
E(HF/CBS) = -77.9605336556
E(DLPNO-CCSD(T)/CBS) = -78.3531896549
Enthalpic correction = 0.04932792 (a.u.)
Entropy = 56.38043 (cal/(mol*K))

C	0.590235	0.021948	-0.030876
C	-0.844287	-0.190791	-0.038694
H	-1.312295	0.812257	0.004113
H	0.609326	0.077729	1.090958
H	1.023563	0.964733	-0.386805
H	1.203721	-0.841665	-0.290846

460-12-80_C4H2

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -153.554447827 (a.u.)
E(HF/CC-PVTZ) = -152.55140096
E(DLPNO-CCSD(T)/CC-PVTZ) = -153.194115650980
T1 (CC-PVTZ)= 0.013586123
T2 (CC-PVTZ)= 0.045576
E(HF/CC-PVQZ) = -152.56077819
E(DLPNO-CCSD(T)/CC-PVQZ) = -153.236122106792
E(HF/TZ-AUG) = -152.55263655
E(DLPNO-CCSD(T)/TZ-AUG) = -153.202716092
E(HF/TZ-CORE) = -152.55316215
E(DLPNO-CCSD(T)/TZ-CORE) = -153.39823934
E(HF/TZ-IT) = -152.55140096
E(DLPNO-CCSD(T)/TZ-IT) = -153.196066273
T1 (CC-PVQZ)= 0.013734466
T2 (CC-PVQZ)= 0.045900
E(HF/CBS) = -152.563063166
E(DLPNO-CCSD(T)/CBS) = -153.262217599
Enthalpic correction = 0.04164809 (a.u.)
Entropy = 59.32305 (cal/(mol*K))

C	0.000000	0.000000	0.681774
C	0.000000	0.000000	-0.681774
C	0.000000	0.000000	1.886590
C	0.000000	0.000000	-1.886590
H	0.000000	0.000000	2.948827
H	0.000000	0.000000	-2.948827

462-80-60_C6H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -231.015927666 (a.u.)
E(HF/CC-PVTZ) = -229.46258992
E(DLPNO-CCSD(T)/CC-PVTZ) = -230.473432792524
T1 (CC-PVTZ)= 0.012334678
T2 (CC-PVTZ)= 0.133319
E(HF/CC-PVQZ) = -229.47699533
E(DLPNO-CCSD(T)/CC-PVQZ) = -230.538261175845
E(HF/TZ-AUG) = -229.46477566
E(DLPNO-CCSD(T)/TZ-AUG) = -230.487764807
E(HF/TZ-CORE) = -229.46448657
E(DLPNO-CCSD(T)/TZ-CORE) = -230.778582691
E(HF/TZ-IT) = -229.46258992
E(DLPNO-CCSD(T)/TZ-IT) = -230.476883132
T1 (CC-PVQZ)= 0.012497919
T2 (CC-PVQZ)= 0.131852
E(HF/CBS) = -229.480505537
E(DLPNO-CCSD(T)/CBS) = -230.578566525
Enthalpic correction = 0.07818102 (a.u.)
Entropy = 67.85137 (cal/(mol*K))

C	0.000000	0.620711	-1.231424
C	0.000000	-0.620711	-1.231424
C	0.000000	1.455157	-0.133522
C	0.000000	-1.455157	-0.133522
C	0.000000	0.700441	1.053780
C	0.000000	-0.700441	1.053780
H	0.000000	2.535532	-0.134912
H	0.000000	-2.535532	-0.134912
H	0.000000	1.224941	2.001908
H	0.000000	-1.224941	2.001908

462-80-62_C6H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -231.015927666 (a.u.)

E(HF/CC-PVTZ) = -229.46258992
E(DLPNO-CCSD(T)/CC-PVTZ) = -230.473432792524
T1 (CC-PVTZ)= 0.012334678
T2 (CC-PVTZ)= 0.133319
E(HF/CC-PVQZ) = -229.47699533
E(DLPNO-CCSD(T)/CC-PVQZ) = -230.538261175845
E(HF/TZ-AUG) = -229.46477566
E(DLPNO-CCSD(T)/TZ-AUG) = -230.487764807
E(HF/TZ-CORE) = -229.46448657
E(DLPNO-CCSD(T)/TZ-CORE) = -230.778582691
E(HF/TZ-IT) = -229.46258992
E(DLPNO-CCSD(T)/TZ-IT) = -230.476883132
T1 (CC-PVQZ)= 0.012497919
T2 (CC-PVQZ)= 0.131852
E(HF/CBS) = -229.480505537
E(DLPNO-CCSD(T)/CBS) = -230.578566525
Enthalpic correction = 0.07818102 (a.u.)
Entropy = 67.85137 (cal/(mol*K))

C	0.000000	0.620711	-1.231424
C	0.000000	-0.620711	-1.231424
C	0.000000	1.455157	-0.133522
C	0.000000	-1.455157	-0.133522
C	0.000000	0.700441	1.053780
C	0.000000	-0.700441	1.053780
H	0.000000	2.535532	-0.134912
H	0.000000	-2.535532	-0.134912
H	0.000000	1.224941	2.001908
H	0.000000	-1.224941	2.001908

463-49-00_C3H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -116.714224469
(a.u.)
E(HF/CC-PVTZ) = -115.90585138
E(DLPNO-CCSD(T)/CC-PVTZ) = -116.432347344470
T1 (CC-PVTZ)= 0.012005610
T2 (CC-PVTZ)= 0.057621
E(HF/CC-PVQZ) = -115.91335958
E(DLPNO-CCSD(T)/CC-PVQZ) = -116.465640460120
E(HF/TZ-AUG) = -115.90704617
E(DLPNO-CCSD(T)/TZ-AUG) = -116.439837309
E(HF/TZ-CORE) = -115.90692885
E(DLPNO-CCSD(T)/TZ-CORE) = -116.584953892
E(HF/TZ-IT) = -115.90585138
E(DLPNO-CCSD(T)/TZ-IT) = -116.433446886
T1 (CC-PVQZ)= 0.012174036
T2 (CC-PVQZ)= 0.056171
E(HF/CBS) = -115.915189124
E(DLPNO-CCSD(T)/CBS) = -116.486286024
Enthalpic correction = 0.05802232 (a.u.)
Entropy = 58.13173 (cal/(mol*K))

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.300138
C	0.000000	0.000000	-1.300138
H	0.000000	0.926258	1.863173
H	0.000000	-0.926258	1.863173
H	-0.926258	0.000000	-1.863173
H	0.926258	0.000000	-1.863173

463-82-10_C5H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -197.871859702
(a.u.)
E(HF/CC-PVTZ) = -196.40358602
E(DLPNO-CCSD(T)/CC-PVTZ) = -197.398625026699
T1 (CC-PVTZ)= 0.007948522
T2 (CC-PVTZ)= 0.033940
E(HF/CC-PVQZ) = -196.41604714
E(DLPNO-CCSD(T)/CC-PVQZ) = -197.457834886462
E(HF/TZ-AUG) = -196.40454097
E(DLPNO-CCSD(T)/TZ-AUG) = -197.413164699
E(HF/TZ-CORE) = -196.40494188
E(DLPNO-CCSD(T)/TZ-CORE) = -197.651297399
E(HF/TZ-IT) = -196.40358602
E(DLPNO-CCSD(T)/TZ-IT) = -197.399662351
T1 (CC-PVQZ)= 0.008334099
T2 (CC-PVQZ)= 0.029281
E(HF/CBS) = -196.419083576
E(DLPNO-CCSD(T)/CBS) = -197.494985268
Enthalpic correction = 0.16180144 (a.u.)
Entropy = 78.54028 (cal/(mol*K))

C	0.000000	0.000000	0.000000
C	0.874151	1.252481	-0.134952
H	1.645072	1.277525	0.638730
H	1.373002	1.279329	-1.106523
H	0.274567	2.160839	-0.040546
C	0.875254	-1.251413	-0.137685
H	1.646198	-1.277466	0.635941
H	0.276470	-2.160502	-0.045263
H	1.374128	-1.275700	-1.109312
C	-1.067487	0.000731	-1.100696
H	-1.705933	-0.882795	-1.027947
H	-1.706711	0.883533	-1.026019
H	-0.608259	0.002016	-2.091980
C	-0.681918	-0.001800	1.373333
H	-1.313268	0.880956	1.498516
H	-1.312490	-0.885382	1.496588
H	0.057221	-0.002352	2.177816

477-75-8-C20H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -770.929799170
(a.u.)
E(HF/CC-PVTZ) = -765.77271098
E(DLPNO-CCSD(T)/CC-PVTZ) = -769.117589298663
T1 (CC-PVTZ)= 0.010058340
T2 (CC-PVTZ)= 0.035910
E(HF/CC-PVQZ) = -765.81826567
E(DLPNO-CCSD(T)/CC-PVQZ) = -769.332801680056
E(HF/TZ-AUG) = -765.77814001
E(DLPNO-CCSD(T)/TZ-AUG) = -769.169169578
E(HF/TZ-CORE) = -765.77834382
E(DLPNO-CCSD(T)/TZ-CORE) = -770.133390174
E(HF/TZ-IT) = -765.77271098
E(DLPNO-CCSD(T)/TZ-IT) = -769.127314644
T1 (CC-PVQZ)= 0.010065148
T2 (CC-PVQZ)= 0.037868
E(HF/CBS) = -765.82936611
E(DLPNO-CCSD(T)/CBS) = -769.467706381
Enthalpic correction = 0.28183447 (a.u.)
Entropy = 114.81089 (cal/(mol*K))

C	0.000156	0.000116	-1.293599
C	-1.366069	-0.319986	-0.699770
C	0.406008	1.343349	-0.699770
C	0.960417	-1.023052	-0.699770

C	-1.366069	-0.319986	0.699770
C	-2.527165	-0.592201	-1.398416
C	0.406008	1.343349	0.699770
C	0.750792	2.484990	-1.398433
C	0.960417	-1.023052	0.699770
C	1.776377	-1.892791	-1.398433
C	0.000156	0.000116	1.293599
C	-2.527165	-0.592201	1.398416
C	-3.700736	-0.867337	-0.693992
C	0.750792	2.484990	1.398433
C	1.099263	3.638910	-0.693997
C	1.776377	-1.892791	1.398433
C	2.601065	-2.771896	-0.693995
C	-3.700736	-0.867337	0.693992
C	1.099263	3.638910	0.693997
C	2.601065	-2.771896	0.693995
H	0.000184	0.000112	-2.381545
H	-2.526955	-0.592203	-2.481690
H	0.750696	2.484803	-2.481709
H	1.776176	-1.892698	-2.481709
H	0.000184	0.000112	2.381545
H	-2.526955	-0.592203	2.481690
H	-4.613859	-1.081452	-1.234136
H	0.750696	2.484803	2.481709
H	1.370378	4.536764	-1.234138
H	1.776176	-1.892698	2.481709
H	3.242739	-3.455931	-1.234134
H	-4.613859	-1.081452	1.234136
H	1.370378	4.536764	1.234138
H	3.242739	-3.455931	1.234134

479-23-2-C20H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -770.952159275 (a.u.)
E(HF/CC-PVTZ) = -765.79262999
E(DLPNO-CCSD(T)/CC-PVTZ) = -769.132155806913
T1 (CC-PVTZ)= 0.010259877
T2 (CC-PVTZ)= 0.036860
E(HF/CC-PVQZ) = -765.83791531
E(DLPNO-CCSD(T)/CC-PVQZ) = -769.347675193539
E(HF/TZ-AUG) = -765.79787305
E(DLPNO-CCSD(T)/TZ-AUG) = -769.183286481
E(HF/TZ-CORE) = -765.79823272
E(DLPNO-CCSD(T)/TZ-CORE) = -770.147854862
E(HF/TZ-IT) = -765.79262999
E(DLPNO-CCSD(T)/TZ-IT) = -769.142343631
T1 (CC-PVQZ)= 0.010290005
T2 (CC-PVQZ)= 0.038253
E(HF/CBS) = -765.848950111
E(DLPNO-CCSD(T)/CBS) = -769.482934854
Enthalpic correction = 0.28189771 (a.u.)
Entropy = 118.22892 (cal/(mol*K))

C	2.179023	2.355061	-0.000004
C	3.632108	1.777074	0.000040
C	3.452313	0.273851	0.000010
C	2.485003	-2.376485	-0.000021
C	3.829610	-2.098647	-0.000022
C	4.337454	-0.767603	-0.000006
C	2.069522	-0.008958	0.000007
C	1.281171	1.136570	0.000007
C	0.139354	-1.427488	-0.000007
C	1.537128	-1.316156	-0.000006
C	-0.685708	-0.302873	0.000002
C	-0.103561	1.020902	0.000003
C	-0.956176	2.172291	-0.000010
C	-2.300817	2.052120	-0.000023
C	-2.142558	-0.413223	0.000005
C	-2.933176	0.764885	-0.000013
C	-4.335989	0.663696	-0.000018
C	-4.962116	-0.562003	0.000001
C	-4.188709	-1.727737	0.000027
C	-2.811978	-1.650044	0.000029
H	1.999651	2.983449	0.875450
H	1.999687	2.983389	-0.875510
H	4.192605	2.109584	-0.875785
H	4.192527	2.109545	0.875930
H	2.140775	-3.403374	-0.000033
H	4.536238	-2.919252	-0.000036
H	5.408222	-0.605728	-0.000006
H	-0.293305	-2.417547	-0.000020
H	-0.495947	3.151922	-0.000012
H	-2.932784	2.931787	-0.000036
H	-4.920458	1.575836	-0.000034
H	-6.042483	-0.624757	-0.000002
H	-4.670686	-2.696843	0.000047
H	-2.245424	-2.569409	0.000054

496-11-7_C9H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -349.148871546 (a.u.)
E(HF/CC-PVTZ) = -346.75754623
E(DLPNO-CCSD(T)/CC-PVTZ) = -348.323413902805
T1 (CC-PVTZ)= 0.009365599
T2 (CC-PVTZ)= 0.035227
E(HF/CC-PVQZ) = -346.7785865
E(DLPNO-CCSD(T)/CC-PVQZ) = -348.422901621098
E(HF/TZ-AUG) = -346.75988795
E(DLPNO-CCSD(T)/TZ-AUG) = -348.346625281
E(HF/TZ-CORE) = -346.76005813
E(DLPNO-CCSD(T)/TZ-CORE) = -348.779956125
E(HF/TZ-IT) = -346.75754623
E(DLPNO-CCSD(T)/TZ-IT) = -348.326978168
T1 (CC-PVQZ)= 0.009514788
T2 (CC-PVQZ)= 0.037412
E(HF/CBS) = -346.783713442
E(DLPNO-CCSD(T)/CBS) = -348.485273998
Enthalpic correction = 0.16685268 (a.u.)
Entropy = 82.64428 (cal/(mol*K))

C	0.148789	-0.698127	0.051902
C	0.148789	0.698127	0.051902
C	1.560636	-1.225286	0.128892
C	-1.046528	-1.400403	0.004700
C	1.560636	1.225286	0.128892
C	-1.046528	1.400403	0.004700
C	2.413659	0.000000	-0.266470
C	-2.246920	-0.695908	-0.047079
C	-2.246920	0.695908	-0.047079
H	1.786980	-1.543772	1.152616
H	1.732442	-2.087576	-0.517176
H	-1.050280	-2.483934	0.001131
H	1.732442	2.087576	-0.517176
H	1.786980	1.543772	1.152616
H	-1.050280	2.483934	0.001131
H	3.398787	0.000000	0.199421
H	2.560213	0.000000	-1.348757
H	-3.185481	-1.233443	-0.092977
H	-3.185481	1.233443	-0.092977

503-17-30_C4H6

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -156.052814572
(a.u.)
E(HF/CC-PVTZ) = -154.96514326
E(DLPNO-CCSD(T)/CC-PVTZ) = -155.680596845733
T1 (CC-PVTZ)= 0.010333587
T2 (CC-PVTZ)= 0.058169
E(HF/CC-PVQZ) = -154.97507097
E(DLPNO-CCSD(T)/CC-PVQZ) = -155.725753259235
E(HF/TZ-AUG) = -154.96644741
E(DLPNO-CCSD(T)/TZ-AUG) = -155.690791971
E(HF/TZ-CORE) = -154.96681619
E(DLPNO-CCSD(T)/TZ-CORE) = -155.884303854
E(HF/TZ-IT) = -154.96514326
E(DLPNO-CCSD(T)/TZ-IT) = -155.681828102
T1 (CC-PVQZ)= 0.010574733
T2 (CC-PVQZ)= 0.057363
E(HF/CBS) = -154.977490083
E(DLPNO-CCSD(T)/CBS) = -155.753879805
Enthalpic correction = 0.08801187 (a.u.)
Entropy = 72.27955 (cal/(mol*K))
```

C	0.000000	0.000000	0.600632
C	0.000000	0.000000	-0.600632
C	0.000000	0.000000	-2.056501
H	0.000000	1.018886	-2.450383
H	-0.882381	-0.509443	-2.450383
H	0.882381	-0.509443	-2.450383
C	0.000000	0.000000	2.056501
H	0.000000	1.018886	2.450383
H	0.882381	-0.509443	2.450383
H	-0.882381	-0.509443	2.450383

50-32-8-C20H12

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -769.764398338
(a.u.)
E(HF/CC-PVTZ) = -764.64548998
E(DLPNO-CCSD(T)/CC-PVTZ) = -767.944836023808
T1 (CC-PVTZ)= 0.010238658
T2 (CC-PVTZ)= 0.034497
E(HF/CC-PVQZ) = -764.69057153
E(DLPNO-CCSD(T)/CC-PVQZ) = -768.159005191167
E(HF/TZ-AUG) = -764.65078938
E(DLPNO-CCSD(T)/TZ-AUG) = -767.995024404
E(HF/TZ-CORE) = -764.65108984
E(DLPNO-CCSD(T)/TZ-CORE) = -768.961101388
E(HF/TZ-IT) = -764.64548998
E(DLPNO-CCSD(T)/TZ-IT) = -767.955746098
T1 (CC-PVQZ)= 0.010248619
T2 (CC-PVQZ)= 0.037636
E(HF/CBS) = -764.701556678
E(DLPNO-CCSD(T)/CBS) = -768.293378601
Enthalpic correction = 0.25964800 (a.u.)
Entropy = 112.56865 (cal/(mol*K))
```

C	-4.773748	0.156795	0.000003
C	-4.370187	-1.193010	0.000018
C	-3.829511	1.146915	-0.000007
C	-3.038317	-1.521384	0.000016
C	-2.032082	-0.527159	0.000001
C	-2.446020	0.839761	-0.000007
C	-0.628632	-0.830704	-0.000005
C	-1.479540	1.864436	-0.000011
C	-0.129741	1.590033	-0.000005
C	0.311834	0.223303	-0.000003
C	0.855480	2.636019	-0.000001
C	1.708141	-0.055913	-0.000001
C	-0.134692	-2.168882	-0.000015
C	2.656666	1.006333	0.000005
C	2.166349	-1.400131	-0.000004
C	2.177300	2.360678	0.000005
C	4.016468	0.704651	0.000010
C	1.196945	-2.442047	-0.000014
C	3.546828	-1.657307	0.000001
C	4.456557	-0.617442	0.000009
H	-5.827062	0.405281	0.000003
H	-5.116753	-1.976574	0.000031
H	-4.125582	2.188850	-0.000015
H	-2.762271	-2.565418	0.000033
H	-1.813447	2.895540	-0.000016
H	0.507112	3.661644	-0.000002
H	-0.832561	-2.992773	-0.000029
H	2.906236	3.161865	0.000009
H	4.735372	1.514708	0.000016
H	1.540685	-3.469218	-0.000023
H	3.889642	-2.684587	-0.000001
H	5.518047	-0.828986	0.000013

519-73-3_C19H16

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -734.008223552
(a.u.)
E(HF/CC-PVTZ) = -729.05281041
E(DLPNO-CCSD(T)/CC-PVTZ) = -732.271257781353
T1 (CC-PVTZ)= 0.009809736
T2 (CC-PVTZ)= 0.035504
E(HF/CC-PVQZ) = -729.09674091
E(DLPNO-CCSD(T)/CC-PVQZ) = -732.477803477789
E(HF/TZ-AUG) = -729.05815381
E(DLPNO-CCSD(T)/TZ-AUG) = -732.320566255
E(HF/TZ-CORE) = -729.05824514
E(DLPNO-CCSD(T)/TZ-CORE) = -733.236362046
E(HF/TZ-IT) = -729.05281041
E(DLPNO-CCSD(T)/TZ-IT) = -732.280092845
T1 (CC-PVQZ)= 0.009874068
T2 (CC-PVQZ)= 0.036566
E(HF/CBS) = -729.107445579
E(DLPNO-CCSD(T)/CBS) = -732.60717329
Enthalpic correction = 0.29729255 (a.u.)
Entropy = 131.52524 (cal/(mol*K))
```

C	0.000037	-0.000156	-0.775937
C	-1.238091	-0.774991	-0.349237
C	1.290111	-0.684836	-0.348979
C	-0.051947	1.459503	-0.349121
C	-2.418855	-0.616012	-1.074858
C	-1.248965	-1.608778	0.765469
C	1.743522	-1.786398	-1.074901
C	2.017001	-0.277564	0.766227
C	0.677583	2.402297	-1.073641
C	-0.770183	1.886079	0.764464
C	-3.582886	-1.269460	-0.696287
C	-2.414736	-2.262806	1.150804
C	2.891619	-2.467415	-0.696219
C	3.166446	-0.959802	1.151666
C	0.693447	3.737125	-0.695167
C	-0.753985	3.222725	1.149681
C	-3.585135	-2.095969	0.422671

C	3.607921	-2.056273	0.423173
C	-0.022919	4.152626	0.422604
H	0.000139	-0.000149	-1.869813
H	-2.424041	0.034436	-1.941633
H	-0.340095	-1.753490	1.333474
H	1.183275	-2.115935	-1.942049
H	1.687301	0.581515	1.334481
H	1.244819	2.081277	-1.939438
H	-1.351033	1.171533	1.331597
H	-4.488262	-1.135588	-1.274572
H	-2.404284	-2.907446	2.020545
H	3.229028	-3.317979	-1.274782
H	3.719036	-0.628567	2.021752
H	1.263194	4.454067	-1.272593
H	-1.318783	3.536217	2.018501
H	-4.490884	-2.608508	0.719894
H	4.504837	-2.584089	0.720449
H	-0.014158	5.193330	0.719721

536-74-30_C8H6

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -308.536950139 (a.u.)
E(HF/CC-PVTZ) = -306.47885924
E(DLPNO-CCSD(T)/CC-PVTZ) = -307.807593856137
T1 (CC-PVTZ)= 0.010831876
T2 (CC-PVTZ)= 0.058263
E(HF/CC-PVQZ) = -306.49747624
E(DLPNO-CCSD(T)/CC-PVQZ) = -307.893811499123
E(HF/TZ-AUG) = -306.4812142
E(DLPNO-CCSD(T)/TZ-AUG) = -307.82670483
E(HF/TZ-CORE) = -306.48145557
E(DLPNO-CCSD(T)/TZ-CORE) = -308.214491296
E(HF/TZ-IT) = -306.47885924
E(DLPNO-CCSD(T)/TZ-IT) = -307.811302346
T1 (CC-PVQZ)= 0.010944040
T2 (CC-PVQZ)= 0.054981
E(HF/CBS) = -306.502012697
E(DLPNO-CCSD(T)/CBS) = -307.947678155
Enthalpic correction = 0.11334598 (a.u.)
Entropy = 80.18899 (cal/(mol*K))

C	0.000000	-0.591123	0.000000
C	1.207551	0.119100	0.000000
C	-1.207551	0.119099	0.000000
C	1.203204	1.505525	0.000000
C	-1.203204	1.505525	0.000000
C	0.000000	2.202891	0.000000
H	2.140567	-0.427676	0.000000
H	-2.140566	-0.427677	0.000000
H	2.142017	2.043967	0.000000
H	-2.142017	2.043966	0.000000
H	0.000000	3.285065	0.000000
C	0.000000	-2.015822	0.000000
C	0.000000	-3.218122	0.000000
H	0.000001	-4.280087	0.000000

53-70-3-C22H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -847.214050971 (a.u.)
E(HF/CC-PVTZ) = -841.56869512
E(DLPNO-CCSD(T)/CC-PVTZ) = -845.210850540102
T1 (CC-PVTZ)= 0.010127162
T2 (CC-PVTZ)= 0.036494
E(HF/CC-PVQZ) = -841.61844291
E(DLPNO-CCSD(T)/CC-PVQZ) = -845.446980687069
E(HF/TZ-AUG) = -841.57449644
E(DLPNO-CCSD(T)/TZ-AUG) = -845.266002395
E(HF/TZ-CORE) = -841.57487032
E(DLPNO-CCSD(T)/TZ-CORE) = -846.328633061
E(HF/TZ-IT) = -841.56869512
E(DLPNO-CCSD(T)/TZ-IT) = -845.222420535
T1 (CC-PVQZ)= 0.010152031
T2 (CC-PVQZ)= 0.037676
E(HF/CBS) = -841.630565094
E(DLPNO-CCSD(T)/CBS) = -845.595111618
Enthalpic correction = 0.29457823 (a.u.)
Entropy = 124.10687 (cal/(mol*K))

C	-2.866154	0.303558	0.000006
C	-3.523342	1.546714	0.000029
C	-4.899109	1.632321	0.000025
C	-3.661409	-0.871243	-0.000010
C	-1.416819	0.176246	0.000000
C	-5.063781	-0.760775	-0.000016
C	-3.029709	-2.158133	-0.000013
C	-5.679536	0.470019	-0.000001
C	-0.833628	-1.127261	0.000005
C	-0.554098	1.267865	-0.000013
C	-1.684105	-2.280039	0.000001
C	0.554098	-1.267864	0.000006
C	0.833628	1.127262	-0.000014
C	1.416820	-0.176247	-0.000002
C	1.684105	2.280039	-0.000023
C	2.866154	-0.303558	-0.000001
C	3.029709	2.158133	-0.000014
C	3.661409	0.871243	-0.000002
C	5.063781	0.760774	0.000007
C	3.523342	-1.546714	0.000002
C	5.679536	-0.470019	0.000014
C	4.899109	-1.632321	0.000010
H	-2.946906	2.460493	0.000059
H	-5.376529	2.603629	0.000044
H	-5.655573	-1.668122	-0.000030
H	-3.661771	-3.037717	-0.000023
H	-6.759406	0.540642	-0.000008
H	-0.950688	2.273641	-0.000029
H	-1.219772	-3.258641	0.000005
H	0.950688	-2.273641	0.000014
H	1.219773	3.258641	-0.000034
H	3.661771	3.037717	-0.000018
H	5.655573	1.668122	0.000007
H	2.946906	-2.460494	-0.000006
H	6.759406	-0.540641	0.000023
H	5.376529	-2.603629	0.000012

542-92-70_C5H6

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -194.192114705 (a.u.)
E(HF/CC-PVTZ) = -192.85812043
E(DLPNO-CCSD(T)/CC-PVTZ) = -193.734023659948
T1 (CC-PVTZ)= 0.010726162
T2 (CC-PVTZ)= 0.046364
E(HF/CC-PVQZ) = -192.87025927
E(DLPNO-CCSD(T)/CC-PVQZ) = -193.789698615509
E(HF/TZ-AUG) = -192.85979199
E(DLPNO-CCSD(T)/TZ-AUG) = -193.746553327

E(HF/TZ-CORE) = -192.85953726
E(DLPNO-CCSD(T)/TZ-CORE) = -193.987628578
E(HF/TZ-IT) = -192.85812043
E(DLPNO-CCSD(T)/TZ-IT) = -193.735925897
T1 (CC-PVQZ)= 0.010881254
T2 (CC-PVQZ)= 0.046334
E(HF/CBS) = -192.873217175
E(DLPNO-CCSD(T)/CBS) = -193.824426119
Enthalpic correction = 0.09456619 (a.u.)
Entropy = 65.62713 (cal/(mol*K))

C	0.000000	0.000000	1.212800
C	-0.000001	1.176418	0.280788
C	0.000001	-1.176418	0.280788
C	0.000000	0.732551	-0.987490
C	0.000000	-0.732551	-0.987490
H	0.875782	0.000001	1.872935
H	-0.875782	-0.000001	1.872935
H	-0.000002	2.205552	0.606789
H	0.000002	-2.205552	0.606789
H	0.000000	1.345128	-1.877912
H	0.000000	-1.345128	-1.877912

56179-83-0-C14H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -540.973134296 (a.u.)
E(HF/CC-PVTZ) = -537.31893241
E(DLPNO-CCSD(T)/CC-PVTZ) = -539.694258620655
T1 (CC-PVTZ)= 0.010051958
T2 (CC-PVTZ)= 0.037735
E(HF/CC-PVQZ) = -537.35121687
E(DLPNO-CCSD(T)/CC-PVQZ) = -539.846547537272
E(HF/TZ-AUG) = -537.32281188
E(DLPNO-CCSD(T)/TZ-AUG) = -539.730155109
E(HF/TZ-CORE) = -537.32286047
E(DLPNO-CCSD(T)/TZ-CORE) = -540.405049424
E(HF/TZ-IT) = -537.31893241
E(DLPNO-CCSD(T)/TZ-IT) = -539.700810547
T1 (CC-PVQZ)= 0.010118497
T2 (CC-PVQZ)= 0.038807
E(HF/CBS) = -537.359083715
E(DLPNO-CCSD(T)/CBS) = -539.941985202
Enthalpic correction = 0.22099753 (a.u.)
Entropy = 99.32731 (cal/(mol*K))

C	-1.319699	0.872694	-0.104056
C	-2.822618	0.881600	-0.235717
C	-0.646453	-0.341987	-0.121869
C	-0.601488	2.080003	-0.031458
C	-3.467655	-0.326885	0.438908
C	-2.748297	-1.585140	0.046577
C	-1.437518	-1.570660	-0.212899
C	0.781882	-0.362491	-0.051583
C	0.766721	2.087297	0.024966
C	1.492284	0.875701	0.017510
C	2.906029	0.864244	0.083025
C	1.539150	-1.560266	-0.035992
C	2.908481	-1.537877	0.029052
C	3.603729	-0.313490	0.086335
H	-3.229021	1.811440	0.165639
H	-3.074065	0.863598	-1.304368
H	-1.149227	3.014960	-0.023325
H	-3.426356	-0.214135	1.531018
H	-4.525231	-0.386377	0.175926
H	-3.300604	-2.516336	0.011177
H	-0.939963	-2.492994	-0.477303
H	1.310395	3.022426	0.080408
H	3.427861	1.812344	0.133132
H	1.032964	-2.513838	-0.065254
H	3.461132	-2.468608	0.039513
H	4.684827	-0.308930	0.136654

56-55-3-C18H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -693.495950345 (a.u.)
E(HF/CC-PVTZ) = -688.86722415
E(DLPNO-CCSD(T)/CC-PVTZ) = -691.854608631210
T1 (CC-PVTZ)= 0.010194048
T2 (CC-PVTZ)= 0.036557
E(HF/CC-PVQZ) = -688.90810396
E(DLPNO-CCSD(T)/CC-PVQZ) = -692.048228860074
E(HF/TZ-AUG) = -688.87200935
E(DLPNO-CCSD(T)/TZ-AUG) = -691.89954649
E(HF/TZ-CORE) = -688.87228907
E(DLPNO-CCSD(T)/TZ-CORE) = -692.769185551
E(HF/TZ-IT) = -688.86722415
E(DLPNO-CCSD(T)/TZ-IT) = -691.86401575
T1 (CC-PVQZ)= 0.010214148
T2 (CC-PVQZ)= 0.038103
E(HF/CBS) = -688.918065258
E(DLPNO-CCSD(T)/CBS) = -692.169649383
Enthalpic correction = 0.24639335 (a.u.)
Entropy = 110.14671 (cal/(mol*K))

C	-0.341474	-0.060151	0.000002
C	-1.765599	-0.376650	0.000003
C	0.062141	1.318616	0.000006
C	0.647933	-1.031678	-0.000005
C	-2.709077	0.681473	-0.000007
C	-2.252863	-1.694554	0.000016
C	1.411296	1.643202	0.000009
C	-0.939763	2.345821	0.000002
C	2.012662	-0.713110	-0.000004
C	-2.254654	2.043588	-0.000008
C	-4.083612	0.387430	-0.000013
C	-3.606075	-1.962253	0.000012
C	2.408763	0.662792	0.000005
C	3.021553	-1.713106	-0.000011
C	-4.532664	-0.914464	-0.000004
C	3.793916	0.977599	0.000008
C	4.344994	-1.373835	-0.000009
C	4.735997	-0.011638	0.000001
H	0.382262	-2.079679	-0.000015
H	-1.561484	-2.524694	0.000032
H	1.700051	2.688075	0.000012
H	-0.611238	3.377913	0.000005
H	-2.999865	2.829654	-0.000014
H	-4.789814	1.208888	-0.000022
H	-3.949959	-2.988462	0.000022
H	2.720987	-2.753899	-0.000018
H	-5.593860	-1.126472	-0.000009
H	4.089711	2.019673	0.000015
H	5.103743	-2.145654	-0.000015
H	5.788629	0.240167	0.000003

56-56-4-C20H16

Charge of molecule: 0
Multiplicity: 1

E (B3LYP-D3/def2tzvp, G09)= -772.170653972
(a.u.)
E(HF/CC-PVTZ) = -766.96641488
E(DLPNO-CCSD(T)/CC-PVTZ) = -770.341810486679
T1 (CC-PVTZ)= 0.009961572
T2 (CC-PVTZ)= 0.036673
E(HF/CC-PVQZ) = -767.01203948
E(DLPNO-CCSD(T)/CC-PVQZ) = -770.558723056176
E(HF/TZ-AUG) = -766.97150334
E(DLPNO-CCSD(T)/TZ-AUG) = -770.39305492
E(HF/TZ-CORE) = -766.97201931
E(DLPNO-CCSD(T)/TZ-CORE) = -771.357627124
E(HF/TZ-IT) = -766.96641488
E(DLPNO-CCSD(T)/TZ-IT) = -770.351790246
T1 (CC-PVQZ)= 0.010013056
T2 (CC-PVQZ)= 0.038039
E(HF/CBS) = -767.023156955
E(DLPNO-CCSD(T)/CBS) = -770.694834455
Enthalpic correction = 0.30314961 (a.u.)
Entropy = 125.41765 (cal/(mol*K))

C	-2.448703	-0.405228	0.000003
C	-3.459345	0.589335	-0.000009
C	-3.094364	1.977806	-0.000012
C	-1.801297	2.363944	-0.000002
C	-0.735029	1.404213	0.000005
C	0.591187	1.815662	0.000008
C	1.647801	0.900578	0.000007
C	3.010725	1.294470	0.000010
C	4.032917	0.384959	0.000004
C	3.727072	-1.017182	-0.000005
C	2.418908	-1.418722	-0.000007
C	1.342296	-0.494677	-0.000001
C	0.002667	-0.903215	-0.000003
C	-1.048432	0.002640	0.000003
C	-4.811946	0.206201	-0.000014
C	-5.175603	-1.122006	-0.000004
C	-4.182639	-2.107360	0.000014
C	-2.849807	-1.752155	0.000018
C	4.837946	-2.028971	-0.000015
C	5.464148	0.842421	0.000005
H	-3.888778	2.714147	-0.000021
H	-1.540286	3.415246	-0.000001
H	0.811746	2.877119	0.000011
H	3.238077	2.354604	0.000016
H	2.185518	-2.477627	-0.000012
H	-0.194228	-1.966366	-0.000012
H	-5.570049	0.980093	-0.000025
H	-6.220804	-1.402574	-0.000008
H	-4.459032	-3.153825	0.000026
H	-2.105757	-2.535490	0.000036
H	5.481121	-1.918436	0.877005
H	5.481078	-1.918462	-0.877071
H	4.440141	-3.042973	0.000009
H	5.524544	1.929983	0.000001
H	6.002854	0.474136	-0.877035
H	6.002851	0.474144	0.877050

567-79-3_C14H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -540.969618681
(a.u.)
E(HF/CC-PVTZ) = -537.31531966
E(DLPNO-CCSD(T)/CC-PVTZ) = -539.695989272873
T1 (CC-PVTZ)= 0.009846251
T2 (CC-PVTZ)= 0.031160
E(HF/CC-PVQZ) = -537.3471554
E(DLPNO-CCSD(T)/CC-PVQZ) = -539.848104926566
E(HF/TZ-AUG) = -537.31875331
E(DLPNO-CCSD(T)/TZ-AUG) = -539.732239787
E(HF/TZ-CORE) = -537.31924948
E(DLPNO-CCSD(T)/TZ-CORE) = -540.406262708
E(HF/TZ-IT) = -537.31531966
E(DLPNO-CCSD(T)/TZ-IT) = -539.702401781
T1 (CC-PVQZ)= 0.009900253
T2 (CC-PVQZ)= 0.036829
E(HF/CBS) = -537.354912904
E(DLPNO-CCSD(T)/CBS) = -539.94363426
Enthalpic correction = 0.22116470 (a.u.)
Entropy = 96.28759 (cal/(mol*K))

C	2.895095	0.790185	0.000000
C	1.426116	1.187253	0.000000
C	0.688431	0.000000	0.000000
C	1.426116	-1.187253	0.000000
C	2.895095	-0.790185	0.000000
C	0.717446	2.370955	0.000000
C	-0.688431	0.000000	0.000000
C	-1.426116	1.187253	0.000000
C	-0.717446	2.370955	0.000000
C	-2.895095	0.790185	0.000000
H	-3.416821	1.180784	0.875916
C	-2.895095	-0.790185	0.000000
C	-1.426116	-1.187253	0.000000
C	-0.717446	-2.370955	0.000000
C	0.717446	-2.370955	0.000000
H	1.226990	-3.327234	0.000000
H	-1.226990	-3.327234	0.000000
H	1.226990	3.327234	0.000000
H	3.416821	1.180784	0.875916
H	3.416821	-1.180784	0.875916
H	-1.226990	3.327234	0.000000
H	-3.416821	-1.180784	-0.875916
H	-3.416821	-1.180784	0.875916
H	-3.416821	1.180784	-0.875916
H	3.416821	1.180784	-0.875916
H	3.416821	-1.180784	-0.875916

569-41-5-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.733130621
(a.u.)
E(HF/CC-PVTZ) = -461.5605987
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.630160903830
T1 (CC-PVTZ)= 0.009838738
T2 (CC-PVTZ)= 0.034328
E(HF/CC-PVQZ) = -461.58849152
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.761933007801
E(HF/TZ-AUG) = -461.56378473
E(DLPNO-CCSD(T)/TZ-AUG) = -463.661211132
E(HF/TZ-CORE) = -461.56396492
E(DLPNO-CCSD(T)/TZ-CORE) = -464.239285775
E(HF/TZ-IT) = -461.5605987
E(DLPNO-CCSD(T)/TZ-IT) = -463.635692963
T1 (CC-PVQZ)= 0.009913631
T2 (CC-PVQZ)= 0.037685
E(HF/CBS) = -461.595288242
E(DLPNO-CCSD(T)/CBS) = -463.844533532
Enthalpic correction = 0.20766858 (a.u.)
Entropy = 98.54241 (cal/(mol*K))

C	-1.280154	0.832409	-0.000002
C	-1.479171	2.329193	0.000003
C	0.000000	0.175602	0.000002

C	-2.428551	0.070000	-0.000003
C	0.000000	-1.263519	0.000002
C	1.280154	0.832409	0.000002
C	-2.413175	-1.333565	-0.000002
C	1.215738	-1.986075	0.000002
C	-1.215737	-1.986076	0.000001
C	1.479170	2.329194	-0.000002
C	2.428551	0.070001	-0.000002
C	2.413176	-1.333564	-0.000001
H	-2.545586	2.550183	-0.000005
H	-1.047572	2.807174	0.878546
H	-1.047555	2.807185	-0.878526
H	-3.384544	0.578720	-0.000005
H	-3.345560	-1.883217	-0.000004
H	1.171216	-3.068069	0.000003
H	-1.171214	-3.068070	0.000003
H	2.545584	2.550185	0.000005
H	1.047568	2.807176	-0.878543
H	1.047555	2.807183	0.878529
H	3.384543	0.578722	-0.000005
H	3.345561	-1.883216	-0.000003

571-58-4-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.742774307 (a.u.)
E(HF/CC-PVTZ) = -461.5726009
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.639465810977
T1 (CC-PVTZ)= 0.009763675
T2 (CC-PVTZ)= 0.034394
E(HF/CC-PVQZ) = -461.60053903
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.771306601522
E(HF/TZ-AUG) = -461.57584198
E(DLPNO-CCSD(T)/TZ-AUG) = -463.67052908
E(HF/TZ-CORE) = -461.57597204
E(DLPNO-CCSD(T)/TZ-CORE) = -464.248676655
E(HF/TZ-IT) = -461.5726009
E(DLPNO-CCSD(T)/TZ-IT) = -463.644965833
T1 (CC-PVQZ)= 0.009854180
T2 (CC-PVQZ)= 0.037788
E(HF/CBS) = -461.607346793
E(DLPNO-CCSD(T)/CBS) = -463.853935225
Enthalpic correction = 0.20740063 (a.u.)
Entropy = 97.45696 (cal/(mol*K))

C	1.520451	0.850145	0.000000
C	3.018474	0.727155	-0.000001
C	0.687375	-0.308945	-0.000001
C	0.921560	2.083707	0.000002
C	-0.735709	-0.163080	0.000000
C	1.231822	-1.615602	-0.000001
C	-0.479679	2.227339	0.000002
C	-1.316345	1.140909	0.000000
C	-1.533960	-1.332080	0.000000
C	0.427207	-2.726446	0.000001
C	-2.808203	1.324197	-0.000002
C	-0.971493	-2.583074	0.000001
H	3.379088	0.187121	0.879150
H	3.482016	1.712957	-0.000015
H	3.379085	0.187099	-0.879140
H	1.539054	2.973974	0.000003
H	2.305579	-1.739320	-0.000002
H	-0.903698	3.224372	0.000002
H	-2.610470	-1.235291	0.000001
H	0.868151	-3.715025	0.000001
H	-3.270815	0.868445	-0.879128
H	-3.062338	2.383487	-0.000014
H	-3.270816	0.868465	0.879133
H	-1.603838	-3.461628	0.000003

571-61-9-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.742769508 (a.u.)
E(HF/CC-PVTZ) = -461.572513
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.639431771903
T1 (CC-PVTZ)= 0.009780046
T2 (CC-PVTZ)= 0.034618
E(HF/CC-PVQZ) = -461.60046228
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.771279814598
E(HF/TZ-AUG) = -461.57577831
E(DLPNO-CCSD(T)/TZ-AUG) = -463.670551134
E(HF/TZ-CORE) = -461.57587951
E(DLPNO-CCSD(T)/TZ-CORE) = -464.248641863
E(HF/TZ-IT) = -461.572513
E(DLPNO-CCSD(T)/TZ-IT) = -463.644932337
T1 (CC-PVQZ)= 0.009868194
T2 (CC-PVQZ)= 0.037732
E(HF/CBS) = -461.60727276
E(DLPNO-CCSD(T)/CBS) = -463.85390831
Enthalpic correction = 0.20739062 (a.u.)
Entropy = 97.48355 (cal/(mol*K))

C	1.879221	-0.165146	0.000001
C	2.940962	-1.229794	-0.000001
C	0.495596	-0.515661	0.000001
C	2.232410	1.162930	0.000000
C	-0.495597	0.515661	-0.000001
C	0.071142	-1.866565	0.000001
C	1.261118	2.180923	0.000000
C	-1.879220	0.165146	-0.000003
C	-0.071142	1.866566	0.000000
C	-1.261119	-2.180923	0.000002
C	-2.940962	1.229794	-0.000001
C	-2.232409	-1.162930	0.000000
H	3.933104	-0.780226	0.000038
H	2.864296	-1.874468	-0.879062
H	2.864252	-1.874522	0.879015
H	3.281661	1.432355	0.000002
H	0.807504	-2.657279	-0.000001
H	1.574615	3.217110	0.000002
H	-0.807504	2.657279	0.000003
H	-1.574614	-3.217110	0.000002
H	-3.933104	0.780224	-0.000054
H	-2.864244	1.874531	-0.879009
H	-2.864306	1.874458	0.879068
H	-3.281661	-1.432354	-0.000002

573-98-8-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.740619370 (a.u.)
E(HF/CC-PVTZ) = -461.56974157
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.637262780359
T1 (CC-PVTZ)= 0.009760301
T2 (CC-PVTZ)= 0.034866
E(HF/CC-PVQZ) = -461.59765065
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.769106606424
E(HF/TZ-AUG) = -461.57296936

E(DLPNO-CCSD(T)/TZ-AUG) = -463.668377555
E(HF/TZ-CORE) = -461.5731065
E(DLPNO-CCSD(T)/TZ-CORE) = -464.246517014
E(HF/TZ-IT) = -461.56974157
E(DLPNO-CCSD(T)/TZ-IT) = -463.642774921
T1 (CC-PVQZ)= 0.009846542
T2 (CC-PVQZ)= 0.037806
E(HF/CBS) = -461.604451334
E(DLPNO-CCSD(T)/CBS) = -463.851751565
Enthalpic correction = 0.20730619 (a.u.)
Entropy = 98.70679 (cal/(mol*K))

C	1.016105	0.709781	0.000000
C	1.454811	2.150095	0.000004
C	-0.381114	0.412673	0.000000
C	1.935792	-0.323707	-0.000002
C	-0.819338	-0.945424	0.000001
C	-1.372146	1.426685	-0.000002
C	3.424143	-0.078369	-0.000003
C	1.479944	-1.664415	0.000000
C	0.149441	-1.972697	0.000002
C	-2.204641	-1.231372	0.000001
C	-2.708657	1.118292	-0.000002
C	-3.133562	-0.224885	-0.000001
H	2.536461	2.246992	0.000007
H	1.076400	2.679082	-0.878370
H	1.076396	2.679077	0.878379
H	-1.072150	2.464624	-0.000003
H	3.743763	0.485474	0.879275
H	3.966464	-1.023190	-0.000030
H	3.743756	0.485520	-0.879252
H	2.214900	-2.460167	-0.000001
H	-0.177532	-3.005339	0.000003
H	-2.518135	-2.268480	0.000002
H	-3.444132	1.912677	-0.000004
H	-4.190865	-0.456209	-0.000001

575-37-1-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.743675843 (a.u.)
E(HF/CC-PVTZ) = -461.57479881
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.640016591890
T1 (CC-PVTZ)= 0.009763596
T2 (CC-PVTZ)= 0.035919
E(HF/CC-PVQZ) = -461.60271234
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.771840797899
E(HF/TZ-AUG) = -461.57798499
E(DLPNO-CCSD(T)/TZ-AUG) = -463.670917282
E(HF/TZ-CORE) = -461.57816796
E(DLPNO-CCSD(T)/TZ-CORE) = -464.249318941
E(HF/TZ-IT) = -461.57479881
E(DLPNO-CCSD(T)/TZ-IT) = -463.64549741
T1 (CC-PVQZ)= 0.009849183
T2 (CC-PVQZ)= 0.037605
E(HF/CBS) = -461.609514108
E(DLPNO-CCSD(T)/CBS) = -463.854469276
Enthalpic correction = 0.20715350 (a.u.)
Entropy = 99.11006 (cal/(mol*K))

C	1.465662	1.025175	0.000001
C	1.449827	2.528265	0.000001
C	0.246615	0.283722	0.000001
C	2.659130	0.342281	0.000000
C	0.297893	-1.141867	0.000001
C	-1.023806	0.910932	0.000000
C	2.709596	-1.066055	-0.000001
C	-0.918222	-1.865395	0.000001
C	1.551850	-1.795125	-0.000001
C	-2.194975	0.192486	0.000000
C	-2.124643	-1.221381	0.000001
C	-3.535866	0.871694	-0.000001
H	2.465209	2.922645	0.000016
H	0.935267	2.924745	-0.878994
H	0.935239	2.924746	0.878978
H	3.586803	0.901904	0.000000
H	-1.075739	1.991461	-0.000001
H	3.670286	-1.564800	-0.000003
H	-0.877154	-2.948108	0.000001
H	1.578362	-2.877971	-0.000001
H	-3.043945	-1.795262	0.000001
H	-4.120462	0.587889	-0.878873
H	-4.120466	0.587884	0.878866
H	-3.431767	1.956479	0.000002

575-41-7-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.743790322 (a.u.)
E(HF/CC-PVTZ) = -461.57512624
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.640192572302
T1 (CC-PVTZ)= 0.009863987
T2 (CC-PVTZ)= 0.035673
E(HF/CC-PVQZ) = -461.60304612
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.772001885903
E(HF/TZ-AUG) = -461.57832333
E(DLPNO-CCSD(T)/TZ-AUG) = -463.671050443
E(HF/TZ-CORE) = -461.57849615
E(DLPNO-CCSD(T)/TZ-CORE) = -464.249489865
E(HF/TZ-IT) = -461.57512624
E(DLPNO-CCSD(T)/TZ-IT) = -463.645668218
T1 (CC-PVQZ)= 0.009942893
T2 (CC-PVQZ)= 0.037760
E(HF/CBS) = -461.609849436
E(DLPNO-CCSD(T)/CBS) = -463.85461641
Enthalpic correction = 0.20716570 (a.u.)
Entropy = 99.08266 (cal/(mol*K))

C	-0.567958	1.359454	0.000000
C	-0.401245	2.853334	0.000001
C	0.572505	0.500299	0.000000
C	-1.820791	0.800934	0.000000
C	0.371883	-0.912101	0.000001
C	1.899344	0.991719	-0.000001
C	-2.035917	-0.599525	0.000001
C	-0.946079	-1.428888	0.000001
C	1.499481	-1.765641	0.000001
C	2.973262	0.137153	-0.000001
C	-3.440647	-1.133588	-0.000002
C	2.772331	-1.256492	0.000000
H	-1.371521	3.348329	0.000006
H	0.151044	3.195129	0.878951
H	0.151035	3.195130	-0.878956
H	-2.685982	1.455164	0.000001
H	2.070164	2.059241	-0.000001
H	-1.080612	-2.504551	0.000002
H	1.338142	-2.836979	0.000001
H	3.980212	0.534285	-0.000002
H	-3.450723	-2.223274	0.000020
H	-3.992017	-0.789701	0.878919
H	-3.992000	-0.789736	-0.878947
H	3.625243	-1.922995	-0.000001

575-43-9-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.743694242 (a.u.)
E(HF/CC-PVTZ) = -461.5749849
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.639993535475
T1 (CC-PVTZ)= 0.009842906
T2 (CC-PVTZ)= 0.035789
E(HF/CC-PVQZ) = -461.60290532
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.771821399630
E(HF/TZ-AUG) = -461.57817656
E(DLPNO-CCSD(T)/TZ-AUG) = -463.670867008
E(HF/TZ-CORE) = -461.57835603
E(DLPNO-CCSD(T)/TZ-CORE) = -464.249305249
E(HF/TZ-IT) = -461.5749849
E(DLPNO-CCSD(T)/TZ-IT) = -463.645472713
T1 (CC-PVQZ)= 0.009921853
T2 (CC-PVQZ)= 0.037644
E(HF/CBS) = -461.609708767
E(DLPNO-CCSD(T)/CBS) = -463.854449198
Enthalpic correction = 0.20715409 (a.u.)
Entropy = 99.17981 (cal/(mol*K))

C	1.874290	-0.605041	0.000003
C	2.480028	-1.980812	0.000003
C	0.458696	-0.433213	0.000001
C	2.678519	0.510106	0.000002
C	-0.090250	0.883534	-0.000001
C	-0.444433	-1.524539	-0.000003
C	2.138367	1.811792	-0.000001
C	-1.496021	1.047158	-0.000003
C	0.782736	1.996762	-0.000002
C	-1.799193	-1.326250	-0.000006
C	-2.353916	-0.023909	-0.000004
C	-3.846158	0.154415	0.000007
H	3.567660	-1.921144	0.000031
H	2.174895	-2.554134	0.879036
H	2.174939	-2.554112	-0.879060
H	3.754684	0.386003	0.000005
H	-0.057759	-2.534170	-0.000007
H	2.805349	2.664466	-0.000002
H	-1.894136	2.055755	-0.000005
H	0.359886	2.993951	-0.000004
H	-2.465622	-2.181004	-0.000011
H	-4.297980	-0.312514	-0.878888
H	-4.297940	-0.312312	0.879032
H	-4.119969	1.209202	-0.000105

581-40-8-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.744092265 (a.u.)
E(HF/CC-PVTZ) = -461.57513827
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.640266169857
T1 (CC-PVTZ)= 0.009745445
T2 (CC-PVTZ)= 0.035056
E(HF/CC-PVQZ) = -461.60303275
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.772148957278
E(HF/TZ-AUG) = -461.57827744
E(DLPNO-CCSD(T)/TZ-AUG) = -463.671099553
E(HF/TZ-CORE) = -461.57851029
E(DLPNO-CCSD(T)/TZ-CORE) = -464.249612068
E(HF/TZ-IT) = -461.57513827
E(DLPNO-CCSD(T)/TZ-IT) = -463.645738004
T1 (CC-PVQZ)= 0.009827830
T2 (CC-PVQZ)= 0.037757
E(HF/CBS) = -461.609829876
E(DLPNO-CCSD(T)/CBS) = -463.854829443
Enthalpic correction = 0.20708413 (a.u.)
Entropy = 98.09425 (cal/(mol*K))

C	1.690560	0.714241	0.000001
C	2.989992	1.469524	0.000000
C	0.493580	1.385368	0.000001
C	1.690560	-0.714241	0.000002
C	-0.749377	0.711776	0.000000
C	2.989992	-1.469524	-0.000002
C	0.493580	-1.385368	0.000002
C	-0.749377	-0.711776	0.000001
C	-1.987020	1.396497	0.000000
C	-1.987020	-1.396497	0.000000
C	-3.171116	0.705419	-0.000001
C	-3.171116	-0.705419	-0.000001
H	3.595404	1.226027	0.877063
H	3.595401	1.226026	-0.877065
H	2.815052	2.544673	-0.000001
H	0.490693	2.469737	0.000001
H	2.815052	-2.544673	0.000026
H	3.595387	-1.226047	-0.877083
H	3.595418	-1.226006	0.877046
H	0.490693	-2.469737	0.000003
H	-1.984167	2.479963	0.000000
H	-1.984167	-2.479963	0.000000
H	-4.112100	1.240396	-0.000001
H	-4.112100	-1.240396	-0.000001

581-42-0-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.744243288 (a.u.)
E(HF/CC-PVTZ) = -461.57680236
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.640236037672
T1 (CC-PVTZ)= 0.009738101
T2 (CC-PVTZ)= 0.034921
E(HF/CC-PVQZ) = -461.60468792
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.772046842731
E(HF/TZ-AUG) = -461.57990588
E(DLPNO-CCSD(T)/TZ-AUG) = -463.670890007
E(HF/TZ-CORE) = -461.58017744
E(DLPNO-CCSD(T)/TZ-CORE) = -464.249626789
E(HF/TZ-IT) = -461.57680236
E(DLPNO-CCSD(T)/TZ-IT) = -463.645695243
T1 (CC-PVQZ)= 0.009815194
T2 (CC-PVQZ)= 0.037554
E(HF/CBS) = -461.611482873
E(DLPNO-CCSD(T)/CBS) = -463.854679137
Enthalpic correction = 0.20695349 (a.u.)
Entropy = 100.75307 (cal/(mol*K))

C	2.542948	-0.076758	0.000000
C	4.000719	-0.443137	0.000000
C	1.556949	-1.032239	0.000000
C	2.161238	1.288292	0.000000
C	0.184971	-0.687290	0.000000
C	0.843872	1.658895	0.000000
C	-0.184971	0.687290	0.000000
C	-0.843872	-1.658895	0.000000
C	-1.556949	1.032239	0.000000
C	-2.161238	-1.288291	0.000000
C	-2.542948	0.076758	0.000000

C	-4.000719	0.443137	0.000000
H	4.508500	-0.037793	-0.878969
H	4.508497	-0.037803	0.878976
H	4.138220	-1.524208	-0.000006
H	1.824816	-2.083001	0.000000
H	2.933789	2.048447	-0.000001
H	0.571882	2.707726	0.000000
H	-0.571882	-2.707726	0.000000
H	-1.824816	2.083001	0.000001
H	-2.933789	-2.048447	0.000001
H	-4.508497	0.037805	-0.878976
H	-4.508501	0.037793	0.878968
H	-4.138219	1.524208	0.000007

5821-51-2-C20H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -768.495497402 (a.u.)
E(HF/CC-PVTZ) = -763.41334417
E(DLPNO-CCSD(T)/CC-PVTZ) = -766.689396070950
T1 (CC-PVTZ)= 0.010472784
T2 (CC-PVTZ)= 0.041275
E(HF/CC-PVQZ) = -763.45826184
E(DLPNO-CCSD(T)/CC-PVQZ) = -766.902831331558
E(HF/TZ-AUG) = -763.41875405
E(DLPNO-CCSD(T)/TZ-AUG) = -766.739821591
E(HF/TZ-CORE) = -763.4189723
E(DLPNO-CCSD(T)/TZ-CORE) = -767.705886528
E(HF/TZ-IT) = -763.41334417
E(DLPNO-CCSD(T)/TZ-IT) = -766.700805776
T1 (CC-PVQZ)= 0.010492048
T2 (CC-PVQZ)= 0.040340
E(HF/CBS) = -763.469207055
E(DLPNO-CCSD(T)/CBS) = -767.036748842
Enthalpic correction = 0.23715873 (a.u.)
Entropy = 104.68252 (cal/(mol*K))

C	-0.216355	-1.185237	0.648544
C	1.060370	-0.572036	0.648599
C	0.871693	0.831697	0.648569
C	-0.521628	1.086057	0.648554
C	-1.194074	-0.160481	0.648528
C	-0.443927	-2.431936	0.102154
C	2.175754	-1.173727	0.102264
C	-2.450087	-0.329301	0.102186
C	-1.070304	2.228422	0.102161
C	1.788605	1.706539	0.102189
C	0.748165	-3.153522	-0.267486
C	1.993796	-2.555257	-0.267442
C	3.230395	-0.262964	-0.267408
C	3.046302	1.106572	-0.267461
C	1.248340	2.991041	-0.267404
C	-0.111055	3.239177	-0.267444
C	-1.814107	-2.685832	-0.267406
C	-2.768013	-1.686049	-0.267399
C	-3.114966	0.895332	-0.267426
C	-2.458884	2.111505	-0.267450
H	0.660047	-4.164297	-0.647748
H	2.837842	-3.118315	-0.647687
H	4.164463	-0.659125	-0.647675
H	3.842621	1.735298	-0.647738
H	1.913762	3.756998	-0.647603
H	-0.462933	4.190830	-0.647661
H	-2.088814	-3.662576	-0.647590
H	-3.756585	-1.914607	-0.647553
H	-4.128791	0.854748	-0.647609
H	-2.981732	2.981046	-0.647663

582-16-1-C12H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -464.744311372 (a.u.)
E(HF/CC-PVTZ) = -461.57696389
E(DLPNO-CCSD(T)/CC-PVTZ) = -463.640280381393
T1 (CC-PVTZ)= 0.009861917
T2 (CC-PVTZ)= 0.035848
E(HF/CC-PVQZ) = -461.6048558
E(DLPNO-CCSD(T)/CC-PVQZ) = -463.772111715165
E(HF/TZ-AUG) = -461.58007739
E(DLPNO-CCSD(T)/TZ-AUG) = -463.670955811
E(HF/TZ-CORE) = -461.58033804
E(DLPNO-CCSD(T)/TZ-CORE) = -464.249682568
E(HF/TZ-IT) = -461.57696389
E(DLPNO-CCSD(T)/TZ-IT) = -463.645738119
T1 (CC-PVQZ)= 0.009942679
T2 (CC-PVQZ)= 0.037524
E(HF/CBS) = -461.6116523
E(DLPNO-CCSD(T)/CBS) = -463.854755903
Enthalpic correction = 0.20693038 (a.u.)
Entropy = 100.76460 (cal/(mol*K))

C	2.436960	-0.423047	0.000000
C	3.751455	-1.151998	0.000000
C	1.239263	-1.094634	0.000000
C	2.420680	0.994328	0.000000
C	0.000000	-0.411058	0.000000
C	1.241920	1.689376	0.000000
C	0.000000	1.012523	0.000000
C	-1.239263	-1.094634	0.000000
C	-1.241919	1.689376	0.000000
C	-2.436960	-0.423046	0.000000
C	-2.420680	0.994328	0.000000
C	-3.751455	-1.151998	0.000000
H	4.346143	-0.890257	-0.878934
H	4.346144	-0.890255	0.878933
H	3.606693	-2.232087	0.000001
H	1.230356	-2.178931	0.000000
H	3.362704	1.530061	0.000000
H	1.246322	2.772921	0.000000
H	-1.230357	-2.178931	0.000000
H	-1.246323	2.772921	0.000000
H	-3.362703	1.530062	0.000000
H	-4.346139	-0.890262	0.878939
H	-4.346147	-0.890251	-0.878929
H	-3.606692	-2.232088	-0.000007

594-11-60_C4H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -157.286818242 (a.u.)
E(HF/CC-PVTZ) = -156.15107757
E(DLPNO-CCSD(T)/CC-PVTZ) = -156.911917893252
T1 (CC-PVTZ)= 0.007665910
T2 (CC-PVTZ)= 0.035234
E(HF/CC-PVQZ) = -156.1609841
E(DLPNO-CCSD(T)/CC-PVQZ) = -156.958188327886
E(HF/TZ-AUG) = -156.15191892
E(DLPNO-CCSD(T)/TZ-AUG) = -156.922231885
E(HF/TZ-CORE) = -156.15219595

E(DLPNO-CCSD(T)/TZ-CORE) = -157.114383848
E(HF/TZ-IT) = -156.15107757
E(DLPNO-CCSD(T)/TZ-IT) = -156.912835055
T1 (CC-PVQZ)= 0.008032606
T2 (CC-PVQZ)= 0.030851
E(HF/CBS) = -156.163398052
E(DLPNO-CCSD(T)/CBS) = -156.987138102
Enthalpic correction = 0.11140887 (a.u.)
Entropy = 67.90528 (cal/(mol*K))

C	-0.346502	0.402265	0.000000
C	-0.346502	-0.897760	0.753731
C	-0.346502	-0.897760	-0.753731
H	-1.249898	-1.201989	1.264949
H	0.567899	-1.183949	1.257771
H	-1.249898	-1.201989	-1.264949
H	0.567899	-1.183949	-1.257771
H	-1.286817	0.942444	0.000000
C	0.879951	1.278930	0.000000
H	1.789152	0.673043	0.000000
H	0.909500	1.921168	0.883638
H	0.909500	1.921168	-0.883638

602-55-1_C20H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -770.938378648 (a.u.)
E(HF/CC-PVTZ) = -765.77736631
E(DLPNO-CCSD(T)/CC-PVTZ) = -769.114396702220
T1 (CC-PVTZ)= 0.010210318
T2 (CC-PVTZ)= 0.039273
E(HF/CC-PVQZ) = -765.82296769
E(DLPNO-CCSD(T)/CC-PVQZ) = -769.329667656449
E(HF/TZ-AUG) = -765.78288059
E(DLPNO-CCSD(T)/TZ-AUG) = -769.165255416
E(HF/TZ-CORE) = -765.78304108
E(DLPNO-CCSD(T)/TZ-CORE) = -770.130529286
E(HF/TZ-IT) = -765.77736631
E(DLPNO-CCSD(T)/TZ-IT) = -769.124751737
T1 (CC-PVQZ)= 0.010240061
T2 (CC-PVQZ)= 0.041280
E(HF/CBS) = -765.834079507
E(DLPNO-CCSD(T)/CBS) = -769.464592406
Enthalpic correction = 0.28131242 (a.u.)
Entropy = 127.91545 (cal/(mol*K))

C	-0.107692	0.000004	0.000000
C	0.590910	1.219517	-0.013374
C	0.590891	-1.219524	0.013374
C	-1.596084	0.000013	0.000003
C	2.030309	1.214800	-0.010666
C	-0.075092	2.481021	-0.039064
C	2.030289	-1.214831	0.010665
C	-0.075131	-2.481012	0.039065
C	-2.305976	-0.177650	-1.187320
C	-2.305977	0.177679	1.187322
C	2.709950	-0.000020	-0.000001
C	2.723805	2.459105	-0.022797
C	0.627646	3.649651	-0.051836
C	2.723765	-2.459144	0.022796
C	0.627588	-3.649656	0.051837
C	-3.695482	-0.177324	-1.188487
C	-3.695484	0.177371	1.188484
C	2.047055	3.641450	-0.041278
C	2.046994	-3.641479	0.041278
C	-4.394114	0.000029	-0.000002
H	-1.155491	2.497903	-0.050433
H	-1.155531	-2.497878	0.050433
H	-1.760742	-0.316230	-2.112224
H	-1.760748	0.316249	2.112230
H	3.793900	-0.000030	-0.000001
H	3.806932	2.443331	-0.018199
H	0.101414	4.595333	-0.072248
H	3.806892	-2.443389	0.018198
H	0.101338	-4.595328	0.072250
H	-4.232349	-0.314771	-2.118404
H	-4.232350	0.314822	2.118401
H	2.587110	4.579389	-0.050713
H	2.587034	-4.579427	0.050714
H	-5.476420	0.000038	-0.000006

604-83-1-C16H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -618.453022690 (a.u.)
E(HF/CC-PVTZ) = -614.26308542
E(DLPNO-CCSD(T)/CC-PVTZ) = -616.988518449873
T1 (CC-PVTZ)= 0.009847615
T2 (CC-PVTZ)= 0.035794
E(HF/CC-PVQZ) = -614.29990119
E(DLPNO-CCSD(T)/CC-PVQZ) = -617.162804916967
E(HF/TZ-AUG) = -614.26737709
E(DLPNO-CCSD(T)/TZ-AUG) = -617.029982538
E(HF/TZ-CORE) = -614.26756334
E(DLPNO-CCSD(T)/TZ-CORE) = -617.800792886
E(HF/TZ-IT) = -614.26308542
E(DLPNO-CCSD(T)/TZ-IT) = -616.996215668
T1 (CC-PVQZ)= 0.009914621
T2 (CC-PVQZ)= 0.037790
E(HF/CBS) = -614.308872192
E(DLPNO-CCSD(T)/CBS) = -617.272092374
Enthalpic correction = 0.25582506 (a.u.)
Entropy = 113.40977 (cal/(mol*K))

C	-0.684411	1.610776	0.000003
C	-1.508238	2.872882	0.000007
C	-1.412826	0.358524	0.000003
C	0.684409	1.610777	-0.000002
C	-0.724026	-0.880742	-0.000001
C	-2.824835	0.339343	0.000004
C	1.508232	2.872885	-0.000008
C	1.412826	0.358526	-0.000002
C	0.724028	-0.880741	0.000002
C	-1.474550	-2.072135	-0.000007
C	-3.532899	-0.840351	0.000000
C	2.824836	0.339346	-0.000004
C	1.474553	-2.072133	0.000007
C	-2.850295	-2.060442	-0.000007
C	3.532900	-0.840348	0.000000
C	2.850298	-2.060440	0.000006
H	-2.157128	2.914466	-0.878138
H	-2.157125	2.914462	0.878154
H	-0.906677	3.773865	0.000008
H	-3.371147	1.269832	0.000007
H	2.157119	2.914467	-0.878154
H	0.906670	3.773868	-0.000010
H	2.157122	2.914473	0.878137
H	-0.967705	-3.025351	-0.000015
H	-4.615112	-0.821333	0.000001
H	3.371148	1.269835	-0.000007
H	0.967708	-3.025349	0.000015
H	-3.399300	-2.993131	-0.000012
H	4.615114	-0.821329	-0.000002
H	3.399304	-2.993128	0.000011

605-02-7_C16H12

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -617.231687916
(a.u.)
E(HF/CC-PVTZ) = -613.09181758
E(DLPNO-CCSD(T)/CC-PVTZ) = -615.770243462409
T1 (CC-PVTZ)= 0.010002031
T2 (CC-PVTZ)= 0.039327
E(HF/CC-PVQZ) = -613.12856393
E(DLPNO-CCSD(T)/CC-PVQZ) = -615.943117676277
E(HF/TZ-AUG) = -613.09623319
E(DLPNO-CCSD(T)/TZ-AUG) = -615.810396319
E(HF/TZ-CORE) = -613.09637882
E(DLPNO-CCSD(T)/TZ-CORE) = -616.58317633
E(HF/TZ-IT) = -613.09181758
E(DLPNO-CCSD(T)/TZ-IT) = -615.778192094
T1 (CC-PVQZ)= 0.010043937
T2 (CC-PVQZ)= 0.041054
E(HF/CBS) = -613.137518017
E(DLPNO-CCSD(T)/CBS) = -616.051408312
Enthalpic correction = 0.23347115 (a.u.)
Entropy = 108.39865 (cal/(mol*K))

 C    -0.072986     0.745762     0.063695
 C     1.038707    -0.147179    -0.033572
 C     0.159075     2.097588     0.191846
 C    -1.471627     0.253105     0.034629
 C     2.362764     0.385805     0.046741
 C     0.890592    -1.540956    -0.242820
 C     1.464819     2.618708     0.258868
 C    -2.368553     0.731385    -0.922774
 C    -1.934970    -0.663790     0.982291
 C     2.544347     1.779960     0.198596
 C     3.467611    -0.494447    -0.043652
 C     1.982701    -2.364206    -0.334495
 C    -3.690051     0.302753    -0.937137
 C    -3.255841    -1.090236     0.971004
 C     3.286157    -1.839431    -0.224391
 C    -4.138195    -0.610177     0.009414
 H    -0.686156     2.769296     0.269399
 H    -0.102390    -1.954025    -0.343322
 H     1.606907     3.685782     0.371425
 H    -2.018774     1.434939    -1.667366
 H    -1.255253    -1.030703     1.740256
 H     3.552487     2.170990     0.260752
 H     4.465792    -0.079392     0.026411
 H     1.844528    -3.425069    -0.499305
 H    -4.368671     0.679863    -1.691571
 H    -3.598687    -1.794382     1.718389
 H     4.140352    -2.500506    -0.293977
 H    -5.167439    -0.944661    -0.000560
```

612-71-5-C24H18

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -925.849308806
(a.u.)
E(HF/CC-PVTZ) = -919.63914192
E(DLPNO-CCSD(T)/CC-PVTZ) = -923.659304704791
T1 (CC-PVTZ)= 0.009896804
T2 (CC-PVTZ)= 0.038973
E(HF/CC-PVQZ) = -919.69421319
E(DLPNO-CCSD(T)/CC-PVQZ) = -923.918640857874
E(HF/TZ-AUG) = -919.64569793
E(DLPNO-CCSD(T)/TZ-AUG) = -923.719848941
E(HF/TZ-CORE) = -919.64600319
E(DLPNO-CCSD(T)/TZ-CORE) = -924.878898601
E(HF/TZ-IT) = -919.63914192
E(DLPNO-CCSD(T)/TZ-IT) = -923.670985819
T1 (CC-PVQZ)= 0.009975008
T2 (CC-PVQZ)= 0.040691
E(HF/CBS) = -919.707632561
E(DLPNO-CCSD(T)/CBS) = -924.081118387
Enthalpic correction = 0.35142231 (a.u.)
Entropy = 146.11209 (cal/(mol*K))

 C    -0.010366     1.404273     0.000006
 C     1.194442     0.701606    -0.038233
 C    -1.204645     0.683851     0.038213
 C    -0.021323     2.883409     0.000025
 C     1.220791    -0.693369    -0.039176
 C    -1.210357    -0.711359     0.039018
 C     0.936917     3.608397     0.714875
 C    -0.990200     3.594103    -0.714844
 C     0.010270    -1.385552    -0.000126
 C     2.505997    -1.423705    -0.097924
 C    -2.484627    -1.460608     0.097803
 C     0.927000     4.996264     0.715595
 C    -1.000858     4.981962    -0.715591
 C     3.622210    -0.967107     0.609477
 C     2.637045    -2.588324    -0.860344
 C    -2.598389    -2.627073     0.860176
 C    -3.607555    -1.020483    -0.609416
 C    -0.042125     5.689619    -0.000002
 C     4.828426    -1.651689     0.557520
 C     3.843147    -3.273161    -0.913904
 C    -3.794264    -3.329604     0.913897
 C    -4.803549    -1.722762    -0.557297
 C     4.944491    -2.808168    -0.204817
 C    -4.902453    -2.880851     0.205013
 H     2.123910     1.248594    -0.117842
 H    -2.142101     1.217009     0.117923
 H     1.680706     3.077669     1.294655
 H    -1.726023     3.052408    -1.294642
 H     0.018279    -2.466922    -0.000189
 H     1.673118     5.537711     1.283073
 H    -1.754918     5.512279    -1.283083
 H     3.535127    -0.080922     1.224464
 H     1.792527    -2.944998    -1.435313
 H    -1.748634    -2.971296     1.435017
 H    -3.533654    -0.133083    -1.224377
 H    -0.050146     6.771799    -0.000010
 H     5.677717    -1.285416     1.120064
 H     3.925243    -4.167844    -1.517796
 H    -3.863075    -4.225427     1.517759
 H    -5.658231    -1.369012    -1.119692
 H     5.884940    -3.342052    -0.246176
 H    -5.834934    -3.428524     0.246501
```

6232-48-0-C16H12

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -617.243823803
(a.u.)
E(HF/CC-PVTZ) = -613.10389087
E(DLPNO-CCSD(T)/CC-PVTZ) = -615.786383663675
T1 (CC-PVTZ)= 0.010069151
T2 (CC-PVTZ)= 0.033261
E(HF/CC-PVQZ) = -613.14027785
E(DLPNO-CCSD(T)/CC-PVQZ) = -615.959389961225
```

```
E(HF/TZ-AUG) = -613.10806424
E(DLPNO-CCSD(T)/TZ-AUG) = -615.827093112
E(HF/TZ-CORE) = -613.10837484
E(DLPNO-CCSD(T)/TZ-CORE) = -616.598910496
E(HF/TZ-IT) = -613.10389087
E(DLPNO-CCSD(T)/TZ-IT) = -615.794207642
T1 (CC-PVQZ)= 0.010107122
T2 (CC-PVQZ)= 0.037726
E(HF/CBS) = -613.149144368
E(DLPNO-CCSD(T)/CBS) = -616.067951657
Enthalpic correction = 0.23390525 (a.u.)
Entropy = 104.73475 (cal/(mol*K))

 C     3.617041     0.975361     0.000004
 C     3.910827    -0.395104    -0.000002
 C     2.307062     1.399671     0.000006
 C     1.239665     0.484087     0.000002
 C     2.888138    -1.315002    -0.000005
 C    -0.638704     2.221026    -0.000004
 C    -0.147276     0.900039     0.000002
 C    -2.000574     2.462713    -0.000005
 C     1.537606    -0.912208    -0.000003
 C    -2.947538     1.419777    -0.000002
 C    -1.112145    -0.115774     0.000004
 C     0.489856    -1.897408    -0.000004
 C    -2.493274     0.121002     0.000003
 C    -0.806242    -1.504351     0.000002
 C    -3.228755    -1.201594     0.000003
 C    -2.103652    -2.285015     0.000001
 H     4.420199     1.700795     0.000008
 H     4.940798    -0.727860    -0.000003
 H     2.095471     2.460194     0.000012
 H     3.111053    -2.375232    -0.000008
 H     0.042461     3.060724    -0.000009
 H    -2.350617     3.487356    -0.000010
 H    -4.005561     1.651003    -0.000004
 H     0.770665    -2.944298    -0.000009
 H    -3.874251    -1.295287     0.875716
 H    -3.874256    -1.295285    -0.875705
 H    -2.174087    -2.932712    -0.875810
 H    -2.174086    -2.932714     0.875810
```

624-64-60_C4H8

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -157.302938365
(a.u.)
E(HF/CC-PVTZ) = -156.16781176
E(DLPNO-CCSD(T)/CC-PVTZ) = -156.924534807245
T1 (CC-PVTZ)= 0.009332957
T2 (CC-PVTZ)= 0.059856
E(HF/CC-PVQZ) = -156.177898
E(DLPNO-CCSD(T)/CC-PVQZ) = -156.970927496922
E(HF/TZ-AUG) = -156.16896389
E(DLPNO-CCSD(T)/TZ-AUG) = -156.935093301
E(HF/TZ-CORE) = -156.16897286
E(DLPNO-CCSD(T)/TZ-CORE) = -157.127131402
E(HF/TZ-IT) = -156.16781176
E(DLPNO-CCSD(T)/TZ-IT) = -156.925591069
T1 (CC-PVQZ)= 0.009627347
T2 (CC-PVQZ)= 0.058193
E(HF/CBS) = -156.180355742
E(DLPNO-CCSD(T)/CBS) = -156.999879135
Enthalpic correction = 0.11063434 (a.u.)
Entropy = 70.24350 (cal/(mol*K))

 C    -0.323526     0.579987     0.000000
 C     0.323526    -0.579987     0.000000
 H    -1.411701     0.568590     0.000000
 H     1.411701    -0.568590     0.000000
 C     0.323526     1.929103     0.000000
 C    -0.323526    -1.929103     0.000000
 H     1.411647     1.848653     0.000000
 H     0.025645     2.510971     0.877363
 H     0.025645     2.510971    -0.877363
 H    -1.411647    -1.848653     0.000000
 H    -0.025645    -2.510971     0.877363
 H    -0.025645    -2.510971    -0.877363
```

630-76-2_C25H20

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -965.155704890
(a.u.)
E(HF/CC-PVTZ) = -958.63956485
E(DLPNO-CCSD(T)/CC-PVTZ) = -962.876149851844
T1 (CC-PVTZ)= 0.009785775
T2 (CC-PVTZ)= 0.037631
E(HF/CC-PVQZ) = -958.69694692
E(DLPNO-CCSD(T)/CC-PVQZ) = -963.146443049922
E(HF/TZ-AUG) = -958.64665765
E(DLPNO-CCSD(T)/TZ-AUG) = -962.943004844
E(HF/TZ-CORE) = -958.64674698
E(DLPNO-CCSD(T)/TZ-CORE) = -964.145725574
E(HF/TZ-IT) = -958.63956485
E(DLPNO-CCSD(T)/TZ-IT) = -962.888231619
T1 (CC-PVQZ)= 0.009828280
T2 (CC-PVQZ)= 0.037853
E(HF/CBS) = -958.710929371
E(DLPNO-CCSD(T)/CBS) = -963.31579308
Enthalpic correction = 0.38029594 (a.u.)
Entropy = 149.58669 (cal/(mol*K))

 C     0.853237    -1.430873    -1.982857
 C     1.740529    -2.364139    -2.515462
 C     2.725996    -2.930088    -1.722615
 C     0.933325    -1.046853    -0.648525
 C     1.947236    -1.611076     0.134016
 C     0.000006     0.000003    -0.000011
 C     2.826595    -2.544823    -0.388914
 C    -2.826407    -0.389067     2.544972
 C    -1.947143     0.133911     1.611161
 C    -0.933183    -0.648553     1.046925
 C    -2.725655    -1.722742     2.930289
 C    -1.740140    -2.515517     2.364320
 C    -0.852947    -1.982864     1.430988
 C     0.933195     1.046982     0.648475
 C     1.947044     1.611293    -0.134078
 C     2.826307     2.545142     0.388835
 C     0.853072     1.431007     1.982803
 C     1.740268     2.364374     2.515390
 C     2.725670     2.930419     1.722528
 C    -2.726023     1.722402    -2.930178
 C    -1.740633     2.515323    -2.364200
 C    -0.853326     1.982783    -1.430910
 C    -2.826536     0.388694    -2.544915
 C    -1.947163    -0.134172    -1.611145
 C    -0.933320     0.648442    -1.046902
 H     0.105644    -0.996446    -2.628117
 H     1.656794    -2.639951    -3.559013
 H     3.415262    -3.654500    -2.136758
 H     2.052395    -1.303706     1.165781
 H     3.598260    -2.966145     0.242759
 H    -3.598113     0.242548     2.966302
 H    -2.052420     1.165653     1.303750
 H    -3.414842    -2.136923     3.654753
```

H	-1.656288	-3.559048	2.640171
H	-0.105314	-2.628068	0.996545
H	2.052235	1.303915	-1.165839
H	3.597924	2.966533	-0.242850
H	0.105530	0.996501	2.628071
H	1.656509	2.640191	3.558938
H	3.414857	3.654914	2.136656
H	-3.415302	2.136494	-3.654606
H	-1.656969	3.558880	-2.640006
H	-0.105795	2.628098	-0.996457
H	-3.598145	-0.243035	-2.966254
H	-2.052256	-1.165944	-1.303775

641-48-5-C16H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -617.234260547 (a.u.)
E(HF/CC-PVTZ) = -613.09118103
E(DLPNO-CCSD(T)/CC-PVTZ) = -615.776030459082
T1 (CC-PVTZ)= 0.010439750
T2 (CC-PVTZ)= 0.036161
E(HF/CC-PVQZ) = -613.12760628
E(DLPNO-CCSD(T)/CC-PVQZ) = -615.949072568701
E(HF/TZ-AUG) = -613.09542507
E(DLPNO-CCSD(T)/TZ-AUG) = -615.816914539
E(HF/TZ-CORE) = -613.09567075
E(DLPNO-CCSD(T)/TZ-CORE) = -616.588528771
E(HF/TZ-IT) = -613.09118103
E(DLPNO-CCSD(T)/TZ-IT) = -615.784048726
T1 (CC-PVQZ)= 0.010464490
T2 (CC-PVQZ)= 0.037616
E(HF/CBS) = -613.136482123
E(DLPNO-CCSD(T)/CBS) = -616.057641796
Enthalpic correction = 0.23370001 (a.u.)
Entropy = 104.14743 (cal/(mol*K))

C	-0.517434	2.396065	-0.000002
C	-2.073270	2.247376	0.000003
C	-2.321168	0.754032	0.000001
C	-3.462518	0.007352	-0.000001
C	-3.353555	-1.416735	-0.000001
C	-2.146654	-2.064390	-0.000001
C	-0.931145	-1.318507	0.000000
C	0.370150	-1.821085	0.000001
C	1.477588	-0.960391	0.000001
C	2.807250	-1.470968	0.000001
C	3.888466	-0.638841	0.000000
C	3.714218	0.769314	-0.000001
C	2.460317	1.307852	-0.000001
C	1.305552	0.477524	0.000000
C	0.001557	0.976108	0.000000
C	-1.068704	0.093773	0.000001
H	-0.167778	2.948666	-0.875398
H	-0.167772	2.948672	0.875388
H	-2.518723	2.722906	0.875872
H	-2.518730	2.722911	-0.875859
H	-4.443577	0.465906	-0.000001
H	-4.264932	-2.001720	-0.000002
H	-2.108088	-3.146653	-0.000001
H	0.539527	-2.891536	0.000001
H	2.944876	-2.545518	0.000002
H	4.889444	-1.050825	0.000001
H	4.583641	1.413968	-0.000002
H	2.328226	2.382359	-0.000002

643-58-3-C13H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -502.854862936 (a.u.)
E(HF/CC-PVTZ) = -499.44506013
E(DLPNO-CCSD(T)/CC-PVTZ) = -501.662304343052
T1 (CC-PVTZ)= 0.009696382
T2 (CC-PVTZ)= 0.039415
E(HF/CC-PVQZ) = -499.47531121
E(DLPNO-CCSD(T)/CC-PVQZ) = -501.804329763853
E(HF/TZ-AUG) = -499.44864701
E(DLPNO-CCSD(T)/TZ-AUG) = -501.695392623
E(HF/TZ-CORE) = -499.44876791
E(DLPNO-CCSD(T)/TZ-CORE) = -502.322639988
E(HF/TZ-IT) = -499.44506013
E(DLPNO-CCSD(T)/TZ-IT) = -501.668221788
T1 (CC-PVQZ)= 0.009801802
T2 (CC-PVQZ)= 0.041237
E(HF/CBS) = -499.482682576
E(DLPNO-CCSD(T)/CBS) = -501.893266189
Enthalpic correction = 0.21379468 (a.u.)
Entropy = 103.22931 (cal/(mol*K))

C	0.864829	2.240782	0.600569
C	1.462443	0.909195	0.226865
C	0.669469	-0.215637	-0.061434
C	2.850296	0.771806	0.192271
C	-0.813894	-0.163048	-0.045268
C	1.291486	-1.431182	-0.359574
C	3.458131	-0.436382	-0.118813
C	-1.539783	-1.040797	0.763664
C	-1.519728	0.732095	-0.852316
C	2.672968	-1.547865	-0.394028
C	-2.928687	-1.019506	0.772352
C	-2.907864	0.752076	-0.848861
C	-3.618163	-0.122048	-0.033877
H	1.581311	2.831152	1.171898
H	0.592550	2.824217	-0.282321
H	-0.039913	2.123381	1.196343
H	3.465086	1.632581	0.427470
H	0.672225	-2.290665	-0.582981
H	4.537908	-0.509839	-0.138244
H	-1.005549	-1.734995	1.399809
H	-0.974806	1.404952	-1.500992
H	3.131132	-2.498191	-0.635566
H	-3.472381	-1.702970	1.412096
H	-3.436299	1.448127	-1.487843
H	-4.700294	-0.104698	-0.028963

702-79-4-C12H20

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -469.588810826 (a.u.)
E(HF/CC-PVTZ) = -466.24537275
E(DLPNO-CCSD(T)/CC-PVTZ) = -468.491875876574
T1 (CC-PVTZ)= 0.008653968
T2 (CC-PVTZ)= 0.031755
E(HF/CC-PVQZ) = -466.27347998
E(DLPNO-CCSD(T)/CC-PVQZ) = -468.627885196535
E(HF/TZ-AUG) = -466.24741525
E(DLPNO-CCSD(T)/TZ-AUG) = -468.526946623
E(HF/TZ-CORE) = -466.24856461
E(DLPNO-CCSD(T)/TZ-CORE) = -469.098370535

E(HF/TZ-IT) = -466.24537275
E(DLPNO-CCSD(T)/TZ-IT) = -468.494977084
T1 (CC-PVQZ)= 0.008846574
T2 (CC-PVQZ)= 0.030937
E(HF/CBS) = -466.280328948
E(DLPNO-CCSD(T)/CBS) = -468.713473527
Enthalpic correction = 0.29960542 (a.u.)
Entropy = 95.15932 (cal/(mol*K))

C	-0.000001	1.218317	1.251997
C	-1.251420	0.332109	1.248550
C	-0.000001	2.105124	0.000000
C	1.251420	0.332109	1.248550
C	-1.274428	-0.567786	0.000000
C	0.000001	-1.429267	0.000001
C	-2.515567	-1.452936	0.000000
C	-1.251420	0.332107	-1.248551
C	1.274429	-0.567784	-0.000001
C	1.251420	0.332109	-1.248550
C	2.515568	-1.452935	0.000000
C	-0.000002	1.218317	-1.251997
H	0.000000	1.846065	2.147312
H	-1.273391	-0.291036	2.148355
H	-2.152519	0.953269	1.268440
H	-0.879992	2.755113	0.000001
H	0.879989	2.755113	-0.000001
H	1.273388	-0.291038	2.148354
H	2.152518	0.953269	1.268444
H	0.000002	-2.082691	0.879189
H	0.000001	-2.082693	-0.879185
H	-2.538280	-2.095760	-0.883581
H	-2.538250	-2.095802	0.883551
H	-3.426958	-0.849836	0.000030
H	-1.273386	-0.291040	-2.148354
H	-2.152520	0.953264	-1.268446
H	2.152517	0.953270	-1.268443
H	1.273389	-0.291036	-2.148355
H	2.538261	-2.095787	-0.883561
H	3.426960	-0.849835	-0.000011
H	2.538271	-2.095772	0.883572
H	0.000000	1.846065	-2.147312

7343-06-8-C18H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -697.109449995 (a.u.)
E(HF/CC-PVTZ) = -692.33536399
E(DLPNO-CCSD(T)/CC-PVTZ) = -695.457582553738
T1 (CC-PVTZ)= 0.009639200
T2 (CC-PVTZ)= 0.036997
E(HF/CC-PVQZ) = -692.3769175
E(DLPNO-CCSD(T)/CC-PVQZ) = -695.654988435443
E(HF/TZ-AUG) = -692.33995005
E(DLPNO-CCSD(T)/TZ-AUG) = -695.505910909
E(HF/TZ-CORE) = -692.34039168
E(DLPNO-CCSD(T)/TZ-CORE) = -696.371273287
E(HF/TZ-IT) = -692.33536399
E(DLPNO-CCSD(T)/TZ-IT) = -695.466042856
T1 (CC-PVQZ)= 0.009740472
T2 (CC-PVQZ)= 0.038065
E(HF/CBS) = -692.387042961
E(DLPNO-CCSD(T)/CBS) = -695.778844005
Enthalpic correction = 0.31203877 (a.u.)
Entropy = 122.64576 (cal/(mol*K))

C	1.017566	-1.991964	-1.059900
C	1.546139	-0.804139	-0.296184
C	0.730577	0.317008	0.017729
C	2.921187	-0.754978	-0.050767
C	-0.730578	0.317008	-0.017727
C	1.380203	1.555033	0.288920
C	3.800631	-1.940012	-0.345497
C	3.505541	0.426995	0.420993
C	-1.380202	1.555034	-0.288919
C	-1.546141	-0.804137	0.296186
C	0.647293	2.780851	0.192659
C	2.760868	1.576228	0.531910
C	-0.647292	2.780852	-0.192655
C	-2.760866	1.576228	-0.531914
C	-1.017568	-1.991957	1.059911
C	-2.921188	-0.754978	0.050763
C	-3.505539	0.426994	-0.421002
C	-3.800631	-1.940012	0.345492
H	1.057581	-2.921285	-0.488806
H	-0.005151	-1.839693	-1.390402
H	1.633679	-2.145913	-1.948627
H	4.810915	-1.771363	0.025688
H	3.419782	-2.855580	0.112217
H	3.870714	-2.131422	-1.420454
H	4.569532	0.447364	0.622902
H	1.179328	3.709432	0.358975
H	3.235338	2.518286	0.777886
H	-1.179327	3.709433	-0.358968
H	-3.235337	2.518286	-0.777891
H	-1.633673	-2.145889	1.948646
H	-1.057597	-2.921285	0.488830
H	0.005153	-1.839689	1.390401
H	-4.569529	0.447363	-0.622917
H	-3.870720	-2.131418	1.420449
H	-4.810913	-1.771367	-0.025700
H	-3.419777	-2.855581	-0.112216

7396-38-5-C18H18

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -697.111529363 (a.u.)
E(HF/CC-PVTZ) = -692.34227261
E(DLPNO-CCSD(T)/CC-PVTZ) = -695.459094644991
T1 (CC-PVTZ)= 0.009752414
T2 (CC-PVTZ)= 0.036709
E(HF/CC-PVQZ) = -692.3837947
E(DLPNO-CCSD(T)/CC-PVQZ) = -695.656452955389
E(HF/TZ-AUG) = -692.34675022
E(DLPNO-CCSD(T)/TZ-AUG) = -695.506796829
E(HF/TZ-CORE) = -692.34731039
E(DLPNO-CCSD(T)/TZ-CORE) = -696.372863943
E(HF/TZ-IT) = -692.34227261
E(DLPNO-CCSD(T)/TZ-IT) = -695.4675029
T1 (CC-PVQZ)= 0.009851717
T2 (CC-PVQZ)= 0.037788
E(HF/CBS) = -692.393912505
E(DLPNO-CCSD(T)/CBS) = -695.780289083
Enthalpic correction = 0.31194380 (a.u.)
Entropy = 127.83804 (cal/(mol*K))

C	0.972638	2.353537	1.110387
C	1.525571	1.130349	0.418686
C	0.727801	0.015763	0.042578
C	2.904735	1.041412	0.314169
C	-0.727801	0.015760	-0.042600
C	1.405454	-1.221675	-0.155616
C	3.568854	-0.124494	-0.086308
C	-1.405449	-1.221680	0.155599
C	-1.525576	1.130344	-0.418696

C	2.804822	-1.258087	-0.263412
C	0.663560	-2.445442	-0.126586
C	5.063645	-0.141961	-0.240153
C	-2.804815	-1.258093	0.263415
C	-0.663552	-2.445444	0.126560
C	-0.972653	2.353526	-1.110416
C	-2.904738	1.041410	-0.314152
C	-3.568850	-0.124498	0.086331
C	-5.063639	-0.141966	0.240203
H	1.015769	3.246778	0.486371
H	1.572268	2.554429	1.999634
H	-0.057092	2.212659	1.428705
H	3.497751	1.900740	0.609720
H	3.283852	-2.211869	-0.452801
H	1.207163	-3.375671	-0.237298
H	5.555561	0.354822	0.598734
H	5.368048	0.383431	-1.149551
H	5.444039	-1.161569	-0.303109
H	-3.283843	-2.211876	0.452806
H	-1.207153	-3.375675	0.237269
H	-1.015824	3.246783	-0.486426
H	-1.572267	2.554377	-1.999684
H	0.057086	2.212665	-1.428708
H	-3.497759	1.900740	-0.609689
H	-5.368025	0.383435	1.149601
H	-5.444030	-1.161574	0.303177
H	-5.555571	0.354808	-0.598680

74-84-00_C2H6

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -79.8694018125 (a.u.)
E(HF/CC-PVTZ) = -79.25979437
E(DLPNO-CCSD(T)/CC-PVTZ) = -79.674322459919
T1 (CC-PVTZ)= 0.007468817
T2 (CC-PVTZ)= 0.029721
E(HF/CC-PVQZ) = -79.26503231
E(DLPNO-CCSD(T)/CC-PVQZ) = -79.698640378013
E(HF/TZ-AUG) = -79.26023815
E(DLPNO-CCSD(T)/TZ-AUG) = -79.6797993171
E(HF/TZ-CORE) = -79.26035116
E(DLPNO-CCSD(T)/TZ-CORE) = -79.7753161013
E(HF/TZ-IT) = -79.25979437
E(DLPNO-CCSD(T)/TZ-IT) = -79.6746382195
T1 (CC-PVQZ)= 0.007995563
T2 (CC-PVQZ)= 0.028737
E(HF/CBS) = -79.2663086536
E(DLPNO-CCSD(T)/CBS) = -79.7138399489
Enthalpic correction = 0.07651313 (a.u.)
Entropy = 54.54643 (cal/(mol*K))

C	0.000000	0.000000	0.763099
C	0.000000	0.000000	-0.763099
H	0.000000	1.017118	1.160146
H	-0.880850	-0.508559	1.160146
H	0.880850	-0.508559	1.160146
H	0.000000	-1.017118	-1.160146
H	-0.880850	0.508559	-1.160146
H	0.880850	0.508559	-1.160146

74-85-10_C2H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -78.6277014591 (a.u.)
E(HF/CC-PVTZ) = -78.06404123
E(DLPNO-CCSD(T)/CC-PVTZ) = -78.438255919400
T1 (CC-PVTZ)= 0.010513348
T2 (CC-PVTZ)= 0.061502
E(HF/CC-PVQZ) = -78.06932711
E(DLPNO-CCSD(T)/CC-PVQZ) = -78.461284165719
E(HF/TZ-AUG) = -78.06488964
E(DLPNO-CCSD(T)/TZ-AUG) = -78.4431354463
E(HF/TZ-CORE) = -78.06464178
E(DLPNO-CCSD(T)/TZ-CORE) = -78.5396237336
E(HF/TZ-IT) = -78.06404123
E(DLPNO-CCSD(T)/TZ-IT) = -78.4388114947
T1 (CC-PVQZ)= 0.010825703
T2 (CC-PVQZ)= 0.058788
E(HF/CBS) = -78.0706151353
E(DLPNO-CCSD(T)/CBS) = -78.4755193232
Enthalpic correction = 0.05332291 (a.u.)
Entropy = 52.36377 (cal/(mol*K))

C	0.000000	0.000000	0.662305
C	0.000000	0.000000	-0.662305
H	0.000000	0.921446	1.232034
H	0.000000	-0.921446	1.232034
H	0.000000	0.921446	-1.232034
H	0.000000	-0.921446	-1.232034

74-86-20_C2H2

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -77.3667641761 (a.u.)
E(HF/CC-PVTZ) = -76.84989563
E(DLPNO-CCSD(T)/CC-PVTZ) = -77.186755060251
T1 (CC-PVTZ)= 0.012858840
T2 (CC-PVTZ)= 0.057507
E(HF/CC-PVQZ) = -76.85492814
E(DLPNO-CCSD(T)/CC-PVQZ) = -77.208539643564
E(HF/TZ-AUG) = -76.8506596
E(DLPNO-CCSD(T)/TZ-AUG) = -77.1912499349
E(HF/TZ-CORE) = -76.85073435
E(DLPNO-CCSD(T)/TZ-CORE) = -77.288695467
E(HF/TZ-IT) = -76.84989563
E(DLPNO-CCSD(T)/TZ-IT) = -77.1875143735
T1 (CC-PVQZ)= 0.013193045
T2 (CC-PVQZ)= 0.056344
E(HF/CBS) = -76.8561544259
E(DLPNO-CCSD(T)/CBS) = -77.2219904154
Enthalpic correction = 0.02978192 (a.u.)
Entropy = 47.99326 (cal/(mol*K))

C	0.000000	0.000000	0.598395
C	0.000000	0.000000	-0.598395
H	0.000000	0.000000	1.661067
H	0.000000	0.000000	-1.661067

74-98-60_C3H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -119.202217139 (a.u.)
E(HF/CC-PVTZ) = -118.30770703
E(DLPNO-CCSD(T)/CC-PVTZ) = -118.913730475735

T1 (CC-PVTZ)= 0.007667828
T2 (CC-PVTZ)= 0.033347
E(HF/CC-PVQZ) = -118.31536037
E(DLPNO-CCSD(T)/CC-PVQZ) = -118.949681910864
E(HF/TZ-AUG) = -118.30834728
E(DLPNO-CCSD(T)/TZ-AUG) = -118.922081596
E(HF/TZ-CORE) = -118.3085252
E(DLPNO-CCSD(T)/TZ-CORE) = -119.065232296
E(HF/TZ-IT) = -118.30770703
E(DLPNO-CCSD(T)/TZ-IT) = -118.914263194
T1 (CC-PVQZ)= 0.008129613
T2 (CC-PVQZ)= 0.028479
E(HF/CBS) = -118.317225281
E(DLPNO-CCSD(T)/CBS) = -118.972196783
Enthalpic correction = 0.10534460 (a.u.)
Entropy = 64.44976 (cal/(mol*K))

C	0.000000	0.000000	0.585912
C	0.000000	1.271080	-0.259327
C	0.000000	-1.271080	-0.259327
H	0.874497	0.000000	1.243454
H	-0.874497	0.000000	1.243454
H	0.000000	2.167755	0.363361
H	0.881358	1.312736	-0.904295
H	-0.881358	1.312736	-0.904295
H	0.000000	-2.167755	0.363361
H	-0.881358	-1.312736	-0.904295
H	0.881358	-1.312736	-0.904295

74-99-70_C3H4

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -116.710837216 (a.u.)
E(HF/CC-PVTZ) = -115.90847834
E(DLPNO-CCSD(T)/CC-PVTZ) = -116.434388304442
T1 (CC-PVTZ)= 0.011196701
T2 (CC-PVTZ)= 0.057320
E(HF/CC-PVQZ) = -115.91599453
E(DLPNO-CCSD(T)/CC-PVQZ) = -116.467887066847
E(HF/TZ-AUG) = -115.90957522
E(DLPNO-CCSD(T)/TZ-AUG) = -116.441830407
E(HF/TZ-CORE) = -115.90973183
E(DLPNO-CCSD(T)/TZ-CORE) = -116.587210937
E(HF/TZ-IT) = -115.90847834
E(DLPNO-CCSD(T)/TZ-IT) = -116.435384246
T1 (CC-PVQZ)= 0.011457088
T2 (CC-PVQZ)= 0.055951
E(HF/CBS) = -115.917826021
E(DLPNO-CCSD(T)/CBS) = -116.488678814
Enthalpic correction = 0.05868222 (a.u.)
Entropy = 59.21671 (cal/(mol*K))

C	0.000000	0.000000	0.218081
C	0.000000	0.000000	1.417592
H	0.000000	0.000000	2.479508
C	0.000000	0.000000	-1.236015
H	0.000000	1.019902	-1.625819
H	0.883261	-0.509951	-1.625819
H	-0.883261	-0.509951	-1.625819

75-19-40_C3H6

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -117.951257515 (a.u.)
E(HF/CC-PVTZ) = -117.10117277
E(DLPNO-CCSD(T)/CC-PVTZ) = -117.669818752381
T1 (CC-PVTZ)= 0.007339641
T2 (CC-PVTZ)= 0.034685
E(HF/CC-PVQZ) = -117.10866617
E(DLPNO-CCSD(T)/CC-PVQZ) = -117.704491008395
E(HF/TZ-AUG) = -117.1018316
E(DLPNO-CCSD(T)/TZ-AUG) = -117.677302282
E(HF/TZ-CORE) = -117.10201641
E(DLPNO-CCSD(T)/TZ-CORE) = -117.821682022
E(HF/TZ-IT) = -117.10117277
E(DLPNO-CCSD(T)/TZ-IT) = -117.670490606
T1 (CC-PVQZ)= 0.007715158
T2 (CC-PVQZ)= 0.031540
E(HF/CBS) = -117.110492108
E(DLPNO-CCSD(T)/CBS) = -117.726150166
Enthalpic correction = 0.08294267 (a.u.)
Entropy = 56.79218 (cal/(mol*K))

C	0.000000	0.867980	0.000000
C	-0.751693	-0.433990	0.000000
C	0.751693	-0.433990	0.000000
H	0.000000	1.455242	0.908313
H	0.000000	1.455242	-0.908313
H	-1.260277	-0.727621	0.908313
H	-1.260277	-0.727621	-0.908313
H	1.260277	-0.727621	0.908313
H	1.260277	-0.727621	-0.908313

75-28-50_C4H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -158.536778562 (a.u.)
E(HF/CC-PVTZ) = -157.35599425
E(DLPNO-CCSD(T)/CC-PVTZ) = -158.155493374039
T1 (CC-PVTZ)= 0.007829647
T2 (CC-PVTZ)= 0.039710
E(HF/CC-PVQZ) = -157.36605928
E(DLPNO-CCSD(T)/CC-PVQZ) = -158.203114648471
E(HF/TZ-AUG) = -157.3568116
E(DLPNO-CCSD(T)/TZ-AUG) = -158.166893498
E(HF/TZ-CORE) = -157.35707673
E(DLPNO-CCSD(T)/TZ-CORE) = -158.357542049
E(HF/TZ-IT) = -157.35599425
E(DLPNO-CCSD(T)/TZ-IT) = -158.156267715
T1 (CC-PVQZ)= 0.008249061
T2 (CC-PVQZ)= 0.035107
E(HF/CBS) = -157.368511854
E(DLPNO-CCSD(T)/CBS) = -158.232973131
Enthalpic correction = 0.13370051 (a.u.)
Entropy = 70.46708 (cal/(mol*K))

C	0.000000	0.000000	0.373534
H	0.000000	0.000000	1.469717
C	0.000000	1.454988	-0.095651
C	-1.260057	-0.727494	-0.095651
C	1.260057	-0.727494	-0.095651
H	0.000000	1.507399	-1.188251
H	-0.883264	1.988106	0.262592
H	0.883264	1.988106	0.262592
H	-1.305446	-0.753700	-1.188251
H	-1.280119	-1.758982	0.262592
H	-2.163382	-0.229124	0.262592
H	1.305446	-0.753700	-1.188251
H	2.163382	-0.229124	0.262592

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 H     1.280119    -1.758982     0.262592
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776-35-2-C14H12

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Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -540.990252919
(a.u.)
E(HF/CC-PVTZ) = -537.33782746
E(DLPNO-CCSD(T)/CC-PVTZ) = -539.711810079969
T1 (CC-PVTZ)= 0.009720534
T2 (CC-PVTZ)= 0.039122
E(HF/CC-PVQZ) = -537.37008425
E(DLPNO-CCSD(T)/CC-PVQZ) = -539.864152068711
E(HF/TZ-AUG) = -537.34161918
E(DLPNO-CCSD(T)/TZ-AUG) = -539.747657914
E(HF/TZ-CORE) = -537.34175649
E(DLPNO-CCSD(T)/TZ-CORE) = -540.422740928
E(HF/TZ-IT) = -537.33782746
E(DLPNO-CCSD(T)/TZ-IT) = -539.718186381
T1 (CC-PVQZ)= 0.009815009
T2 (CC-PVQZ)= 0.040313
E(HF/CBS) = -537.377944353
E(DLPNO-CCSD(T)/CBS) = -539.959641911
Enthalpic correction = 0.22139237 (a.u.)
Entropy = 98.57623 (cal/(mol*K))

 C     0.738486    -0.412452     0.012007
 C    -0.738486    -0.412453    -0.012000
 C     1.425742     0.795990    -0.200642
 C     1.479473    -1.574538     0.244979
 C    -1.425744     0.795990     0.200643
 C    -1.479471    -1.574539    -0.244973
 C     0.628817     2.052261    -0.432843
 C     2.815857     0.805583    -0.199771
 C     2.866222    -1.553117     0.243589
 C    -0.628817     2.052259     0.432850
 C    -2.815858     0.805583     0.199763
 C    -2.866221    -1.553118    -0.243591
 C     3.540528    -0.359824     0.015127
 C    -3.540528    -0.359824    -0.015137
 H     0.966638    -2.504486     0.449668
 H    -0.966636    -2.504489    -0.449656
 H     1.243080     2.930060    -0.226566
 H     0.335066     2.108191    -1.488006
 H     3.336401     1.741547    -0.365421
 H     3.419106    -2.464598     0.430711
 H    -1.243080     2.930061     0.226581
 H    -0.335063     2.108181     1.488012
 H    -3.336404     1.741548     0.365407
 H    -3.419104    -2.464600    -0.430713
 H     4.622541    -0.334112     0.016931
 H    -4.622541    -0.334112    -0.016950
```

78-78-40_C5H12

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -197.868714870
(a.u.)
E(HF/CC-PVTZ) = -196.40171903
E(DLPNO-CCSD(T)/CC-PVTZ) = -197.394151484240
T1 (CC-PVTZ)= 0.007943602
T2 (CC-PVTZ)= 0.038752
E(HF/CC-PVQZ) = -196.41419033
E(DLPNO-CCSD(T)/CC-PVQZ) = -197.453388464018
E(HF/TZ-AUG) = -196.40272295
E(DLPNO-CCSD(T)/TZ-AUG) = -197.408587817
E(HF/TZ-CORE) = -196.40306717
E(DLPNO-CCSD(T)/TZ-CORE) = -197.646713868
E(HF/TZ-IT) = -196.40171903
E(DLPNO-CCSD(T)/TZ-IT) = -197.395155576
T1 (CC-PVQZ)= 0.008330928
T2 (CC-PVQZ)= 0.030361
E(HF/CBS) = -196.417229247
E(DLPNO-CCSD(T)/CBS) = -197.490553688
Enthalpic correction = 0.16266597 (a.u.)
Entropy = 80.37067 (cal/(mol*K))

 C     2.087284    -0.035999    -0.110174
 C     0.755967    -0.670715     0.283633
 C    -0.480823    -0.002941    -0.330985
 H     2.926612    -0.602888     0.296764
 H     2.175281     0.987249     0.257862
 H     2.201440    -0.008698    -1.196950
 H     0.653309    -0.662891     1.374907
 H     0.762735    -1.724307    -0.012447
 H    -0.349173    -0.004383    -1.420307
 C    -0.641223     1.449131     0.121622
 C    -1.740131    -0.807608    -0.008282
 H    -0.741175     1.503421     1.209757
 H    -1.535492     1.897445    -0.316107
 H     0.211254     2.064991    -0.166696
 H    -1.913839    -0.836410     1.071235
 H    -2.623654    -0.366356    -0.474267
 H    -1.653741    -1.838378    -0.358642
```

78-79-50_C5H8

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -195.406284756
(a.u.)
E(HF/CC-PVTZ) = -194.02826483
E(DLPNO-CCSD(T)/CC-PVTZ) = -194.938592598251
T1 (CC-PVTZ)= 0.010441118
T2 (CC-PVTZ)= 0.049287
E(HF/CC-PVQZ) = -194.04072726
E(DLPNO-CCSD(T)/CC-PVQZ) = -194.995255295364
E(HF/TZ-AUG) = -194.02993387
E(DLPNO-CCSD(T)/TZ-AUG) = -194.951610032
E(HF/TZ-CORE) = -194.02974026
E(DLPNO-CCSD(T)/TZ-CORE) = -195.192094168
E(HF/TZ-IT) = -194.02826483
E(DLPNO-CCSD(T)/TZ-IT) = -194.940283984
T1 (CC-PVQZ)= 0.010647643
T2 (CC-PVQZ)= 0.047888
E(HF/CBS) = -194.043764015
E(DLPNO-CCSD(T)/CBS) = -195.0305463
Enthalpic correction = 0.11656829 (a.u.)
Entropy = 74.71167 (cal/(mol*K))

 C    -0.585060     1.726678     0.000000
 C     0.000000     0.523512     0.000000
 C    -0.824030    -0.684350     0.000000
 H    -0.005913     2.640919     0.000000
 H    -1.663345     1.827292     0.000000
 C     1.495155     0.374854     0.000000
 H     1.984110     1.347865     0.000000
 H     1.833629    -0.179832     0.878709
 H     1.833629    -0.179832    -0.878709
 C    -0.372098    -1.939180     0.000000
 H    -1.896597    -0.514242     0.000000
 H    -1.054043    -2.778816     0.000000
 H     0.684732    -2.172431     0.000000
```

822-35-50_C4H6

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -156.044569978
(a.u.)
E(HF/CC-PVTZ) = -154.95335
E(DLPNO-CCSD(T)/CC-PVTZ) = -155.676304901647
T1 (CC-PVTZ)= 0.009620160
T2 (CC-PVTZ)= 0.059098
E(HF/CC-PVQZ) = -154.96309841
E(DLPNO-CCSD(T)/CC-PVQZ) = -155.721524953372
E(HF/TZ-AUG) = -154.9544504
E(DLPNO-CCSD(T)/TZ-AUG) = -155.686447591
E(HF/TZ-CORE) = -154.95451068
E(DLPNO-CCSD(T)/TZ-CORE) = -155.878684051
E(HF/TZ-IT) = -154.95335
E(DLPNO-CCSD(T)/TZ-IT) = -155.677533818
T1 (CC-PVQZ)= 0.009917183
T2 (CC-PVQZ)= 0.059039
E(HF/CBS) = -154.965473833
E(DLPNO-CCSD(T)/CBS) = -155.749785087
Enthalpic correction = 0.08834250 (a.u.)
Entropy = 62.79414 (cal/(mol*K))
```

C	0.000000	0.667529	0.812381
C	0.000000	-0.667529	0.812381
H	0.000000	1.411836	1.598299
H	0.000000	-1.411836	1.598299
C	0.000000	0.784715	-0.698487
C	0.000000	-0.784715	-0.698487
H	-0.887405	1.242437	-1.140831
H	0.887405	-1.242437	-1.140831
H	0.887405	1.242437	-1.140831
H	-0.887405	-1.242437	-1.140831

832-64-4-C15H12

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -579.113199542
(a.u.)
E(HF/CC-PVTZ) = -575.21159326
E(DLPNO-CCSD(T)/CC-PVTZ) = -577.741532172138
T1 (CC-PVTZ)= 0.009955380
T2 (CC-PVTZ)= 0.036171
E(HF/CC-PVQZ) = -575.24598207
E(DLPNO-CCSD(T)/CC-PVQZ) = -577.904153321270
E(HF/TZ-AUG) = -575.21563374
E(DLPNO-CCSD(T)/TZ-AUG) = -577.77963264
E(HF/TZ-CORE) = -575.21581178
E(DLPNO-CCSD(T)/TZ-CORE) = -578.503334827
E(HF/TZ-IT) = -575.21159326
E(DLPNO-CCSD(T)/TZ-IT) = -577.748971374
T1 (CC-PVQZ)= 0.010009231
T2 (CC-PVQZ)= 0.038047
E(HF/CBS) = -575.254361688
E(DLPNO-CCSD(T)/CBS) = -578.00610789
Enthalpic correction = 0.22739609 (a.u.)
Entropy = 103.84290 (cal/(mol*K))
```

C	-1.201032	2.664986	0.245744
C	-1.585525	1.218626	0.053861
C	-0.669687	0.123008	-0.013824
C	-2.947706	0.968076	-0.005546
C	0.788850	0.231706	-0.028343
C	-1.229587	-1.191614	-0.045353
C	-3.476922	-0.318429	-0.109617
C	1.577325	-0.953187	0.080007
C	1.502235	1.440722	-0.188044
C	-0.389315	-2.345593	0.021074
C	-2.620435	-1.387823	-0.110120
C	0.951375	-2.234148	0.117140
C	2.982782	-0.875111	0.106146
C	2.879731	1.491128	-0.178188
C	3.635734	0.327562	-0.009958
H	-2.086831	3.240937	0.510334
H	-0.787390	3.111962	-0.661157
H	-0.469657	2.793040	1.043875
H	-3.626440	1.810109	0.048099
H	-4.548166	-0.463576	-0.159722
H	0.978766	2.361441	-0.352647
H	-0.864289	-3.318815	0.013561
H	-2.998399	-2.401855	-0.147971
H	1.579239	-3.113279	0.193081
H	3.544387	-1.796194	0.204345
H	3.375008	2.444657	-0.309477
H	4.716821	0.372120	0.007805

83-32-9-C12H10

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -463.525695390
(a.u.)
E(HF/CC-PVTZ) = -460.4025436
E(DLPNO-CCSD(T)/CC-PVTZ) = -462.430496982766
T1 (CC-PVTZ)= 0.010199378
T2 (CC-PVTZ)= 0.033754
E(HF/CC-PVQZ) = -460.43005732
E(DLPNO-CCSD(T)/CC-PVQZ) = -462.560981133785
E(HF/TZ-AUG) = -460.40571799
E(DLPNO-CCSD(T)/TZ-AUG) = -462.460941381
E(HF/TZ-CORE) = -460.40591285
E(DLPNO-CCSD(T)/TZ-CORE) = -463.039759488
E(HF/TZ-IT) = -460.4025436
E(DLPNO-CCSD(T)/TZ-IT) = -462.436145147
T1 (CC-PVQZ)= 0.010234150
T2 (CC-PVQZ)= 0.037662
E(HF/CBS) = -460.436761666
E(DLPNO-CCSD(T)/CBS) = -462.642826064
Enthalpic correction = 0.18579335 (a.u.)
Entropy = 90.97428 (cal/(mol*K))
```

C	0.000000	0.091046	0.000000
C	-1.170780	0.870390	0.000001
C	1.170780	0.870390	-0.000001
C	0.000000	-1.317169	0.000000
C	-0.781935	2.333914	0.000013
C	-2.386385	0.236488	-0.000001
C	0.781935	2.333914	-0.000013
C	2.386385	0.236487	0.000001
C	1.270514	-1.944142	0.000002
C	-1.270515	-1.944142	-0.000002
C	-2.416986	-1.181482	-0.000004
C	2.416986	-1.181482	0.000004
H	-1.180719	2.849798	-0.875722
H	-1.180683	2.849765	0.875785
H	-3.316609	0.791194	-0.000001
H	1.180719	2.849797	0.875722
H	1.180684	2.849765	-0.875785
H	3.316609	0.791195	0.000000
H	1.336437	-3.025208	0.000003
H	-1.336437	-3.025208	-0.000003

H	-3.379316	-1.678182	-0.000007
H	3.379316	-1.678182	0.000006

84-15-1-C18H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -694.682558776 (a.u.)
E(HF/CC-PVTZ) = -690.0122868
E(DLPNO-CCSD(T)/CC-PVTZ) = -693.037888622725
T1 (CC-PVTZ)= 0.009796064
T2 (CC-PVTZ)= 0.037743
E(HF/CC-PVQZ) = -690.05373283
E(DLPNO-CCSD(T)/CC-PVQZ) = -693.232659816169
E(HF/TZ-AUG) = -690.01731944
E(DLPNO-CCSD(T)/TZ-AUG) = -693.083843582
E(HF/TZ-CORE) = -690.01744737
E(DLPNO-CCSD(T)/TZ-CORE) = -693.952576864
E(HF/TZ-IT) = -690.0122868
E(DLPNO-CCSD(T)/TZ-IT) = -693.046588374
T1 (CC-PVQZ)= 0.009873487
T2 (CC-PVQZ)= 0.041035
E(HF/CBS) = -690.063832101
E(DLPNO-CCSD(T)/CBS) = -693.354645017
Enthalpic correction = 0.26837836 (a.u.)
Entropy = 119.45444 (cal/(mol*K))

C	0.703494	1.225003	-0.033034
C	-0.703514	1.224993	0.033027
C	1.377524	2.449228	-0.052139
C	1.499985	-0.023683	-0.119955
C	-1.377561	2.449209	0.052139
C	-1.499987	-0.023704	0.119953
C	0.693931	3.655433	-0.023314
C	1.217668	-0.995872	-1.082744
C	2.572692	-0.238297	0.747868
C	-0.693984	3.655423	0.023317
C	-1.217645	-0.995892	1.082735
C	-2.572698	-0.238332	-0.747861
C	1.981866	-2.149901	-1.170668
C	3.335635	-1.396426	0.664723
C	-1.981824	-2.149933	1.170661
C	-3.335622	-1.396472	-0.664713
C	3.042080	-2.357322	-0.294691
C	-3.042044	-2.357368	0.294694
H	2.457688	2.445208	-0.121163
H	-2.457725	2.445174	0.121166
H	1.241977	4.588421	-0.046762
H	0.392470	-0.843448	-1.764699
H	2.795961	0.501541	1.506141
H	-1.242044	4.588404	0.046770
H	-0.392441	-0.843458	1.764681
H	-2.795986	0.501506	-1.506130
H	1.749464	-2.889952	-1.925679
H	4.156757	-1.549336	1.353459
H	-1.749402	-2.889985	1.925667
H	-4.156748	-1.549392	-1.353442
H	3.634665	-3.260576	-0.360623
H	-3.634613	-3.260631	0.360628

85-01-8-C14H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -539.785929491 (a.u.)
E(HF/CC-PVTZ) = -536.17554214
E(DLPNO-CCSD(T)/CC-PVTZ) = -538.507554746145
T1 (CC-PVTZ)= 0.010059980
T2 (CC-PVTZ)= 0.036374
E(HF/CC-PVQZ) = -536.20756908
E(DLPNO-CCSD(T)/CC-PVQZ) = -538.658675012759
E(HF/TZ-AUG) = -536.17937587
E(DLPNO-CCSD(T)/TZ-AUG) = -538.542213333
E(HF/TZ-CORE) = -536.17948515
E(DLPNO-CCSD(T)/TZ-CORE) = -539.218902613
E(HF/TZ-IT) = -536.17554214
E(DLPNO-CCSD(T)/TZ-IT) = -538.514642297
T1 (CC-PVQZ)= 0.010096503
T2 (CC-PVQZ)= 0.037699
E(HF/CBS) = -536.215373175
E(DLPNO-CCSD(T)/CBS) = -538.753385048
Enthalpic correction = 0.19847233 (a.u.)
Entropy = 96.62079 (cal/(mol*K))

C	-2.867565	-1.523918	-0.000013
C	-1.491345	-1.559984	-0.000018
C	-0.725457	-0.377818	-0.000003
C	-3.544568	-0.296351	0.000006
C	-2.825210	0.874739	0.000014
C	-1.416538	0.862943	0.000008
C	-0.676559	2.086116	0.000005
C	0.725456	-0.377818	0.000001
C	1.416538	0.862942	-0.000008
C	1.491344	-1.559984	0.000016
C	0.676560	2.086116	-0.000008
C	2.825211	0.874739	-0.000012
C	3.544569	-0.296352	-0.000002
C	2.867565	-1.523918	0.000014
H	-3.428797	-2.449378	-0.000026
H	-0.997983	-2.520965	-0.000041
H	-4.626528	-0.273344	0.000012
H	-3.335186	1.830478	0.000024
H	-1.227243	3.018859	0.000011
H	0.997986	-2.520967	0.000036
H	1.227243	3.018859	-0.000016
H	3.335183	1.830479	-0.000020
H	4.626529	-0.273344	-0.000004
H	3.428795	-2.449379	0.000027

86-73-7-C13H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -501.651702761 (a.u.)
E(HF/CC-PVTZ) = -498.28778667
E(DLPNO-CCSD(T)/CC-PVTZ) = -500.466186658544
T1 (CC-PVTZ)= 0.009903520
T2 (CC-PVTZ)= 0.038166
E(HF/CC-PVQZ) = -498.31760982
E(DLPNO-CCSD(T)/CC-PVQZ) = -500.607109174735
E(HF/TZ-AUG) = -498.29136506
E(DLPNO-CCSD(T)/TZ-AUG) = -500.498863959
E(HF/TZ-CORE) = -498.29144935
E(DLPNO-CCSD(T)/TZ-CORE) = -501.126555541
E(HF/TZ-IT) = -498.28778666
E(DLPNO-CCSD(T)/TZ-IT) = -500.472298547
T1 (CC-PVQZ)= 0.009978091
T2 (CC-PVQZ)= 0.039346
E(HF/CBS) = -498.324876911
E(DLPNO-CCSD(T)/CBS) = -500.695448776
Enthalpic correction = 0.19167678 (a.u.)

Entropy = 93.76831 (cal/(mol*K))

C	0.732226	-0.448401	-0.000001
C	-0.732228	-0.448399	-0.000003
C	1.180597	0.883668	0.000001
C	1.643842	-1.498379	-0.000003
C	-1.180597	0.883670	-0.000004
C	-1.643843	-1.498379	0.000001
C	0.000001	1.825607	-0.000001
C	2.535054	1.167837	0.000003
C	3.003517	-1.207065	-0.000001
C	-2.535055	1.167837	-0.000002
C	-3.003517	-1.207066	0.000003
C	3.447154	0.113932	0.000003
C	-3.447153	0.113932	0.000002
H	1.305214	-2.526802	-0.000006
H	-1.305210	-2.526801	0.000001
H	0.000004	2.478783	-0.877888
H	-0.000002	2.478786	0.877883
H	2.886514	2.192648	0.000006
H	3.725506	-2.013546	-0.000001
H	-2.886516	2.192648	-0.000002
H	-3.725508	-2.013545	0.000006
H	4.509198	0.322534	0.000005
H	-4.509197	0.322533	0.000005

91-20-3_C10H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -386.069669453 (a.u.)
E(HF/CC-PVTZ) = -383.47627459
E(DLPNO-CCSD(T)/CC-PVTZ) = -385.153447969824
T1 (CC-PVTZ)= 0.010106921
T2 (CC-PVTZ)= 0.035182
E(HF/CC-PVQZ) = -383.49942061
E(DLPNO-CCSD(T)/CC-PVQZ) = -385.262035988863
E(HF/TZ-AUG) = -383.47908833
E(DLPNO-CCSD(T)/TZ-AUG) = -385.17779883
E(HF/TZ-CORE) = -383.47910602
E(DLPNO-CCSD(T)/TZ-CORE) = -385.66157143
E(HF/TZ-IT) = -383.47627459
E(DLPNO-CCSD(T)/TZ-IT) = -385.158350105
T1 (CC-PVQZ)= 0.010145948
T2 (CC-PVQZ)= 0.037680
E(HF/CBS) = -383.505060666
E(DLPNO-CCSD(T)/CBS) = -385.330025612
Enthalpic correction = 0.15035307 (a.u.)
Entropy = 80.09278 (cal/(mol*K))

C	0.000000	0.000000	0.713635
C	0.000000	0.000000	-0.713635
C	0.000000	1.239507	-1.396673
C	0.000000	-1.239507	-1.396673
C	0.000000	-1.239507	1.396673
C	0.000000	1.239507	1.396673
C	0.000000	2.422570	-0.705666
C	0.000000	-2.422570	-0.705666
C	0.000000	-2.422570	0.705666
C	0.000000	2.422570	0.705666
H	0.000000	1.236956	-2.480020
H	0.000000	-1.236956	-2.480020
H	0.000000	-1.236956	2.480020
H	0.000000	1.236956	2.480020
H	0.000000	3.363690	-1.240308
H	0.000000	-3.363690	-1.240308
H	0.000000	-3.363690	1.240308
H	0.000000	3.363690	1.240308

92-06-8-C18H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -694.684798042 (a.u.)
E(HF/CC-PVTZ) = -690.01960167
E(DLPNO-CCSD(T)/CC-PVTZ) = -693.040067284811
T1 (CC-PVTZ)= 0.009875939
T2 (CC-PVTZ)= 0.039054
E(HF/CC-PVQZ) = -690.06108952
E(DLPNO-CCSD(T)/CC-PVQZ) = -693.235022221564
E(HF/TZ-AUG) = -690.02457921
E(DLPNO-CCSD(T)/TZ-AUG) = -693.085224531
E(HF/TZ-CORE) = -690.02475238
E(DLPNO-CCSD(T)/TZ-CORE) = -693.954749135
E(HF/TZ-IT) = -690.01960167
E(DLPNO-CCSD(T)/TZ-IT) = -693.048713747
T1 (CC-PVQZ)= 0.009962656
T2 (CC-PVQZ)= 0.040728
E(HF/CBS) = -690.071198981
E(DLPNO-CCSD(T)/CBS) = -693.357121178
Enthalpic correction = 0.26845587 (a.u.)
Entropy = 120.39235 (cal/(mol*K))

C	0.000000	0.071699	0.000001
C	-1.219784	0.749440	-0.019831
C	-1.204461	2.147129	-0.018840
C	-2.496608	0.003254	-0.050217
C	1.219784	0.749440	0.019832
C	0.000000	2.835603	0.000000
C	-3.603590	0.447109	0.679595
C	-2.629139	-1.164254	-0.808160
C	1.204461	2.147129	0.018840
C	2.496608	0.003254	0.050218
C	-4.801912	-0.252773	0.653727
C	-3.827354	-1.864281	-0.835527
C	3.603589	0.447109	-0.679597
C	2.629140	-1.164253	0.808162
C	-4.919445	-1.411942	-0.104267
C	4.801911	-0.252773	-0.653730
C	3.827355	-1.864279	0.835528
C	4.919446	-1.411942	0.104265
H	0.000000	-1.010002	0.000001
H	-2.137623	2.693036	-0.058279
H	0.000000	3.918173	0.000000
H	-3.515089	1.335255	1.291549
H	-1.792435	-1.511492	-1.400114
H	2.137624	2.693036	0.058278
H	-5.643738	0.103780	1.233497
H	-3.910712	-2.760985	-1.436264
H	3.515087	1.335254	-1.291550
H	1.792438	-1.511491	1.400118
H	-5.853752	-1.957689	-0.125106
H	5.643736	0.103778	-1.233501
H	3.910714	-2.760983	1.436267
H	5.853752	-1.957689	0.125104

92-24-0-C18H12

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -693.481989362 (a.u.)
E(HF/CC-PVTZ) = -688.8487257

E(DLPNO-CCSD(T)/CC-PVTZ) = -691.839309693424
T1 (CC-PVTZ)= 0.010545059
T2 (CC-PVTZ)= 0.032832
E(HF/CC-PVQZ) = -688.88960782
E(DLPNO-CCSD(T)/CC-PVQZ) = -692.032876142866
E(HF/TZ-AUG) = -688.85346363
E(DLPNO-CCSD(T)/TZ-AUG) = -691.884036359
E(HF/TZ-CORE) = -688.85379855
E(DLPNO-CCSD(T)/TZ-CORE) = -692.753884305
E(HF/TZ-IT) = -688.8487257
E(DLPNO-CCSD(T)/TZ-IT) = -691.849082032
T1 (CC-PVQZ)= 0.010547347
T2 (CC-PVQZ)= 0.037470
E(HF/CBS) = -688.899569681
E(DLPNO-CCSD(T)/CBS) = -692.154256299
Enthalpic correction = 0.24589729 (a.u.)
Entropy = 109.97340 (cal/(mol*K))

C	0.000001	0.723195	0.000000
C	0.000001	-0.723195	0.000000
C	1.229772	-1.400925	0.000000
C	-1.229774	-1.400925	0.000000
C	-1.229773	1.400925	0.000000
C	1.229772	1.400925	0.000000
C	2.438624	-0.722914	0.000000
C	-2.438623	-0.722915	0.000000
C	-2.438623	0.722915	0.000000
C	2.438624	0.722914	0.000000
C	3.694547	-1.403458	0.000000
C	-3.694548	-1.403459	0.000000
C	-3.694548	1.403459	0.000000
C	3.694547	1.403459	0.000000
C	4.866289	-0.712869	0.000000
C	-4.866289	-0.712869	0.000000
C	-4.866289	0.712870	0.000000
C	4.866289	0.712869	0.000000
H	1.230099	-2.484898	0.000000
H	-1.230096	-2.484898	0.000000
H	-1.230097	2.484897	0.000000
H	1.230097	2.484898	-0.000001
H	3.692987	-2.486679	0.000000
H	-3.692988	-2.486680	0.000000
H	-3.692987	2.486680	0.000000
H	3.692986	2.486680	0.000000
H	5.810135	-1.242575	0.000001
H	-5.810135	-1.242575	0.000000
H	-5.810134	1.242576	0.000000
H	5.810135	1.242575	0.000001

92-52-4-C12H10

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -463.520424625 (a.u.)
E(HF/CC-PVTZ) = -460.39972268
E(DLPNO-CCSD(T)/CC-PVTZ) = -462.421361843855
T1 (CC-PVTZ)= 0.009859073
T2 (CC-PVTZ)= 0.039083
E(HF/CC-PVQZ) = -460.42760853
E(DLPNO-CCSD(T)/CC-PVQZ) = -462.551846864794
E(HF/TZ-AUG) = -460.40314091
E(DLPNO-CCSD(T)/TZ-AUG) = -462.451119107
E(HF/TZ-CORE) = -460.40315646
E(DLPNO-CCSD(T)/TZ-CORE) = -463.031088292
E(HF/TZ-IT) = -460.39972268
E(DLPNO-CCSD(T)/TZ-IT) = -462.426991468
T1 (CC-PVQZ)= 0.009949461
T2 (CC-PVQZ)= 0.040758
E(HF/CBS) = -460.434403554
E(DLPNO-CCSD(T)/CBS) = -462.633511554
Enthalpic correction = 0.18544529 (a.u.)
Entropy = 94.79462 (cal/(mol*K))

C	2.845473	1.132510	0.398102
C	1.457515	1.132062	0.397528
C	0.739372	-0.000005	0.000000
C	1.457524	-1.132066	-0.397532
C	2.845482	-1.132505	-0.398099
C	3.546170	0.000004	0.000005
C	-0.739372	-0.000005	-0.000005
C	-1.457522	-1.132066	0.397528
C	-2.845480	-1.132506	0.398102
C	-3.546170	0.000003	0.000002
C	-2.845476	1.132509	-0.398100
C	-1.457517	1.132062	-0.397531
H	-0.921622	2.010590	-0.732350
H	3.381254	2.017050	0.718227
H	0.921618	2.010590	0.732343
H	0.921634	-2.010595	-0.732355
H	3.381271	-2.017039	-0.718224
H	4.628392	0.000006	0.000008
H	-0.921631	-2.010597	0.732348
H	-3.381267	-2.017041	0.718228
H	-4.628392	0.000006	0.000006
H	-3.381258	2.017048	-0.718223

92-94-4-C18H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -694.684943058 (a.u.)
E(HF/CC-PVTZ) = -690.01975959
E(DLPNO-CCSD(T)/CC-PVTZ) = -693.039936704161
T1 (CC-PVTZ)= 0.009853774
T2 (CC-PVTZ)= 0.038952
E(HF/CC-PVQZ) = -690.06123821
E(DLPNO-CCSD(T)/CC-PVQZ) = -693.234887208073
E(HF/TZ-AUG) = -690.02470719
E(DLPNO-CCSD(T)/TZ-AUG) = -693.085032581
E(HF/TZ-CORE) = -690.02490984
E(DLPNO-CCSD(T)/TZ-CORE) = -693.954619477
E(HF/TZ-IT) = -690.01975959
E(DLPNO-CCSD(T)/TZ-IT) = -693.048585105
T1 (CC-PVQZ)= 0.009931470
T2 (CC-PVQZ)= 0.040595
E(HF/CBS) = -690.071345422
E(DLPNO-CCSD(T)/CBS) = -693.356987417
Enthalpic correction = 0.26846995 (a.u.)
Entropy = 120.30403 (cal/(mol*K))

C	0.692565	-1.075404	0.523649
C	1.416368	0.000000	0.000001
C	0.692565	1.075405	-0.523648
C	2.893574	0.000000	0.000000
C	-0.692565	-1.075405	0.523649
C	-0.692565	1.075405	-0.523648
C	3.612285	1.175906	0.238655
C	3.612284	-1.175906	-0.238655
C	-1.416367	0.000000	0.000000
C	5.000101	1.176413	0.238921
C	5.000100	-1.176414	-0.238922
C	-2.893574	0.000000	0.000000
C	5.700901	-0.000001	-0.000001
C	-3.612285	-1.175906	-0.238653
C	-3.612285	1.175906	0.238652
C	-5.000101	-1.176414	-0.238919

C	-5.000101	1.176414	0.238919
C	-5.700901	0.000000	0.000000
H	1.222728	-1.907937	0.967372
H	1.222727	1.907939	-0.967371
H	-1.222727	-1.907938	0.967372
H	-1.222728	1.907938	-0.967372
H	3.076894	2.092122	0.450654
H	3.076892	-2.092122	-0.450651
H	5.535870	2.096489	0.434755
H	5.535868	-2.096491	-0.434756
H	6.783107	-0.000001	-0.000002
H	-3.076893	-2.092123	-0.450649
H	-3.076893	2.092123	0.450647
H	-5.535870	-2.096491	-0.434751
H	-5.535869	2.096491	0.434750
H	-6.783107	0.000000	0.000000

95-13-6_C9H8

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -347.922133568 (a.u.)
E(HF/CC-PVTZ) = -345.57385197
E(DLPNO-CCSD(T)/CC-PVTZ) = -347.099992254849
T1 (CC-PVTZ)= 0.010174751
T2 (CC-PVTZ)= 0.038529
E(HF/CC-PVQZ) = -345.59483226
E(DLPNO-CCSD(T)/CC-PVQZ) = -347.198340815063
E(HF/TZ-AUG) = -345.57646188
E(DLPNO-CCSD(T)/TZ-AUG) = -347.122544243
E(HF/TZ-CORE) = -345.57640067
E(DLPNO-CCSD(T)/TZ-CORE) = -347.557007112
E(HF/TZ-IT) = -345.57385197
E(DLPNO-CCSD(T)/TZ-IT) = -347.10403188
T1 (CC-PVQZ)= 0.010270251
T2 (CC-PVQZ)= 0.038663
E(HF/CBS) = -345.599944586
E(DLPNO-CCSD(T)/CBS) = -347.259911068
Enthalpic correction = 0.14319571 (a.u.)
Entropy = 80.30908 (cal/(mol*K))

C	0.228449	-0.687129	-0.000002
C	0.210993	0.719877	-0.000001
C	1.661475	-1.152184	0.000003
C	-0.952765	-1.404817	-0.000001
C	1.594801	1.191836	0.000003
C	-0.995500	1.410316	-0.000001
C	2.431744	0.142888	-0.000004
C	-2.163225	-0.710302	0.000000
C	-2.182078	0.682337	0.000000
H	1.895860	-1.765664	0.876727
H	1.895863	-1.765665	-0.876720
H	-0.946175	-2.488295	0.000000
H	1.882791	2.233874	0.000004
H	-1.015076	2.493108	0.000000
H	3.510839	0.190943	-0.000006
H	-3.096453	-1.258554	0.000001
H	-3.131008	1.203323	0.000001

959-02-4-C18H14

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -694.699495919 (a.u.)
E(HF/CC-PVTZ) = -690.03127046
E(DLPNO-CCSD(T)/CC-PVTZ) = -693.058419986409
T1 (CC-PVTZ)= 0.009968946
T2 (CC-PVTZ)= 0.035125
E(HF/CC-PVQZ) = -690.07252342
E(DLPNO-CCSD(T)/CC-PVQZ) = -693.253631846160
E(HF/TZ-AUG) = -690.036085
E(DLPNO-CCSD(T)/TZ-AUG) = -693.104441242
E(HF/TZ-CORE) = -690.0363452
E(DLPNO-CCSD(T)/TZ-CORE) = -693.972933169
E(HF/TZ-IT) = -690.03127046
E(DLPNO-CCSD(T)/TZ-IT) = -693.066992008
T1 (CC-PVQZ)= 0.010008403
T2 (CC-PVQZ)= 0.037759
E(HF/CBS) = -690.082575645
E(DLPNO-CCSD(T)/CBS) = -693.376032457
Enthalpic correction = 0.26891725 (a.u.)
Entropy = 112.72474 (cal/(mol*K))

C	-0.033235	0.710369	0.575125
C	-0.033235	-0.710369	0.575124
C	1.266401	-1.410697	0.883569
C	-1.187556	-1.391913	0.292479
C	-1.187556	1.391913	0.292480
C	1.266401	1.410697	0.883570
C	2.439866	-0.699176	0.257657
C	-2.395216	-0.712933	0.007583
C	-2.395216	0.712933	0.007583
C	2.439866	0.699176	0.257656
C	3.505768	-1.385472	-0.313527
C	-3.599094	-1.396397	-0.284056
C	-3.599094	1.396397	-0.284055
C	3.505767	1.385473	-0.313528
C	4.572688	-0.694638	-0.875993
C	-4.750066	-0.705480	-0.560717
C	-4.750066	0.705480	-0.560717
C	4.572687	0.694638	-0.875993
H	1.406482	-1.428605	1.973510
H	1.228036	-2.451511	0.561387
H	-1.185700	-2.476275	0.280051
H	-1.185701	2.476275	0.280052
H	1.228036	2.451512	0.561391
H	1.406483	1.428601	1.973511
H	3.498717	-2.469094	-0.322076
H	-3.596289	-2.479819	-0.284679
H	-3.596290	2.479819	-0.284678
H	3.498715	2.469094	-0.322079
H	5.396168	-1.239299	-1.319511
H	-5.664742	-1.240490	-0.781407
H	-5.664742	1.240491	-0.781406
H	5.396167	1.239299	-1.319513

C2H2

Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -77.3667641761 (a.u.)
E(HF/CC-PVTZ) = -76.84989546
E(DLPNO-CCSD(T)/CC-PVTZ) = -77.186755304477
T1 (CC-PVTZ)= 0.012859011
T2 (CC-PVTZ)= 0.057507
E(HF/CC-PVQZ) = -76.85492796
E(DLPNO-CCSD(T)/CC-PVQZ) = -77.208539864876
E(HF/TZ-AUG) = -76.85065943
E(DLPNO-CCSD(T)/TZ-AUG) = -77.1912500808
E(HF/TZ-CORE) = -76.85073417
E(DLPNO-CCSD(T)/TZ-CORE) = -77.2886956256
E(HF/TZ-IT) = -76.84989546

```
E(DLPNO-CCSD(T)/TZ-IT) = -77.1875184453
T1 (CC-PVQZ)= 0.013193077
T2 (CC-PVQZ)= 0.056345
E(HF/CBS) = -76.8561542434
E(DLPNO-CCSD(T)/CBS) = -77.2219906248
Enthalpic correction = 0.02978190 (a.u.)
Entropy = 47.99323 (cal/(mol*K))

 C     0.000000     0.000000     0.598396
 C     0.000000     0.000000    -0.598396
 H     0.000000     0.000000     1.661069
 H     0.000000     0.000000    -1.661069
```

C2H4

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -78.6277014591
(a.u.)
E(HF/CC-PVTZ) = -78.06404123
E(DLPNO-CCSD(T)/CC-PVTZ) = -78.438256057418
T1 (CC-PVTZ)= 0.010513511
T2 (CC-PVTZ)= 0.061502
E(HF/CC-PVQZ) = -78.06932711
E(DLPNO-CCSD(T)/CC-PVQZ) = -78.461284300650
E(HF/TZ-AUG) = -78.06488964
E(DLPNO-CCSD(T)/TZ-AUG) = -78.4431355059
E(HF/TZ-CORE) = -78.06464178
E(DLPNO-CCSD(T)/TZ-CORE) = -78.5396238957
E(HF/TZ-IT) = -78.06404123
E(DLPNO-CCSD(T)/TZ-IT) = -78.438813997
T1 (CC-PVQZ)= 0.010825788
T2 (CC-PVQZ)= 0.058788
E(HF/CBS) = -78.0706151353
E(DLPNO-CCSD(T)/CBS) = -78.4755194558
Enthalpic correction = 0.05332292 (a.u.)
Entropy = 52.36378 (cal/(mol*K))

 C     0.000000     0.000000     0.662305
 C     0.000000     0.000000    -0.662305
 H     0.000000     0.921446     1.232034
 H     0.000000    -0.921446     1.232034
 H     0.000000     0.921446    -1.232034
 H     0.000000    -0.921446    -1.232034
```

C2H6

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -79.8694018123
(a.u.)
E(HF/CC-PVTZ) = -79.25979416
E(DLPNO-CCSD(T)/CC-PVTZ) = -79.674322525572
T1 (CC-PVTZ)= 0.007468765
T2 (CC-PVTZ)= 0.029720
E(HF/CC-PVQZ) = -79.26503207
E(DLPNO-CCSD(T)/CC-PVQZ) = -79.698640374233
E(HF/TZ-AUG) = -79.26023793
E(DLPNO-CCSD(T)/TZ-AUG) = -79.6797994249
E(HF/TZ-CORE) = -79.26035093
E(DLPNO-CCSD(T)/TZ-CORE) = -79.7753160644
E(HF/TZ-IT) = -79.25979416
E(DLPNO-CCSD(T)/TZ-IT) = -79.6746384612
T1 (CC-PVQZ)= 0.007995504
T2 (CC-PVQZ)= 0.028737
E(HF/CBS) = -79.2663084063
E(DLPNO-CCSD(T)/CBS) = -79.713839909
Enthalpic correction = 0.07651280 (a.u.)
Entropy = 54.54641 (cal/(mol*K))

 C     0.000000     0.000000     0.763109
 C     0.000000     0.000000    -0.763109
 H     0.000000     1.017120     1.160157
 H    -0.880852    -0.508560     1.160157
 H     0.880852    -0.508560     1.160157
 H     0.000000    -1.017120    -1.160157
 H    -0.880852     0.508560    -1.160157
 H     0.880852     0.508560    -1.160157
```

C3H4

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -116.714224469
(a.u.)
E(HF/CC-PVTZ) = -115.90585091
E(DLPNO-CCSD(T)/CC-PVTZ) = -116.432347833417
T1 (CC-PVTZ)= 0.012005709
T2 (CC-PVTZ)= 0.057622
E(HF/CC-PVQZ) = -115.91335909
E(DLPNO-CCSD(T)/CC-PVQZ) = -116.465640886018
E(HF/TZ-AUG) = -115.9070457
E(DLPNO-CCSD(T)/TZ-AUG) = -116.439837834
E(HF/TZ-CORE) = -115.90692836
E(DLPNO-CCSD(T)/TZ-CORE) = -116.584954281
E(HF/TZ-IT) = -115.90585091
E(DLPNO-CCSD(T)/TZ-IT) = -116.433447691
T1 (CC-PVQZ)= 0.012174169
T2 (CC-PVQZ)= 0.056172
E(HF/CBS) = -115.915188629
E(DLPNO-CCSD(T)/CBS) = -116.486286413
Enthalpic correction = 0.05802210 (a.u.)
Entropy = 58.13151 (cal/(mol*K))

 C     0.000000     0.000000     0.000000
 C     0.000000     0.000000     1.300142
 C     0.000000     0.000000    -1.300142
 H     0.000000     0.926262     1.863180
 H     0.000000    -0.926262     1.863180
 H    -0.926262     0.000000    -1.863180
 H     0.926262     0.000000    -1.863180
```

C4H2

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -153.554447827
(a.u.)
E(HF/CC-PVTZ) = -152.55140171
E(DLPNO-CCSD(T)/CC-PVTZ) = -153.194115432570
T1 (CC-PVTZ)= 0.013583813
T2 (CC-PVTZ)= 0.045576
E(HF/CC-PVQZ) = -152.56077893
E(DLPNO-CCSD(T)/CC-PVQZ) = -153.236128548238
E(HF/TZ-AUG) = -152.5526373
E(DLPNO-CCSD(T)/TZ-AUG) = -153.202722578
E(HF/TZ-CORE) = -152.55316291
E(DLPNO-CCSD(T)/TZ-CORE) = -153.398241899
E(HF/TZ-IT) = -152.55140171
E(DLPNO-CCSD(T)/TZ-IT) = -153.196068262
T1 (CC-PVQZ)= 0.013749099
T2 (CC-PVQZ)= 0.045904
```

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E(HF/CBS) = -152.563063904
E(DLPNO-CCSD(T)/CBS) = -153.262228905
Enthalpic correction = 0.04164807 (a.u.)
Entropy = 59.32272 (cal/(mol*K))

 C     0.000000     0.000000     0.681784
 C     0.000000     0.000000    -0.681784
 C     0.000000     0.000000     1.886599
 C     0.000000     0.000000    -1.886599
 H     0.000000     0.000000     2.948841
 H     0.000000     0.000000    -2.948841
```

C6H6

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -232.356304711
(a.u.)
E(HF/CC-PVTZ) = -230.77978009
E(DLPNO-CCSD(T)/CC-PVTZ) = -231.803107791681
T1 (CC-PVTZ)= 0.009859055
T2 (CC-PVTZ)= 0.034815
E(HF/CC-PVQZ) = -230.79406122
E(DLPNO-CCSD(T)/CC-PVQZ) = -231.869180701524
E(HF/TZ-AUG) = -230.78163082
E(DLPNO-CCSD(T)/TZ-AUG) = -231.817412406
E(HF/TZ-CORE) = -230.78149286
E(DLPNO-CCSD(T)/TZ-CORE) = -232.107954621
E(HF/TZ-IT) = -230.77978009
E(DLPNO-CCSD(T)/TZ-IT) = -231.805725951
T1 (CC-PVQZ)= 0.009967886
T2 (CC-PVQZ)= 0.038096
E(HF/CBS) = -230.797541143
E(DLPNO-CCSD(T)/CBS) = -231.910454626
Enthalpic correction = 0.10246743 (a.u.)
Entropy = 64.48581 (cal/(mol*K))

 C     0.000000     1.390481     0.000000
 H     0.000000     2.473049     0.000000
 C     1.204192     0.695240     0.000000
 H     2.141723     1.236524     0.000000
 C     1.204192    -0.695240     0.000000
 H     2.141723    -1.236524     0.000000
 C     0.000000    -1.390481     0.000000
 H     0.000000    -2.473049     0.000000
 C    -1.204192    -0.695240     0.000000
 H    -2.141723    -1.236524     0.000000
 C    -1.204192     0.695240     0.000000
 H    -2.141723     1.236524     0.000000
```

CH4

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -40.5394392207
(a.u.)
E(HF/CC-PVTZ) = -40.21333182
E(DLPNO-CCSD(T)/CC-PVTZ) = -40.438113683313
T1 (CC-PVTZ)= 0.007179930
T2 (CC-PVTZ)= 0.038642
E(HF/CC-PVQZ) = -40.21614423
E(DLPNO-CCSD(T)/CC-PVQZ) = -40.450925036720
E(HF/TZ-AUG) = -40.21356698
E(DLPNO-CCSD(T)/TZ-AUG) = -40.4409277351
E(HF/TZ-CORE) = -40.21362074
E(DLPNO-CCSD(T)/TZ-CORE) = -40.4886521304
E(HF/TZ-IT) = -40.21333182
E(DLPNO-CCSD(T)/TZ-IT) = -40.4382379139
T1 (CC-PVQZ)= 0.007841140
T2 (CC-PVQZ)= 0.028106
E(HF/CBS) = -40.2168295379
E(DLPNO-CCSD(T)/CBS) = -40.4589068709
Enthalpic correction = 0.04697154 (a.u.)
Entropy = 44.48241 (cal/(mol*K))

 C     0.000000     0.000000     0.000000
 H     0.628862     0.628862     0.628862
 H    -0.628862    -0.628862     0.628862
 H    -0.628862     0.628862    -0.628862
 H     0.628862    -0.628862    -0.628862
```

H2

```
Charge of molecule: 0
Multiplicity: 1
E (B3LYP-D3/def2tzvp, G09)= -1.17978981202
(a.u.)
E(HF/CC-PVTZ) = -1.13292558
E(DLPNO-CCSD(T)/CC-PVTZ) = -1.172370827810
T1 (CC-PVTZ)= 0.005666456
T2 (CC-PVTZ)= 0.056538
E(HF/CC-PVQZ) = -1.13342128
E(DLPNO-CCSD(T)/CC-PVQZ) = -1.173834778444
E(HF/TZ-AUG) = -1.13299202
E(DLPNO-CCSD(T)/TZ-AUG) = -1.17266693301
E(HF/TZ-CORE) = -1.13292558
E(DLPNO-CCSD(T)/TZ-CORE) = -1.17234614622
E(HF/TZ-IT) = -1.13292558
E(DLPNO-CCSD(T)/TZ-IT) = -1.17237082781
T1 (CC-PVQZ)= 0.005785357
T2 (CC-PVQZ)= 0.055147
E(HF/CBS) = -1.13354206861
E(DLPNO-CCSD(T)/CBS) = -1.17466212833
Enthalpic correction = 0.01304449 (a.u.)
Entropy = 31.13863 (cal/(mol*K))

 H     0.000000     0.000000     0.371989
 H     0.000000     0.000000    -0.371989
```