

Day 13: Estimation methods for thermochemical and rate parameters

To apply transition state theory and the various unimolecular rate theories, we need to know something about the structure and energies of the reactant(s), product(s), and transition state. If we know the rate constant for an elementary reaction in one direction, we need to know the reaction thermochemistry (ΔH , ΔS , ΔC_p) to get the equilibrium constant and the rate constant in the reverse direction. There are essentially four ways to obtain this information:

- (1) From the literature. Of course, this is the best way because it is the easiest and often the most accurate method. The first place that one should generally look for thermochemical data is in the NIST Chemistry WebBook, available at <http://webbook.nist.gov>. This database contains thermochemical properties for more than 7000 small organic and inorganic compounds, and includes the entire contents of several other databases. For hydrocarbons, the thermodynamic database supplied with process simulators (i.e. Aspen or HYSIS) can be a useful resource. Another online source of thermochemical data useful for high-temperature chemical kinetics is the HiTempThermo page maintained by Sandia National Laboratories at <http://www.ca.sandia.gov/HiTempThermo/>. Another valuable source is the thermochemical property database assembled by Burcat, which is available online at <ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics/>. NIST has also compiled a comprehensive database of gas-phase chemical kinetics, available at <http://www.kinetics.nist.gov>.
- (2) From experiment. This is usually the most reliable method, but also the most difficult, and is usually not an option.
- (3) From *ab initio* molecular orbital calculations. These methods can provide accurate structures and vibrational frequencies for small to moderately large molecules *and transition states*. For small molecules, energies can be calculated with ‘chemical accuracy’, which usually means ± 1 or 2 kcal/mole. This is generally much easier than experiments, but in many cases is still less reliable.
- (4) Empirical estimation methods. There are some simple “quick and dirty” methods of estimating thermochemical quantities for molecules for which no data are available, and for estimating reaction rates for elementary reactions that have not previously been studied. These are not always reliable, but they can often provide better estimates of a rate constant than (a) blind guessing, or (b) neglecting the reaction (effectively assuming a rate constant of 0). In the literature, you will find that option (b) shows up pretty often. This makes no sense, because even if we have to purely guess a rate constant, we can almost always make a guess that is closer to correct than guessing zero.

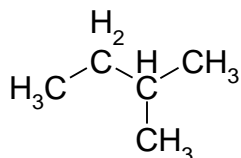
Option (1) is straightforward. First using the references cited above, then using SciFinder Scholar (Chemical Abstracts) and other indexes, you should be able to find out whether the property that you need has been measured. Options (2) and (3) could each have a course of their own. Today we’ll briefly consider option (4). The best source that I have found for this is ‘Thermochemical Kinetics’ by Sidney Benson (Wiley and Sons, New York, 1968; 2nd edition

1976). Parts of this are a bit dated, but I have yet to find anything newer that is also better. Quoting from the preface to the 1st edition of this book (1968):

“Over the last decade, a number of relatively facile methods for the rapid and quantitative estimation of both thermochemical data and kinetic parameters for gas phase reactions have been developed in my laboratories. They have now reached the stage in which they provide a very useful tool for the critical analysis of relatively complex chemical reaction systems. This book is a systematic presentation of these methods with examples of their application.”

Professor Benson is, perhaps, a bit overoptimistic (and not particularly humble), but he did develop a set of useful and simple methods that are still widely used.

First, we'll consider the group additivity or group contribution method for estimating the thermochemical properties of molecules. In this method, the molecule is considered to be made up of several groups, and the thermochemical properties of interest (enthalpy of formation, $\Delta H_f^\circ(298\text{ K})$; standard entropy, $S^\circ(298\text{ K})$; and heat capacity as a function of temperature, $C_p^\circ(T)$) are written as the sum of contributions from each group. This is probably best illustrated by example. Consider isopentane



Each heavy atom (non-hydrogen atom) is a group. Groups are differentiated by what other atoms they are bonded to. Thus, isopentane is made up of

- 3 C-(H)₃(C) groups
- 1 C-(H)₂(C)₂ group, and
- 1 C-(H)(C)₃ group

There are tables of group additivity values for common groups like these. One place that these tables can be found is in the above-mentioned book by Sidney Benson. From that source, we find:

Group	$\Delta H_f^\circ(298)$ kcal mol ⁻¹	$S^\circ(298)$ cal mol ⁻¹ K ⁻¹	$C_p^\circ(T)$ cal mol ⁻¹ K ⁻¹						
			300	400	500	600	800	1000	1500
C-(H) ₃ (C)	-10.08	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
C-(H) ₂ (C) ₂	-4.95	9.42	5.50	6.95	8.25	9.35	11.07	12.34	14.25
C-(H)(C) ₃	-1.90	-12.07	4.54	6.00	7.17	8.05	9.31	10.05	11.17

So, we estimate the thermochemical properties of isopentane as

$$\Delta H_f^\circ(298) = 3(-10.08) + (-4.95) + -1.90 = -37.1 \text{ kcal/mol}$$

$$S^\circ(298) = 3(30.41) + 9.42 - 12.07 = 88.6 \text{ cal/(mol K)}$$

$$C_p^\circ(300) = 3(6.19) + 5.50 + 4.54 = 28.6 \text{ cal/(mol K), etc.}$$

It really is that easy. Separate groups are defined for multiple bonds, atoms in aromatic rings, etc. There are additional corrections that are applied for compounds containing rings, as well as small corrections to account for differences between cis- and tran- isomers, etc. In addition to hydrocarbons, there are tables of group additivity parameters for oxygen, sulfur, phosphorous, boron, and nitrogen containing compounds, and some organometallics. NIST has set up a web-based group additivity calculator at <http://webbook.nist.gov/chemistry/grp-add/>, where you can draw a molecule (containing only known groups) and get group additivity estimates for its properties. For types of compounds that have well established group values based on a substantial database of thermodynamic properties, like hydrocarbons and hydrocarbon derivatives, these group additivity methods do very well – typically predicting heats of formation to within 2-3 kcal/mole. Unfortunately, they cannot be applied to transition states, or to reactive or exotic species that contain groups for which there are no tabulated group values available. A fairly large table of group additivity parameters is included at the end of this set of notes (although this is somewhat obsolete given the web-based utility mentioned above).

Entropies and specific heats can also be calculated using statistical mechanical formulae along with estimated vibrational frequencies and moments of inertia. For entropy, we have, from statistical mechanics

$$\frac{S^\circ}{R} = \ln(Q) + \frac{\partial \ln(Q)}{\partial T} =$$

$$\ln \left(\left(\frac{2\pi mkT}{h^2} \right)^{3/2} \frac{V e^{5/2}}{N} \right) + \ln \left(\frac{e^{3/2} \sqrt{\pi}}{\sigma} \left(\frac{8\pi^2 I_A kT}{h^2} \right)^{1/2} \left(\frac{8\pi^2 I_B kT}{h^2} \right)^{1/2} \left(\frac{8\pi^2 I_C kT}{h^2} \right)^{1/2} \right)$$

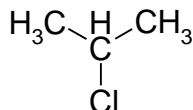
$$+ \sum_{j=1}^{3N-6} \left(\frac{\frac{hv}{kT}}{\exp\left(\frac{hv}{kT}\right) - 1} - \ln \left(1 - \exp\left(-\frac{hv}{kT}\right) \right) \right) + \ln(g_e)$$

Likewise, for heat capacity we have

$$\frac{C_p^\circ}{R} = \frac{\partial}{\partial T} \left(kT^2 \left(\frac{\partial \ln(Q)}{\partial T} \right) \right) = 4 + \sum_{j=1}^{3N-6} \left(\frac{hv}{kT} \right)^2 \frac{\exp\left(\frac{hv}{kT}\right)}{\left(\exp\left(\frac{hv}{kT}\right) - 1 \right)^2}$$

The above equations are for a non-linear molecule. For a linear molecule the expressions are slightly different. These equations, along with the corresponding equations for energy, enthalpy, etc. can be found in statistical mechanics textbooks such as ‘Statistical Mechanics’, by Donald A. McQuarrie (HarperCollins, New York, 1976). Computing the heat capacity only requires estimates of the vibrational frequencies. Computing the entropy also requires estimates of the moments of inertia. If we guess a structure for a molecule, the moments of inertia can be calculated from it. Vibrational frequencies can be assigned based on known vibrational frequencies of similar molecules as follows. We take the total number of vibrational modes (3N-6 for a non-linear molecule) and categorize them as stretches, bends, etc. A molecule of N atoms containing no rings has N - 1 bonds and therefore has N - 1 stretching modes. A molecule with

one ring has N bonds and N stretching modes, etc. The remaining $2N - 5$ modes will either be bending (deformation) modes of various types or internal rotations. An internal rotation is possible around any single bond that is not part of a ring or otherwise constrained from rotating. We usually want to further classify each type of mode based on whether it involves an H atom or only 'heavy' atoms. Due to its small mass, vibrations involving H have much higher frequencies than those involving only heavy atoms. If there are P heavy atoms in our molecule, then there are $3P-6$ modes involving only heavy atoms. For an acyclic molecule, $P-1$ of these will be stretches, and the remaining $2P-5$ will be deformations or internal rotations. As an example of these vibrational assignments, consider isopropyl chloride.



This molecule has 11 atoms, and therefore 27 vibrational frequencies. There are 10 stretching modes (7 C-H stretches, 2 C-C stretches, and 1 C-Cl stretch). There are 2 internal rotations (rotation of the 2 CH₃ groups, these only involve H atoms). There are then 15 bending or deformational modes. Since there are 4 heavy atoms, there are 6 total modes that involve only heavy atoms. Three of these are the stretches listed above, so there must be 3 bending modes involving only heavy atoms (C and Cl) and that leaves 12 bending modes involving H atoms. So, we might assign the frequencies as

- 7 C-H stretches at 3100 cm⁻¹
- 2 C-C stretches at 1000 cm⁻¹
- 1 C-Cl stretch at 650 cm⁻¹
- 4 H-C-H bends at 1450 cm⁻¹
- 8 H-C-C bends at 1150 cm⁻¹
- 2 C-C-Cl bends at 400 cm⁻¹
- 1 C-C-C bend at 420 cm⁻¹

The two internal rotations are treated separately from the vibrations. They are characterized by both a moment of inertia and by a rotational barrier height (the energy needed to rotate the CH₃ group past through the highest energy angle, where the H's overlap with the atoms connected to the adjacent carbon). Making approximate vibrational assignments like these allows us to calculate the vibrational contributions to the entropy, specific heat, and partition functions. If we do this for reactants and products in a reaction, we can often make some educated guesses about the frequencies of the transition state in the same ways. Some modes will be the same in reactants and products. Others will change from one kind to another. For example, consider the reaction



The reactant has

- 1 internal rotation
- 4 H-Si-Si bends (2 near 400 cm⁻¹, 2 near 700 cm⁻¹)
- 1 Si-Si stretch at around 500 cm⁻¹
- 6 H-Si-H bends around 1000 cm⁻¹

6 Si-H stretches around 2300 cm^{-1}

We could have guesstimated these as we did for isopropyl chloride above, except that we would probably not have gotten the H-Si-Si bending frequencies right.

The first product, SiH_4 has

5 H-Si-H bends around 1000 cm^{-1}

4 Si-H stretches around 2300 cm^{-1}

The second product, SiH_2 has

1 H-Si-H bend around 1000 cm^{-1}

2 Si-H stretches around 2300 cm^{-1}

We could have guessed the product frequencies pretty accurately.

Since this reaction converts 1 molecule into 2 molecules, 6 vibrational frequencies are lost. These become the 3 translational and 3 rotational degrees of freedom of the second product molecule. In this case, we see that the six Si-H stretches and 6 H-Si-H bends are conserved during the reaction. The Si-Si stretch, the four H-Si-Si bends, and the internal rotation are lost during the reaction. We could try to guess the transition state frequencies (from which we could calculate a partition function for the TS) by interpolating between the reactant and product frequencies. (How would you do this?) The actual transition state frequencies (calculated using *ab initio* quantum mechanical methods) are:

1 imaginary frequency (reaction coordinate) at $200i\text{ cm}^{-1}$

1 internal rotation

4 H-Si-Si bends around 360, 520, 620, and 700 cm^{-1}

6 H-Si-H bends around 830, 910, 970, 1020, 1050, and 1650 cm^{-1}

1 Si-H stretch around 1450 cm^{-1} (corresponding to the H atom that is moving from one Si to the other)

5 Si-H stretches around 2300 cm^{-1}

In this case, the distinction between H-Si-Si bends and H-Si-H bends is somewhat arbitrary. We see that the Si-Si stretching mode has become the reaction coordinate. 5 of the Si-H stretching modes, three of the H-Si-H bending modes, and 1 of the H-Si-Si bending modes are unchanged. However, several of the other modes are higher than in the reactant or product. In this case, interpolating between reactant and product frequencies would not work very well. In other cases it would work somewhat better.

Rules of thumb for estimating reaction rate parameters (also based mostly on Benson's book)

(1) Unimolecular dissociation of one molecule into two by *simple bond fission*.

Examples: $\text{C}_2\text{H}_6 \rightarrow 2\text{CH}_3$, $\text{C}_2\text{H}_5\text{ONO}_2 \rightarrow \text{C}_2\text{H}_5\text{O} + \text{NO}_2$, $\text{C}_2\text{H}_5\text{I} \rightarrow \text{C}_2\text{H}_5 + \text{I}$

These reactions proceed by the breaking of a single bond. There is no activation barrier beyond the heat of reaction, so the activation energy is approximately equal to the heat of reaction (ΔH_{rxn}). These reactions convert internal (vibrational) degrees of freedom to external (translational and rotational) degrees of freedom. The entropy of the products is therefore substantially greater than that of the reactants. Likewise, the transition state, which is on its way to losing the vibrational modes, is 'looser' and bigger than the reactant, and the entropy of activation is positive. Transition states for reactions like this with no maximum in potential energy along the reaction path are referred to as *loose transition states*. In the thermodynamic formulation of transition state theory, we saw that:

$$k_f = \frac{kT}{h} \exp\left(\frac{\Delta S_o^\ddagger}{R}\right) \exp\left(\frac{-\Delta H_o^\ddagger}{RT}\right)$$

If there is no barrier to reaction beyond the heat of reaction, $E_a \cong \Delta H_o^\ddagger \cong \Delta H_{rxn}$. Because the entropy of the transition state is higher than that of the reactants, the factor $\exp\left(\frac{\Delta S_o^\ddagger}{R}\right)$ is greater than 1, so the pre-exponential factor will be larger than the *universal frequency factor*, $\frac{kT}{h}$. Pre-exponential factors for simple bond fission reactions range from about 10^{15} to 10^{17} s^{-1} . Note that some reactions that might first appear to be simple bond fissions are not. For example, $\text{C}_2\text{H}_5 \rightarrow \text{C}_2\text{H}_4 + \text{H}$ involves the breaking of the C-H bond, but it also involves the formation of a bond between the carbon atoms (the C-C single bond becomes a C-C double bond). This reaction has a pre-exponential around $10^{13.6} \text{ s}^{-1}$, and an activation energy greater than the heat of reaction.

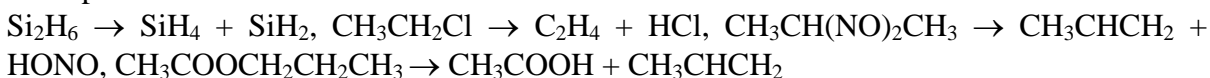
(2) Unimolecular isomerization reactions.

Example: cis-butene \rightarrow trans-butene

In general, isomerization reactions will have an entropy of activation near zero – the transition state will be about the same size and have about the same frequencies as the reactant. There may be a small negative entropy of activation since one vibrational mode in the reactant becomes the reaction coordinate in the transition state. Because there is almost no entropy of activation, pre-exponential factors for isomerizations are typically around 10^{13} s^{-1} . In general, there is no simple way to predict the activation energy of these reactions. However, for the particular class of cis-trans isomerizations, the activation energy is approximately equal to the energy needed to change the double bond into a single bond and a biradical (breaking the pi bond, but not the sigma bond joining the two atoms).

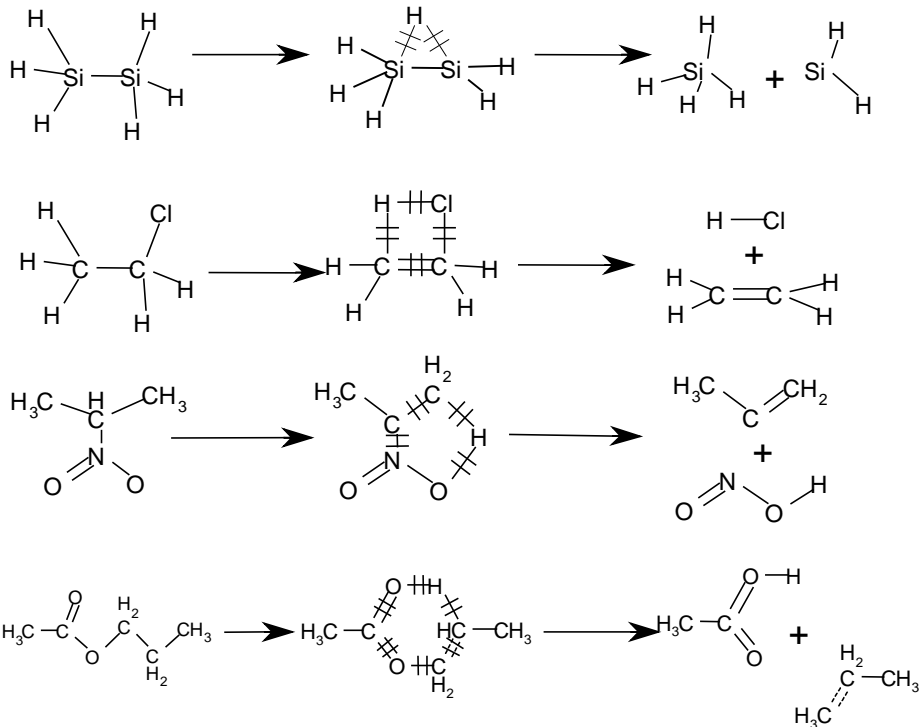
(3) Complex unimolecular dissociation reactions with cyclic transition states

Examples:



These four reactions proceed through transition states with 3, 4, 5, and 6-membered rings, respectively.

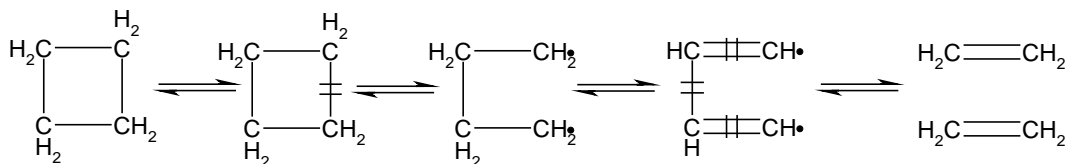
These reactions look like:



There is no simple way to predict the activation energy of these reactions. The best that one can do is to try to find a similar reaction and make a guess by analogy. The entropy of activation for these reactions can be positive or negative. The entropy of reaction is always positive, because we are forming two molecules from one (converting 6 vibrational degrees of freedom to rotational and translational degrees of freedom). This leads to an increase in entropy in going from reactant to transition state, as bonds become longer and looser (lower vibrational frequencies = more entropy contribution from those vibrations). However, there is entropy lost in forming the ring. In the transition state, some number of reactant bonds are replaced by a larger number of partial bonds. The pre-exponential factor is around $10^{13.5}$ for a large number of four-centered eliminations like the HCl elimination shown above. Pre-exponential factors for reactions with 5- and 6-center transition states range from 10^{11} (substantial negative entropy of activation) to 10^{15} (substantial positive entropy of activation).

(4) Unimolecular reactions proceeding through biradical transition states.

Example: cyclobutane decomposition



These involve complete breaking of bonds followed by forming of new bonds in a separate step. They are therefore best considered as multi-step processes, involving one transition state for the bond breaking step and another for the bond forming step as shown above.

(5) Bimolecular association reactions

Example: $C_2H_5 + I \rightarrow C_2H_5I$, or the reverse of any of the other unimolecular decomposition reactions listed above.

These are the reverse of unimolecular decomposition. The decomposition reaction can be analyzed by the means discussed above, and then the rate constant for the association reaction can be obtained using the equilibrium constant. When we do this, we should make sure that the rate of the association reaction does not exceed the collision rate (if it does, then there is a problem with our decomposition rate constant or with the equilibrium constant or both)

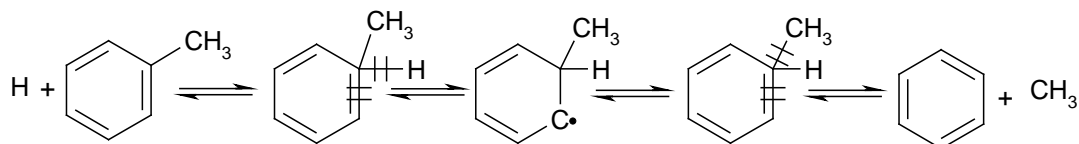
(6) Bimolecular metathesis reactions

Examples: $H + C_2H_6 \rightarrow H_2 + C_2H_5$, $CH_3 + C_2H_6 \rightarrow CH_4 + C_2H_5$, $CH_3 + CCl_4 \rightarrow CH_3Cl + CCl_3$

For bimolecular reactions, the entropy of activation is always negative, because they combine two reactants into one transition state (converting translational and rotational degrees of freedom into vibrations). For atom + molecule metathesis reactions, only translational degrees of freedom are lost. For a large number of atom + molecule metathesis reactions, the pre-exponential factor is about $10^{14} \text{ cm}^3 \text{ mole}^{-1} \text{ s}^{-1}$. For molecule plus molecule metathesis reactions, rotational degrees of freedom are often lost, and therefore the entropy of activation is more negative and the pre-exponential is smaller. You can also think of this as relating to the fact that a molecule + molecule reaction requires a certain orientation of both reactants, while a molecule + atom reaction requires no special orientation of the (spherically symmetric) atom. For a large number of molecule + molecule metathesis reactions, the pre-exponential factor is about $10^{11.5} \text{ cm}^3 \text{ mole}^{-1} \text{ s}^{-1}$. There is no general means of estimating the activation energy for these reactions.

(7) Bimolecular displacement reactions

Example:



These reactions are generally two-step processes. First the reactions undergo an association reaction to form a highly reactive intermediate (which may also be highly vibrationally excited). This then decomposes in a second step to give the products. The two steps need to be analyzed separately as association and decomposition reactions. This can be especially difficult since we are likely to know very little about the reactive intermediate – not to mention the two transition states. If the reactive intermediate is formed in a highly excited state and does not maintain an equilibrium distribution of vibrational energies, then this must be analyzed as a chemically activated reaction system.

As we have seen above, there are some reasonable ways to go about estimating the thermochemistry of a reaction and the pre-exponential factor for certain types of reactions. Unfortunately, there are not similar methods for predicting the activation energies of chemical reactions. For certain classes of reactions, some correlations are available. Sometimes the activation energies of a series of reactions of the same type can be written as

$$E_a = \alpha \Delta H_{rxn}.$$

This is known as an Evans-Polanyi relationship (or sometimes as a linear-free-energy relationship). It is a simple, but not terribly accurate or widely applicable, means of correlating the activation energy with the heat of reaction.

After completing your study of these lecture notes and the associated homework, you should be able to:

- (1) List several methods of obtaining thermochemical and rate parameters and rank the methods in terms of ease of use, accuracy and reliability, and range of applicability.
- (2) Apply a group additivity method to estimate the heat of formation of a compound.
- (3) Identify the types of vibrational degrees of freedom in a molecule, and classify them to make estimates of the molecules vibrational frequencies.
- (4) Use statistical mechanics formulae to estimate the entropy and heat capacity of compounds
- (5) Rationalize the pre-exponential factor and activation energy of a reaction based on the expected structure of reactants, transition state, and products.

Group Additivity parameters from THERM database(E.R. Ritter J. Bozzelli *Int. J. Chem. Kin.* **23** 767 (1991).)UNITS: H_f = kcal/mole; S , C_p = cal/mole/K

H = hydrogen

C = carbon

CD = carbon with double bond

CT = carbon with triple bond

CB = carbon in a benzene (aromatic) ring

N = nitrogen

NO = NO group (treated as a single unit)

NO2 = NO₂ group (treated as a single unit)

NA = azo group (R-N=N)

NI = imino N atom (N=C)

CN = cyano group

O = oxygen

OO = peroxy group

CO = carbonyl group

Groups named CY- and BCY- are ring corrections for cyclic and bicyclic compounds

C3 = cyclopropane ring, C4 = cyclobutane ring, etc.

/E = ring with a double bond in it (cyclo-X-ene)

/DE = ring with two double bonds in it (cyclo-X-diene)

/TE = ring with three double bonds in it (cyclo-X-triene)

Numbers denote locations of functional groups (double bonds, etc.) as in organic chemistry nomenclature.

	H_f	S	C_p :						
			300	400	500	600	800	1000	1500
C-(C)(H) ₃	-10.20	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
C-(CB)(H) ₃	-10.20	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
C-(CD)(H) ₃	-10.20	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
C-(CT)(H) ₃	-10.20	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
C-(C) ₂ (H) ₂	-4.93	9.42	5.50	6.95	8.25	9.35	11.07	12.34	14.20
C-(C) ₃ (H)	-1.90	-12.07	4.54	6.00	7.17	8.05	9.31	10.05	11.18
C-(C)4	0.50	-35.10	4.37	6.13	7.36	8.12	8.77	8.76	8.12
C-(C)(CD)(H) ₂	-4.76	9.80	5.12	6.86	8.32	9.49	11.22	12.48	14.36
C-(CD) ₂ (H) ₂	-4.29	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.40
C-(CB)(CD)(H) ₂	-4.29	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.40
C-(C)(CT)(H) ₂	-4.73	10.30	4.95	6.56	7.93	9.08	10.86	12.19	14.20
C-(C)(CB)(H) ₂	-4.86	9.34	5.84	7.61	8.98	10.01	11.49	12.54	13.76
C-(C) ₂ (CD)(H)	-1.48	-11.69	4.16	5.91	7.34	8.19	9.46	10.19	11.28
C-(C) ₂ (CT)(H)	-1.72	-11.19	3.99	5.61	6.85	7.78	9.10	9.90	11.12
C-(C) ₂ (CB)(H)	-0.98	-12.15	4.88	6.66	7.90	8.75	9.73	10.25	10.68
C-(C)(CB)(CT)(H)	-1.55	-11.65	4.33	6.27	7.58	8.48	9.52	10.1	10.63
C-(C)(CB)(CD)(H)	-1.56	-11.77	4.50	6.57	8.07	8.89	9.88	10.39	10.79
C-(C)(CD)(CT)(H)	-2.36	-11.19	3.61	5.52	7.02	7.92	9.25	9.9	11.23
C-(C)(CD) ₂ (H)	-2.31	-11.31	3.78	5.85	7.51	8.30	9.61	10.33	11.39
C-(C)(CT) ₂ (H)	-2.54	-10.69	3.44	5.22	6.53	7.51	8.89	9.75	11.07
C-(C)(CB) ₂ (H)	-1.06	-12.23	5.22	7.32	8.63	8.45	10.15	10.45	10.19
C-(CB)(CD) ₂ (H)	-1.39	-11.39	4.12	6.51	8.24	9.00	10.03	10.53	10.89
C-(CD) ₃ (H)	-2.14	-10.93	3.4	5.76	7.68	8.44	9.76	10.47	11.5
C-(CB) ₃ (H)	-0.34	-12.31	5.56	7.98	9.36	10.15	10.57	10.65	9.7
C-(C) ₃ (CD)	1.68	-34.72	3.99	6.04	7.43	8.26	8.92	8.96	8.23
C-(C) ₃ (CB)	2.81	-35.18	4.37	6.79	8.09	8.78	9.19	8.96	7.63

C-(C) ₃ (CT)	2.81	-35.18	4.37	6.79	8.09	8.78	9.19	8.96	7.63
C-(C) ₂ (CD) ₂	1.61	-34.34	3.61	5.98	7.51	8.37	9.00	9.02	8.34
C-(C)(CD) ₃	2.54	-33.96	3.32	5.86	7.57	8.54	9.22	9.36	8.45
C-(C) ₂ (CB)(CD)	2.99	-34.8	3.99	6.70	8.16	8.92	9.34	9.16	7.74
C-(C) ₂ (CD)(CT)	2.99	-34.8	3.99	6.70	8.16	8.92	9.34	9.16	7.74
C-(C)(CB) ₂ (CD)	5.1	-34.88	3.99	7.36	8.89	9.58	9.76	9.16	7.25
C-(C)(CB)(CD)(CT)	5.1	-34.88	3.99	7.36	8.89	9.58	9.76	9.16	7.25
C-(C)(CD)(CT) ₂	5.1	-34.88	3.99	7.36	8.89	9.58	9.76	9.16	7.25
C-(C) ₂ (CB) ₂	1.16	-35.26	3.57	5.98	7.51	8.37	9.00	9.02	8.34
C-(C) ₂ (CB)(CT)	1.16	-35.26	3.57	5.98	7.51	8.37	9.00	9.02	8.34
C-(C) ₂ (CT) ₂	1.16	-35.26	3.57	5.98	7.51	8.37	9.00	9.02	8.34
C-(C)(CB) ₃	6.23	-35.34	4.37	8.11	9.55	10.10	10.03	9.36	6.65
C-(C)(CB) ₂ (CT)	6.43	-35.34	4.37	8.11	9.55	10.10	10.03	9.36	6.65
C-(C)(CB)(CT) ₂	6.23	-35.34	4.37	8.11	9.55	10.10	10.03	9.36	6.65
C-(C)(CT) ₃	6.23	-35.34	4.37	8.11	9.55	10.10	10.03	9.36	6.65
C-(CB) ₂ (CD) ₂	5.48	-34.50	3.61	7.30	8.97	9.69	9.84	9.42	7.36
C-(CB)(CD) ₂ (CT)	5.48	-34.50	3.61	7.30	8.97	9.69	9.84	9.42	7.36
C-(CD) ₂ (CT) ₂	5.48	-34.50	3.61	7.30	8.97	9.69	9.84	9.42	7.36
C-(CD)(CT)(H) ₂	-4.26	10.70	4.53	6.47	8.00	9.27	11.01	12.33	14.31
C-(CB) ₂ (H) ₂	-6.30	9.26	6.18	8.27	9.71	10.67	11.91	12.74	13.27
C-(CB)(CT)(H) ₂	-5.66	10.22	5.29	7.22	8.66	9.74	11.28	12.39	13.71
C-(CT) ₂ (H) ₂	-9.80	11.18	4.4	6.17	7.61	8.81	10.65	12.04	14.15
CD-(H) ₂	6.26	27.61	5.10	6.36	7.51	8.50	10.07	11.27	13.19
CD-(C)(H)	8.59	7.97	4.16	5.03	5.81	6.50	7.65	8.45	9.62
CD-(C) ₂	10.34	-12.70	4.10	4.61	4.99	5.26	5.80	6.08	6.36
CD-(CD)(H)	6.78	6.38	4.46	5.79	6.75	7.42	8.35	9.11	10.09
CD-(C)(CD)	8.88	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
CD-(CB)(H)	6.78	6.38	4.46	5.79	6.75	7.42	8.35	9.11	10.09
CD-(C)(CB)	8.64	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
CD-(CB)(CD)	7.18	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CD)(CT)	6.94	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CD)(CB)	8.00	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CB)(CT)	6.70	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CD) ₂	4.60	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CT) ₂	6.46	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CB) ₂	8.00	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(CT)(H)	6.78	8.03	4.46	5.79	6.75	7.42	8.35	9.11	10.09
CD-(C)(CT)	8.53	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
CT-(H)	27.25	24.70	5.28	5.99	6.49	6.87	7.47	7.96	8.85
CT-(C)	27.26	6.35	3.13	3.48	3.81	4.09	4.60	4.92	6.35
CT-(CD)	28.20	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
CT-(CB)	24.67	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
CT-(CT)	25.60	5.88	3.54	4.06	4.40	4.64	5.00	5.23	5.57
CB-(H)	3.30	11.53	3.24	4.44	5.46	6.30	7.54	8.41	9.73
CB-(C)	5.51	-7.69	2.67	3.14	3.68	4.15	4.96	5.44	5.98
CB-(CD)	5.69	-7.80	3.59	3.97	4.38	4.72	5.28	5.61	5.75
CB-(CT)	5.69	-7.80	3.59	3.97	4.38	4.72	5.28	5.61	5.75
CB-(CB)	4.96	-8.64	3.33	4.22	4.89	5.27	5.76	5.95	6.05
C-(H) ₃ (N)	-10.08	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
C-(H) ₃ (NO)	-15.10	68.40	12.59	15.82	18.52	20.66	23.79	25.90	29.80
C-(H) ₃ (NO ₂)	-15.10	68.40	12.59	15.82	18.52	20.66	23.79	25.90	29.80
C-(H) ₂ (N)(O)	-9.80	9.8	4.99	6.85	8.30	9.43	11.11	12.33	
C-(C)(CN)(H) ₂	22.50	40.20	11.10	13.40	15.50	17.20	19.70	21.30	24.56
C-(C)(H) ₂ (N)	-6.60	9.80	5.25	6.90	8.28	9.39	11.09	12.34	14.28
C-(C)(H) ₂ (NO)	-15.10	48.40	12.59	15.82	18.52	20.66	23.79	25.90	29.80
C-(C)(H) ₂ (NO ₂)	-15.10	48.98	12.76	15.74	18.26	20.27	23.29	26.33	

C-(C) ₂ (CN)(H)	25.80	19.80	11.00	12.70	14.10	15.40	17.30	18.60	20.67
C-(C) ₂ (H)(NO)	-15.80	26.90	11.99	15.21	17.72	19.61	22.18	23.70	26.24
C-(C) ₂ (H)(NO ₂)	-15.80	26.85	12.37	15.35	17.71	19.45	21.73	23.23	
C-(C) ₂ (H)(N)	-5.20	-11.70	4.67	6.32	7.64	8.39	9.56	10.23	11.37
C-(C) ₃ (NO)	-10.80	5.90	11.99	15.21	17.72	19.61	22.18	23.70	26.24
C-(C) ₃ (NO ₂)	-12.7	3.96	12.8	15.47	16.96	18.58	20.09	20.81	
C-(C) ₃ (N)	-3.20	-34.10	4.35	6.16	7.31	7.91	8.49	8.50	7.88
C-(C) ₃ (CN)	29.00	-2.80	8.65	11.16	12.89	14.05	15.51	16.1	14.87
CB-(CN)	35.80	20.50	9.80	11.20	12.30	13.10	14.20	14.90	15.27
CB-(N)	-0.50	-9.69	3.95	5.21	5.94	6.32	6.53	6.56	7.21
CB-(NO)	31.50	20.60	10.30	11.30	12.30	13.10	14.20	14.90	15.27
CB-(NO ₂)	4.32	24.39	12.26	14.18	15.58	16.66	18.25	19.24	20.56
CO-(C)(N)	-32.80	16.20	5.36	6.17	7.07	7.66	9.62	11.19	
CO-(H)(N)	-29.60	34.93	7.03	7.87	8.82	9.68	11.16	12.20	
CO-(N)(O)	-35.10	14.61	6.10	6.71	7.40	8.02	8.87	9.36	
CO-(N) ₂	-29.90	11.60	6.10	6.71	7.40	8.02	8.87	9.36	
CD-(CN)(H)	37.40	36.58	9.80	11.70	13.30	14.50	16.30	14.90	16.54
CD-(C)(NO ₂)	4.32	24.39	12.26	14.18	15.58	16.66	18.25	19.24	20.56
CD-(H)(NO ₂)	1.74	45.80	12.86	15.19	17.01	18.47	20.65	22.13	24.21
CD-(C)(CN)	39.15	15.91	9.74	11.28	12.48	13.26	14.45	14.93	15.15
CD-(CN) ₂	84.10	43.00	13.60	16.55	18.68	20.25	22.34	23.59	
CT-(CN)	63.80	35.40	10.30	11.30	12.10	12.70	13.60	14.30	15.08
N-(C)(H) ₂	4.80	29.71	5.72	6.51	7.32	8.07	9.41	10.47	12.28
N-(C) ₂ (H)	15.40	8.94	4.20	5.21	6.13	6.83	7.90	8.65	9.55
N-(C) ₃	24.40	-13.46	3.48	4.56	5.43	5.97	6.56	6.67	6.50
N-(C)(H)(N)	20.90	9.61	4.82	5.80	6.50	7.00	7.80	8.30	9.00
N-(C)(H)(NI)	21.00	9.61	4.82	5.80	6.50	7.00	7.80	8.30	9.00
N-(CB)(H) ₂	4.80	29.71	5.72	6.51	7.32	8.07	9.41	10.47	12.28
N-(CB) ₂ (H)	16.30	8.94	4.20	5.21	6.13	6.83	7.90	8.65	9.55
N-(CO)(H) ₂	-14.90	29.69	4.07	5.74	7.13	8.29	9.96	11.22	13.12
N-(C)(CO)(H)	-4.40	8.66	4.20	5.21	6.13	6.83	7.90	8.65	9.55
N-(H) ₂ (N)	11.40	29.13	6.10	7.38	8.43	9.27	10.54	11.52	13.19
NA-(C)	27.65	6.35	3.13	3.48	3.81	4.09	4.60	4.92	6.35
NA-(H)	25.10	26.80	4.38	4.89	5.44	5.94	6.77	7.42	8.44
NI-(H)	14.30	12.30	2.95	4.58	6.45	7.71	9.13	9.92	
NI-(N)	27.80	6.36	3.13	3.48	3.81	4.07	4.63	6.35	
NI-(C)	21.30	6.36	3.13	3.48	3.81	4.07	4.63	6.35	
O-(C)(NO)	-5.90	41.63	10.66	11.42	12.05	12.64	13.38	13.87	
O-(NO)(O)	11.90	41.90	9.10	10.30	11.20	12.00	13.30	13.70	
O-(NO ₂)(O)	6.06	46.75	13.87	15.77	17.28	18.52	19.73	20.34	
O-(C)(NO ₂)	-19.40	46.47	13.80	15.20	16.25	17.21	18.43	19.17	
O-(CD)(NO ₂)	-11.69	48.51	13.22	14.43	15.45	16.40	17.98	18.99	20.90
O-(O)(NO)	6.27	48.50	9.54	11.54	13.26	15.60	16.39	17.38	
O-(O)(NO ₂)	6.06	46.75	13.87	15.77	17.28	18.52	19.73	20.34	
C-(H) ₃ (OO)	-8.3	30.3	6.19	7.84	9.4	10.79	13.02	14.77	17.58
CD-(H)(OO)	2.03	6.2	4.75	6.46	7.64	8.35	9.1	9.56	
C-(C)(H) ₂ (OO)	-7.89	9.65	4.78	6.34	7.78	9.03	10.95	12.30	14.13
C-(C) ₂ (H)(OO)	-6.08	-11.96	4.21	5.85	7.15	8.10	9.38	10.10	
C-(C) ₃ (OO)	-5.58	-35.11	4.02	5.60	6.60	7.15	7.68	7.74	
C-(CT)(H) ₂ (OO)	-9.06	9.15	4.07	6.03	7.66	9.01	10.92	12.38	
C-(CD)(H) ₂ (OO)	-7.28	10.12	5.1	6.88	8.32	9.5	11.18	12.48	
OO-(C)(H)	-23.50	36.84	9.74	10.47	11.00	11.74	12.19	12.91	
OO-(C) ₂	-9.7	18.13	7.64	8.47	9.03	9.63	9.61	9.34	
OO-(CD)(H)	-15.89	37.31	8.55	9.19	9.94	10.73	12.07	12.91	
O-(H) ₂	-57.80	45.10	8.00	8.40	9.20	9.90	11.20	12.30	
O-(C)(H)	-37.90	29.07	4.30	4.50	4.82	5.23	6.02	6.61	7.44

O-(CD)(H)	-37.90	29.10	4.30	4.50	4.82	5.23	6.02	6.61	7.44
O-(CB)(H)	-37.90	29.10	4.30	4.50	4.82	5.23	6.02	6.61	7.44
O-(CT)(H)	-37.90	29.10	4.30	4.40	4.82	5.23	6.02	6.61	7.44
O-(H)(O)	-16.30	27.83	5.21	5.72	6.17	6.66	7.15	7.61	8.43
O-(CO)(H)	-58.10	24.50	3.80	5.0	5.80	6.30	7.20	7.80	
O-(C) ₂	-23.20	8.68	3.40	3.70	3.70	3.80	4.40	4.60	
O-(C)(O)	-5.25	8.54	3.90	4.31	4.60	4.84	5.32	5.80	
O-(CT)(O)	-6.43	7.44	3.90	4.31	4.60	4.84	5.32	5.80	
O-(CD)(O)	1.64	10.12	3.50	3.87	3.95	4.15	4.73	4.89	
O-(CT)(O)	7.00	10.80	3.90	4.31	4.60	4.84	5.32	5.80	
O-(O) ₂	9.45	9.40	2.20	3.64	4.20	4.34	4.62	4.90	
O-(C)(CO)	-42.19	8.40	3.91	4.31	4.60	4.84	5.32	5.80	
O-(CO)(O)	-19.00	9.76	3.03	4.08	4.68	4.92	5.48	5.67	
O-(C)(CD)	-23.73	9.70	3.91	4.31	4.60	4.84	5.32	5.80	
O-(CB) ₂	-18.77	13.59	1.19	-0.24	-0.72	-0.51	0.43	1.36	1.75
O-(CD) ₂	-32.80	10.0	3.40	3.70	3.70	3.80	4.40	4.60	4.80
O-(C)(CB)	-22.60	9.70	3.40	3.70	3.70	3.80	4.40	4.60	
CO-(H) ₂	-26.00	52.30	8.47	9.38	10.46	11.52	13.37	14.81	
CO-(C)(H)	-29.10	34.90	7.03	7.87	8.82	9.68	11.20	12.20	
CO-(CD)(H)	-30.90	33.40	7.45	8.77	9.82	10.70	12.14	12.90	
CO-(CO)/(H)	-25.30	33.40	7.45	8.77	9.82	10.70	12.14	12.90	
CO-(H)(O)	-32.10	34.90	7.03	7.87	8.82	9.68	11.20	12.20	
CO-(C) ₂	-31.40	15.01	5.59	6.32	7.09	7.76	8.89	9.61	
CO-(CD)(C)	-30.90	14.60	5.46	6.32	7.17	7.88	9.00	9.77	
CO-(CD) ₂	-30.90	14.60	5.46	6.32	7.17	7.88	9.00	9.77	
CO-(CO)(C)	-29.10	14.60	5.46	6.32	7.17	7.88	9.00	9.77	
CO-(CO)(O)	-29.30	14.61	5.46	6.32	7.17	7.88	9.00	9.77	
CO-(C)(O)	-35.10	10.04	6.10	6.70	7.40	8.02	8.87	9.36	
CO-(O) ₂	-31.45	10.78	5.97	6.70	7.40	8.02	8.87	9.36	
CO-(CB)(O)	-36.60	14.78	5.97	6.70	7.40	8.02	8.87	9.36	
CO-(CD)(O)	-32.10	14.78	5.97	6.70	7.40	8.02	8.87	9.36	
C-(H) ₃ (O)	-10.10	30.41	6.19	7.84	9.40	10.79	13.03	14.77	17.58
C-(C)(H) ₂ (O)	-8.10	9.8	4.99	6.85	8.30	9.43	11.11	12.33	
C-(CD)(H) ₂ (O)	-6.76	9.80	5.12	6.86	8.32	9.49	11.22	12.48	14.40
C-(CT)(H) ₂ (O)	-6.76	9.80	5.12	6.86	8.32	9.49	11.22	12.48	14.40
C-(C)(CO)(H) ₂	-5.20	9.60	6.20	7.70	8.70	9.50	11.10	12.20	14.07
C-(C)(O)(H) ₂ (O)	-6.50	9.60	6.20	7.70	8.70	9.50	11.10	12.20	14.07
C-(C)(O)(H) ₂ (O)	-6.76	9.80	5.12	6.86	8.32	9.49	11.22	12.48	14.40
C-(CD)(CO)(H) ₂	-3.80	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.40
C-(H) ₂ (O) ₂	-15.23	9.42	5.50	6.95	8.25	9.35	11.07	12.34	
C-(C)(H)(O) ₂	-16.00	-12.07	5.25	7.10	8.81	9.55	10.31	11.05	
C-(C) ₂ (H)(O)	-7.20	-11.00	4.80	6.64	8.10	8.73	9.81	10.40	11.51
C-(CB)(C)(H)(O)	-6.00	-11.10	4.47	6.82	8.45	9.17	10.24	10.80	11.02
C-(CD)(C)(H)(O)	-6.00	-11.10	4.47	6.82	8.45	9.17	10.24	10.80	11.02
C-(C)(CD)(H)(O)	-6.00	-11.10	4.47	6.82	8.45	9.17	10.24	10.80	11.02
C-(C)(CO)(H)(O)	-6.00	-11.10	4.47	6.82	8.45	9.17	10.24	10.80	11.02
C-(C) ₂ (CO)(H)	-1.7	-11.70	4.16	5.91	7.34	8.19	9.46	10.19	
C-(CD) ₂ (H)(O)	-6.67	-10.42	4.21	6.60	8.26	9.05	10.23	10.86	11.04
C-(H)(O) ₃	-21.23	-12.07	4.54	6.00	7.17	8.05	9.31	10.05	
C-(C) ₃ (O)	-6.60	-33.56	4.33	6.19	7.25	7.70	8.20	8.24	
C-(CD)/(C) ₂ (O)	-6.60	-32.56	4.63	6.79	7.95	8.40	8.80	8.44	
C-(CB)/(C) ₂ (O)	-6.60	-32.56	4.63	6.79	7.95	8.40	8.80	8.44	
C-(C) ₂ (O) ₂	-9.77	-33.18	3.8	6.09	7.30	7.78	8.24	8.24	
C-(CD) ₂ (C)(O)	-8.01	-34.34	3.61	5.98	7.51	8.37	9.00	9.02	8.34
C-(C)(O) ₃	-19.00	-33.56	4.33	6.19	7.25	7.70	8.20	8.24	

C-(C) ₃ (CO)	1.40	-34.72	3.99	6.04	7.43	8.26	8.92	8.96	8.23
C-(C) ₂ (CO)(O)	-3.60	-34.72	3.99	6.04	7.43	8.26	8.92	8.96	8.23
C-(O) ₄	-23.00	-35.56	4.33	6.13	7.25	7.70	8.20	8.24	
C-(C)(O)(H) ₃	-10.08	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
CD-(H)(O)	2.03	6.20	4.75	6.46	7.64	8.35	9.10	9.56	10.46
CD-(C)(O)	3.03	-12.32	3.59	4.56	5.04	5.30	5.84	6.07	6.16
CD-(CO)(H)	4.32	6.38	4.46	5.79	6.75	7.42	8.35	9.11	10.09
CD-(CD)(CO)	4.60	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
CD-(C)(CO)	7.50	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
CD-(CO)(O)	5.13	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
CD-(CD)(O)	1.5	-14.4	4.4	5.37	5.93	6.18	6.5	6.62	6.72
CD-(CB)(O)	1.5	-14.4	4.4	5.37	5.93	6.18	6.5	6.62	6.72
CT-(O)	31.40	4.91	3.64	4.39	4.85	5.63	5.66	5.73	
CB-(O)	-0.90	-10.20	3.90	5.30	6.20	6.60	6.90	6.90	7.07
CB-(CO)	3.69	-7.80	3.59	3.97	4.38	4.72	5.28	5.61	5.75
CY-C ₃	27.53	32.04	-3.13	-2.67	-2.32	-2.11	-1.92	-1.84	-1.38
CY-C ₃ /E	53.34	33.43	-0.32	-0.62	-0.78	-0.93	-1.27	-1.52	-1.58
CY-C ₄	26.51	29.88	-5.02	-4.46	-3.83	-3.31	-2.57	-2.12	-1.20
CY-C ₄ /E	29.79	28.45	-3.05	-2.73	-2.30	-1.97	-1.64	-1.43	-1.02
CY-C ₄ /DE	64.90	37.30	-3.18	-4.02	-4.14	-3.86	-3.25	-3.26	-2.67
CY-C ₅	5.91	22.90	-7.57	-6.51	-5.39	-4.43	-3.06	-2.22	-0.75
CY-C ₅ /E	5.09	25.66	-4.50	-3.94	-3.29	-2.76	-2.08	-1.63	-0.85
CY-C ₅ /DE	4.81	27.97	-3.80	-3.75	-3.30	-2.78	-2.09	-1.94	-1.26
CY-C ₆	0.00	18.38	-7.64	-6.17	-4.40	-2.72	-0.20	1.11	2.48
CY-C ₆ /E	1.10	21.21	-5.14	-4.29	-3.35	-2.54	-1.41	-0.66	0.55
CY-C ₆ /DE/14	0.27	21.28	-3.41	-3.19	-2.54	-1.95	-1.19	-0.76	0.16
CY-C ₆ /DE/13	4.19	25.57	-4.82	-4.64	-4.00	-3.26	-2.17	-1.64	-0.62
CY-C ₇	6.26	17.26	-6.73	-4.86	-3.14	-1.77	0.06	1.07	2.70
CY-C ₇ /E	4.88	15.55	-5.21	-4.17	-3.10	-2.16	-0.84	0.03	1.48
CY-C ₇ /DE/13	6.22	22.28	-4.68	-4.79	-3.89	-3.09	-1.81	-1.15	0.19
CY-C ₇ /TE	3.68	23.92	-5.30	-5.89	-5.50	-4.68	-3.24	-2.71	-1.19
CY-C ₈	9.71	12.31	-8.82	-7.28	-5.52	-3.90	-1.45	0.10	2.68
CY-C ₈ /E	5.61	12.10	-6.17	-4.51	-2.93	-1.65	0.04	1.06	2.64
CY-C ₈ /DE/13	7.88	20.13	-5.09	-4.67	-3.78	-2.79	-1.28	-0.47	1.11
CY-C ₈ /DE/15	-1.32	14.07	-3.84	-2.62	-1.32	-0.25	1.05	1.76	2.56
CY-C ₂ O	26.83	31.08	-2.08	-2.66	-2.40	-2.11	-2.05	-1.80	
CY-C ₂ O/E	69.37	37.68	0.10	-1.50	-2.30	-2.64	-2.98	-2.83	-2.81
CY-CO ₂	35.65	32.57	-2.77	-2.77	-2.67	-2.65	-2.98	-3.59	
CY-C ₃ O	25.09	28.55	-4.08	-4.28	-3.64	-3.02	-2.45	-1.90	
CY-C ₂ O ₂	22.99	26.93	-4.16	-4.52	-4.23	-3.83	-3.37	-3.53	
CY-C ₂ O ₂ /E	19.97	30.10	-3.69	-4.75	-4.71	-4.51	-4.28	-3.57	
CY-C ₄ O	5.06	26.52	-5.93	-5.71	-4.67	-3.72	-2.69	-1.86	
CY-C ₄ O/E23	8.05	26.45	-5.07	-5.50	-5.27	-4.79	-3.94	-3.48	
CY-C ₄ O/E34	2.81	25.11	-3.76	-3.07	-2.16	-1.58	-1.35	-1.04	
CY-C ₄ O/DE	6.84	30.09	-6.08	-6.98	-6.71	-6.00	-4.85	-4.03	-2.95
CY-C ₃ O ₂ /12	4.95	22.57	-4.77	-4.49	-3.79	-3.16	-2.56	-2.59	
CY-C ₃ O ₂ /13	6.61	26.66	-5.20	-5.16	-4.03	-3.09	-2.53	-1.81	
CY-C*CCOO	-2.46	25.53	-4.25	-4.29	-3.84	-3.46	-3.22	-2.98	
CY-C*COCO	10.34	26.27	-5.95	-6.49	-6.41	-5.97	-5.16	-4.88	
CY-C ₂ O ₃ /123	9.60	25.79	-1.26	-2.42	-2.38	-1.99	-1.83	-2.24	
CY-C ₂ O ₃ /124	15.53	23.57	-5.65	-4.78	-3.63	-2.86	-2.64	-2.76	
CY-C ₂ O ₃ /E	-3.26	26.17	-1.76	-3.58	-3.73	-3.45	-3.26	-2.70	
CY-C ₅ O	0.80	17.18	-6.02	-5.48	-4.18	-2.98	-1.56	-0.48	
CY-C*CCCCO	1.00	20.09	-6.26	-6.50	-5.96	-5.14	-3.74	-2.92	
CY-C*CCCOC	-4.24	19.14	-4.20	-3.64	-2.57	-1.72	-0.99	-0.33	
CY-C ₄ O ₂ /12	6.22	18.27	-5.66	-5.11	-4.17	-3.36	-2.52	-2.40	

CY-CCCOCO	0.95	16.64	-6.28	-5.95	-4.46	-3.15	-1.97	-0.83	
CY-CCOCCO	3.32	16.35	-4.60	-4.98	-3.80	-2.62	-1.54	-0.44	
CY-C*CCOOC	3.62	18.72	-5.45	-4.66	-3.81	-3.16	-2.65	-2.68	
CY-C*CCCOO	-3.32	21.26	-4.64	-4.84	-4.28	-3.72	-3.11	-2.62	
CY-C*CCOCO	1.62	20.85	-5.53	-5.09	-4.17	-3.39	-2.75	-2.31	
CY-C*COCCO	2.24	20.67	-6.84	-7.85	-7.78	-7.05	-5.57	-4.80	
CY-C*COC*CO	24.02	27.37	-6.26	-7.87	-7.82	-7.11	-5.92	-4.49	-3.21
CY-COCOCO	3.94	16.83	-7.01	-5.72	-3.63	-2.19	-1.53	-0.62	
CY-C ₆ O	5.73	14.64	-5.45	-4.40	-3.45	-2.31	-0.31	0.87	2.05
CY-C ₇ O	9.17	12.44	-7.54	-6.70	-5.82	-4.48	-1.82	-0.09	1.64
CY-C ₅ O ₂	5.73	14.64	-5.45	-4.40	-3.45	-2.31	-0.31	0.87	2.05
CY-C ₅ O ₂ /E	7.91	18.51	-4.84	-4.21	-3.34	-2.65	-2.05	-2.03	
CY-C ₂ N	27.50	28.99	-2.33	-2.24	-2.13	-2.01	-1.78	-1.57	-1.36
CY-C ₃ N	26.20	29.30	-3.89	-3.52	-3.17	-2.73	-1.89	-1.33	-0.77
CY-C ₄ N	6.80	26.70	-6.17	-5.44	-4.80	-4.08	-2.87	-2.17	-1.47
CY-C ₅ N	1.00	15.74	-5.08	-3.92	-2.93	-1.47	1.09	2.23	3.37
CY-C ₆ N	6.95	16.45	-5.97	-4.36	-3.12	-1.66	0.53	1.18	1.83
CY-C ₇ N	10.39	14.25	-8.07	-6.72	-5.49	-4.01	-1.38	0.24	1.86
CY-C ₄ N/E	11.85	27.27	-6.19	-5.97	-5.73	-4.99	-3.47	-2.73	-1.99
CY-C ₅ N/E	2.42	22.99	-4.49	-3.57	-2.85	-2.05	-0.83	-0.39	0.05
BCY-110C ₄	67.0	68.36	-5.3	-5.43	-5.37	-5.26	-5.16	-4.87	-4.29
BCY-210C ₅	55.3	63.16	-7.25	-6.84	-6.27	-5.77	-5.17	-4.6	-3.6
BCY-310C ₆	32.7	60.08	-8.41	-7.76	-6.91	-6.13	-5.09	-4.24	-2.81
BCY-221C ₇	16.20	51.27	-11.2	-9.67	-8.11	-6.82	-5.17	-3.99	-2.11
BCY-311C ₇	28.77	52.31	-10.48	-9.1	-7.67	-6.49	-4.96	-3.85	-2.05
BCY-410C ₇	28.9	56.28	-8.82	-7.95	-6.9	-5.94	-4.63	-3.6	-1.89
BCY-222C ₈	5.65	48.04	-11.82	-10.16	-8.4	-6.89	-4.87	-3.44	-1.20
BCY-321C ₈	6.55	46.5	-12.05	-10.33	-8.52	-7.00	-4.96	-3.53	-1.27
BCY-420C ₈	31.08	48.77	-10.86	-9.4	-7.83	-6.48	-4.66	-3.35	-1.22
BCY-510C ₈	29.6	50.29	-10.14	-8.86	-7.45	-6.2	-4.48	-3.2	-1.1
BCY-322C ₉	9.79	51.8	-12.00	-10.14	-8.19	-6.53	-4.26	-2.69	-0.21
BCY-331C ₉	10.28	44.17	-12.22	-10.31	-8.34	-6.65	-4.38	-2.8	-0.3
BCY-430C ₉	3.69	45.29	-12.09	-10.38	-8.49	-6.83	-4.57	-2.98	-0.44
BCY-610C ₉	31.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
BCY-440C ₁₀	-0.88	38.85	-13.34	-11.27	-9.04	-7.11	-4.44	-2.62	0.31