Standard Chemical Thermodynamic Properties of Alkyne Isomer Groups

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The chemical thermodynamic properties of alkyne isomer groups from C_2H_2 to C_5H_8 in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of C_6H_{10} to C_8H_{14} have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. For isomer group properties, increments per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Values of C°_P, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species from C_2H_2 to C_8H_{14} in SI units for a standard state pressure of 1 bar.

Key words: alkynes; Benson method; enthalpy of formation; entropy; Gibbs energy of formation; heat capacity; isomer group thermodynamic properties; isomer mole fractions; thermodynamic properties.

Contents

List of Tables

1. Introduction

Earlier papers in this series have presented isomer group thermodynamic properties[1] for the alkanes,[2] alkylbenzenes,[3] alkenes,[4] and alkylnaphthalenes.[5] The alkynes (alkylacetylenes) are of special interest because of their high reactivity. The thermodynamic properties have been calculated for the C_2H_2, C_3H_4, C_4H_6, and C_5H_8 isomer groups, which is as far as existing data on individual species goes.[6] However, since the increments in isomer group properties per carbon vary somewhat for lower members of this homologous series, it is of special interest to see what the Benson

group method[7] can tell us about the properties of higher homologs. The standard thermodynamic properties of all alkynes through C_8H_{14} have been calculated using the Benson method.

2. Standard Thermodynamic Properties of Alkyne Isomer Groups

When isomers are in chemical equilibrium it has been known for some time[8,9] that they can be aggregated in calculations of equilibrium mole fractions by use of the standard Gibbs energy of formation $\Delta_f G^\circ(\mathrm{I})$ of the isomer group defined by

$$\Delta_f G^\circ(\mathrm{I}) = -RT\ln\left[\sum_{i=1}^{N_\mathrm{I}} \exp(-\Delta_f G_i^\circ/RT)\right], \quad (1)$$

where $\Delta_f G_i^\circ$ is the standard Gibbs energy of formation of an individual isomer and N_I is the number of isomers in the group, including stereoisomers. The equilibrium mole fractions r_i of various isomers in a group can be calculated using

$$r_i = \frac{y_i}{y_\mathrm{I}} = \exp[(\Delta_f G^\circ(\mathrm{I}) - \Delta_f G_i^\circ)/RT], \quad (2)$$

where y_I is the sum of the mole fractions of the individual isomers. The corresponding equations for the other standard thermodynamic properties $C_P^\circ(\mathrm{I})$, $S^\circ(\mathrm{I})$, and $\Delta_f H^\circ(\mathrm{I})$ can be derived by differentiating Eq. (1) with respect to temperature.[3] When standard Gibbs energies of formation of isomer groups are used to calculate equilibrium constants for reactions of ideal gases the equilibrium expression is written in terms of equilibrium mole fractions of isomer groups.

For the alkynes, the standard chemical thermodynamic properties for an isomer group are interrelated by

$$\Delta_f G^\circ(\mathrm{I}) = \Delta_f H^\circ(\mathrm{I}) - T[S^\circ(\mathrm{I}) - nS^\circ_{\text{graphite}} - (n-1)S^\circ_{\mathrm{H_2(g)}}], \quad (3)$$

where n is the number of carbon atoms.

To calculate the chemical thermodynamic properties for an isomer group, a term must be included for each molecular species, including stereoisomers. The numbers of chiral molecules and isomers of the alkynes are shown in Table 1. Rather than having a line in a thermodynamic table for each stereoisomer, this article follows the standard practice of giving properties of racemates. Thus $R\ln 2$ is added to the calculated standard entropy and $RT\ln 2$ is subtracted from the standard Gibbs energy of formation of one of the chiral forms at each temperature. Therefore the numbers of lines in tables in this article do not correspond to the total numbers of isomers; the numbers of lines, chiral molecules, and isomers are given in Table 1. The name 3(RS), 4(RS)-dimethyl-1-hexyne represents four isomers, and so the values in the table apply to the equilibrium mixture of the four isomers, which have the same Benson groups.

Table 1. Numbers of isomers, chiral centers, and lines in tables

	Number of lines	One Chiral Center	Two Chiral Centers	Total Isomers
C2H2	1			1
C3H4	1			1
C4H6	2			2
C5H8	3			3
C6H10	7	1		8
C7H12	14	4		18
C8H14	32	12	1	47

The basic information on the chemical thermodynamic properties of the alkynes comes from statistical mechanical calculations and correlations by Rossini, Pitzer, Arnett, Braun, and Pimentel.[10] Only small changes were made by Stull, Westrum, and Sinke.[6]

3. Calculations of Standard Thermodynamic Properties of Alkynes Using the Benson Method

Data are available for the calculation of isomer group properties only for C_2H_2, C_3H_4, C_4H_6, and C_5H_8. Since the increments per carbon atom are still increasing at C_5H_8, these data do not provide an adequate basis for extrapolating to higher carbon numbers. Therefore the Benson group method has been used to calculate the properties for all isomers through C_8H_{14} in the ideal gas state.

In order to make these calculations, the structure of each alkyne species was divided into the following Benson groups; $C(H)_3(C)$, $C(H)_2(C)_2$, $C(H)(C)_3$, $C(C)_4$, $C(C_t)(C)(H)_2$, $C(C_t)(C)_2(H)$, $C(C_t)(C)_3$, $C_t(H)$, and $C_t(C)$. In addition, the total symmetry number (TSN), number of optical isomers (OPT), and *gauche* corrections were tabulated. In view of some of the uncertainties in some of these group values indicated by Benson, the 1,5-H repulsions, which affect only several of the most highly branched species were omitted. In calculating symmetry numbers a report by Davies, Syverud, and Steiner[12] was very helpful.

Values are not available for one Benson group that is needed to estimate thermodynamic properties of alkylacetylenes; that is $C(C)_t(C)_3$. There are three ways to estimate the values for this group, and fortunately they are in good agreement. The progression of values in the series $C(C_d)(C)(H)_2$, $C(C_d)(C)_2(H)$, and $C(C_d)(C)_3$, in the series $C(C_B)(C)(H)_2$, $C(C_B)(C)_2(H)$, and $C(C_B)(C)_3$, and for the pair $C(C_t)(C)(H)_2$ and $C(C_t)(C)_2(H)$ indicate that the values for $\Delta_f H^\circ_{298}$, $S^\circ_{\mathrm{int}\,298}$, C°_{300}, C°_{400}, C°_{500}, C°_{600}, C°_{800}, and C°_{1000} are 1.3, −34.2, 4.0, 5.6, 6.9, 7.8, 9.1, and 9.9, respectively, in the units and for the standard state used by Benson.[7]

The assignment of Benson groups was checked by multiplying the matrix of numbers of groups by a matrix which had in its first column the number of carbon atoms in the group, in the second column the number of hydrogen atoms in each group, and in the third column the number of groups starting with C_t. Matrix multiplication yields a matrix with as many rows as lines in the table for that isomer group and three columns giving the numbers of carbon atoms, hydrogen atoms, and triple bond carbons. This check prevents large errors in the group assignments. The computer programs used in making the Benson calculations are described in the first paper in this series.[2]

Table 2 shows how well the chemical thermodynamic properties calculated using the Benson method agree with the values from Stull, Westrum, and Sinke[6] for C_2H_2 through C_5H_8. The differences between the literature and estimated values at each temperature were squared, divided

Table 2. Root mean square deviations between alkyne thermodynamic properties from Stull, Westrum, and Sinke and from the Benson method

T/K	298	300	400	500	600	700	800	900	1000
	Standard heat capacity at constant pressure in J/K mol								
C2H2	.62	.59	.52	.39	.87	.55	.69	.40	.30
C3H4	.40	.41	.25	.44	.24	.06	.20	.07	.43
C4H6	.40	.39	.31	.36	.14	.44	.69	.60	.33
C5H8	1.19	1.28	1.39	1.35	.99	.43	.90	.70	.63
	Standard entropy in J/K mol								
C2H2	.09	.08	.05	.04	.05	.01	.06	.16	.14
C3H4	.10	.10	.10	.17	.26	.28	.25	.22	.25
C4H6	.28	.25	.28	.25	.27	.30	.37	.45	.49
C5H8	.60	.58	.37	.45	.61	.70	.74	.75	.80
	Standard enthalpy of formation in kJ/mol								
C2H2	1.38	1.39	1.36	1.39	1.39	1.37	1.30	1.23	1.23
C3H4	.17	.17	.14	.14	.19	.17	.16	.14	.18
C4H6	.83	.83	.80	.76	.73	.73	.70	.69	.67
C5H8	2.11	2.10	2.08	2.09	2.11	2.09	2.03	1.95	1.94
	Standard Gibbs energy of formation in kJ/mol								
C2H2	1.40	1.39	1.38	1.39	1.38	1.41	1.40	1.40	1.46
C3H4	.11	.10	.10	.07	.04	.06	.01	.00	.03
C4H6	.84	.85	.86	.88	.89	.93	.95	.99	1.07
C5H8	2.19	2.17	2.21	2.25	2.25	2.30	2.32	2.40	2.47

by the number of pairs of values, and the square root was taken. For C_2H_2 and C_3H_4 this yields the magnitudes of the deviations, and for the higher homologous series it yields the root-mean-square deviations at various temperatures. The average root-mean-square deviation in $\Delta_f G^\circ$ for C_5H_8 over the temperature range is 2.3 kJ mol^{-1}.

4. Tables of Standard Thermodynamic Properties of Alkyne Isomer Groups

Since the International Union of Pure and Applied Chemistry has recently recommended that thermodynamic data be given in SI units for a standard state pressure of 1 bar (10^5 Pa), this has been done for the tables in this article. The change in standard state pressure from 1 atm to 1 bar does not affect C_p° and $\Delta_f H^\circ$, but the standard entropy of an ideal gas is increased by $R \ln(1.013\,25) = 0.109\ \mathrm{J\ K^{-1}\ mol^{-1}}$ at any temperature and the standard Gibbs energy of formation is reduced by $[RT \ln(1.013\,25)]\delta$, where δ is the net increase $(2 - n)$ in moles of gas in the formation reaction[12] and n is the number of carbon atoms.

The remaining tables in this paper have all been calculated using corrected values from Stull, Westrum, and Sinke for C_2H_2 to C_5H_8 and values calculated using the Benson method for C_6H_{10}, C_7H_{12}, and C_8H_{14} species. Tables 3–8 give isomer group properties and the increments per carbon atom. Table 7 gives $H^\circ(I,T) - H^\circ(I,298.15\ K)$, the standard enthalpy for an isomer group relative to the isomer group at 298.15 K. Table 8 gives values for $H^\circ(I,T) - H^\circ(I,298.15\ K) + \Delta_f H^\circ(I,298.15\ K)$, the standard enthalpy of formation for the isomer group relative to the elements at 298.15 K. This quantity allows the direct calcu-

Table 3. Standard heat capacity at constant pressure for alkyne isomer groups in J/K mol

T/K	C2H2	C3H4	C4H6	C5H8	C6H10	C7H12	C8H14
298.15	43.93	60.67	78.53	100.03	137.8	197.5	196.9
300.00	44.06	60.88	78.85	100.46	138.5	197.6	197.7
400.00	50.08	72.51	97.09	124.99	168.2	206.1	233.8
500.00	54.27	82.59	115.48	147.98	191.1	227.1	264.4
600.00	58.45	91.21	132.18	167.86	211.8	251.4	293.5
700.00	60.12	98.66	146.51	185.24	230.8	274.6	320.1
800.00	62.47	105.19	158.40	199.62	247.7	295.1	343.5
900.00	64.64	110.92	167.97	212.29	262.0	312.3	363.1
1000.00	66.61	115.94	175.76	222.57	273.5	326.0	378.6

Table 3a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	16.74	17.87	21.50	37.8	59.7	-.6
300.00	16.82	17.98	21.61	38.1	59.1	.1
400.00	22.43	24.58	27.89	43.2	38.0	27.6
500.00	28.33	32.89	32.50	43.1	36.0	37.4
600.00	32.76	40.97	35.69	44.0	39.6	42.1
700.00	38.53	47.85	38.73	45.6	43.8	45.5
800.00	42.72	53.22	41.22	48.1	47.4	48.4
900.00	46.28	57.05	44.32	49.7	50.4	50.7
1000.00	49.33	59.83	46.81	50.9	52.6	52.5

Table 4. Standard entropy for alkyne isomer groups in J/K mol

T/K	C2H2	C3H4	C4H6	C5H8	C6H10	C7H12	C8H14
298.15	200.94	248.22	283.50	332.33	367.2	401.4	446.3
300.00	201.23	248.60	284.00	332.97	368.1	402.6	447.5
400.00	214.79	267.76	309.17	365.26	412.3	460.3	509.6
500.00	226.42	285.04	332.84	395.69	452.3	508.4	565.1
600.00	236.59	300.90	355.38	424.45	489.0	552.0	615.9
700.00	245.67	315.54	376.86	451.66	523.1	592.5	663.2
800.00	253.87	329.14	397.24	477.35	555.1	630.5	707.5
900.00	261.32	341.86	416.45	501.65	585.1	666.3	749.1
1000.00	268.26	353.83	434.58	524.54	613.3	700.0	788.2

Table 4a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	47.28	35.27	48.84	34.9	34.1	44.9
300.00	47.36	35.40	48.97	35.1	34.5	44.9
400.00	52.97	41.41	56.09	47.0	48.1	49.3
500.00	58.62	47.80	62.85	56.6	56.1	56.7
600.00	64.31	54.48	69.07	64.6	63.0	63.9
700.00	69.87	61.32	74.79	71.5	69.4	70.7
800.00	75.27	68.10	80.12	77.7	75.5	77.0
900.00	80.54	74.59	85.20	83.4	81.2	82.8
1000.00	85.56	80.76	89.96	88.8	86.7	88.2

Table 5. Standard enthalpy of formation for alkyne isomer groups in kJ/mol

T/K	C2H2	C3H4	C4H6	C5H8	C6H10	C7H12	C8H14
298.15	226.73	185.43	146.34	128.97	96.8	71.7	47.7
300.00	226.73	185.39	146.25	128.84	96.7	71.6	47.5
400.00	226.48	183.18	142.21	123.36	91.5	67.1	40.7
500.00	226.10	181.08	138.74	118.66	86.9	61.9	34.5
600.00	225.60	179.20	136.01	114.87	83.0	57.2	29.3
700.00	225.02	177.49	134.08	111.93	79.8	53.5	25.3
800.00	224.35	176.02	132.79	109.76	77.4	50.8	22.4
900.00	223.63	174.77	132.05	108.28	75.8	49.1	20.7
1000.00	222.97	173.76	131.80	107.44	74.9	48.2	19.8

Table 5a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-41.30	-39.10	-17.37	-32.1	-25.1	-24.0
300.00	-41.34	-39.14	-17.41	-32.1	-25.1	-24.1
400.00	-43.30	-40.96	-18.86	-31.9	-24.4	-26.5
500.00	-45.02	-42.34	-20.08	-31.7	-25.0	-27.4
600.00	-46.40	-43.19	-21.15	-31.9	-25.7	-27.9
700.00	-47.53	-43.40	-22.16	-32.1	-26.3	-28.2
800.00	-48.33	-43.23	-23.03	-32.3	-26.6	-28.4
900.00	-48.87	-42.71	-23.77	-32.4	-26.7	-28.5
1000.00	-49.20	-41.96	-24.36	-32.5	-26.7	-28.4

Table 6. Standard Gibbs energy of formation for alkyne isomer groups in kJ/mol

T/K	C2H2	C3H4	C4H6	C5H8	C6H10	C7H12	C8H14
298.15	209.20	194.46	185.50	194.25	192.4	197.8	201.0
300.00	209.07	194.51	185.75	194.62	193.0	198.6	202.0
400.00	203.22	197.90	199.55	217.43	225.9	241.5	254.5
500.00	197.44	201.81	214.30	241.51	260.1	285.7	308.7
600.00	191.75	206.13	229.65	266.42	295.1	331.0	364.1
700.00	186.19	210.78	245.42	291.94	330.7	376.9	420.2
800.00	180.67	215.61	261.42	317.78	366.8	423.3	476.8
900.00	175.23	220.64	277.53	343.90	403.0	469.9	533.7
1000.00	169.91	225.84	293.76	370.15	439.4	516.7	590.7

Table 6a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-14.74	-8.97	8.75	-1.8	5.4	3.2
300.00	-14.67	-8.76	8.88	-1.6	5.5	3.4
400.00	-5.31	1.65	17.88	8.5	15.6	13.0
500.00	4.36	12.49	27.21	18.6	25.6	23.0
600.00	14.37	23.53	36.76	28.7	35.8	33.1
700.00	24.59	34.64	46.51	38.8	46.1	43.3
800.00	34.94	45.81	56.36	49.0	56.5	53.5
900.00	45.41	56.90	66.36	59.1	66.9	63.8
1000.00	55.92	67.92	76.39	69.2	77.3	74.0

Table 7. Standard enthalpy for alkyne isomer groups relative to isomer groups at 298.15 K in kJ/mol

T/K	C2H2	C3H4	C4H6	C5H8	C6H10	C7H12	C8H14
298.15	.00	.00	.00	.00	.0	.0	.0
300.00	.09	.12	.15	.18	.3	.4	.4
400.00	4.78	6.77	8.90	11.41	15.7	20.5	22.0
500.00	9.98	14.51	19.51	25.04	33.7	42.1	47.0
600.00	15.56	23.21	31.68	40.85	53.6	66.0	74.9
700.00	21.46	32.69	45.85	58.53	76.0	92.3	105.6
800.00	27.59	42.90	61.11	77.79	99.9	120.8	138.8
900.00	33.93	53.70	77.44	98.39	125.4	151.2	174.1
1000.00	40.51	65.08	94.69	120.18	152.2	183.2	211.3

Table 7a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	.00	.00	.00	.0	.0	.0
300.00	.03	.03	.03	.1	.1	.0
400.00	1.99	2.13	2.51	4.3	4.8	1.6
500.00	4.52	5.00	5.54	8.6	8.4	4.9
600.00	7.65	8.66	8.98	13.0	12.1	8.9
700.00	11.23	13.16	12.68	17.4	16.3	13.3
800.00	15.31	18.21	16.68	22.1	20.9	18.0
900.00	19.78	23.74	20.95	27.0	25.8	22.9
1000.00	24.57	29.61	25.49	32.1	30.9	28.1

Table 8. Standard enthalpy for alkyne isomer groups relative to the elements at 298.15 K in kJ/mol

T/K	C2H2	C3H4	C4H6	C5H8	C6H10	C7H12	C8H14
298.15	226.73	185.43	146.34	128.97	96.8	71.7	47.7
300.00	226.82	185.55	146.48	129.14	97.1	72.1	48.0
400.00	231.51	192.21	155.24	140.38	112.5	92.2	69.7
500.00	236.71	199.94	165.85	154.01	130.5	113.8	94.6
600.00	242.30	208.65	178.21	169.82	150.7	137.7	122.5
700.00	248.19	218.13	192.19	187.50	172.8	164.0	153.2
800.00	254.32	228.33	207.44	206.75	196.8	192.5	186.4
900.00	260.66	239.14	223.78	227.36	222.3	222.9	221.8
1000.00	267.24	250.51	241.03	249.15	249.1	254.9	258.9

Table 8a. Increments per carbon atom

T/K	C3-C2	C4-C3	C5-C4	C6-C5	C7-C6	C8-C7
298.15	-41.30	-39.10	-17.37	-32.1	-25.1	-24.0
300.00	-41.27	-39.07	-17.34	-32.1	-25.0	-24.0
400.00	-39.31	-36.97	-14.86	-27.9	-20.4	-22.5
500.00	-36.77	-34.10	-11.83	-23.5	-16.8	-19.1
600.00	-33.65	-30.44	-8.39	-19.2	-13.0	-15.1
700.00	-30.07	-25.94	-4.69	-14.7	-8.8	-10.8
800.00	-25.99	-20.69	-.69	-10.0	-4.3	-6.1
900.00	-21.52	-15.36	3.58	-5.1	.6	-1.1
1000.00	-16.73	-9.48	8.12	-.1	5.8	4.1

lation of heat effects when the reactants and products are at different temperatures.

The increments per carbon atom are of interest because they indicate the extent to which we can estimate thermodynamic properties of isomer groups of higher carbon numbers. Since the data for C_5H_8 and below come from earlier calculations and the data for C_6H_{10}, C_7H_{12}, and C_8H_{14} come from the Benson method, the C_6–C_5 and higher increments are in a sense less certain. The increments in the various thermodynamic quantities per carbon atom are quite similar for the alkynes and alkenes.[4] There is a problem with the heat capacities for C_7H_{12} and C_8H_{14} at 298.15 and 300 K. This is apparently due to the fact that the uncertainties in the contributions to the heat capacity are more uncertain for $C-(C_t)(C)_2(H)$ and $C-(C_t)(C)_3$. The heat capacity makes only a small contribution to other properties, and so this problem does appear in other tables. It is important to realize that heat capacity values used in the calculations are obtained from least squaring to $C_p^\circ = a + bT + cT^2$ so that the largest problems might be expected at the lowest or highest temperatures.

5. Equilibrium Mole Fractions Within Alkyne Isomer Groups

The equilibrium mole fractions within isomer groups calculated from standard Gibbs energies of formation are given in Table 9 for the ideal gas state. Since the uncertainties in $\Delta_f G^\circ(I)$ and $\Delta_f G_i^\circ$ are about the same, the uncertainty in the difference is nearly independent of the relative values of the two parameters, but the absolute uncertainty does in-

Table 9. Equilibrium mole fractions within alkyne isomer groups

T/K	298.15	300	400	500	600	700	800	900	1000
C4H6									
1-butyne	.0012	.0013	.0086	.0273	.0591	.1017	.1514	.2026	.2541
2-butyne	.9988	.9987	.9914	.9727	.9409	.8983	.8486	.7974	.7459
C5H8									
1-pentyne	.0015	.0015	.0075	.0200	.0386	.0623	.0887	.1170	.1440
2-pentyne	.9883	.9881	.9702	.9438	.9106	.8721	.8326	.7920	.7542
3-methyl-1-butyne	.0102	.0103	.0223	.0362	.0509	.0656	.0787	.0910	.1018
C6H10									
1-hexyne	.0000	.0000	.0004	.0017	.0046	.0092	.0155	.0231	.0317
2-hexyne	.0720	.0735	.1499	.2077	.2445	.2664	.2788	.2851	.2875
3-hexyne	.0800	.0818	.1797	.2575	.3083	.3389	.3562	.3651	.3685
4-methyl-1-pentyne	.0003	.0003	.0015	.0041	.0077	.0119	.0163	.0209	.0253
3(RS)-methyl-1-pentyne	.0005	.0005	.0031	.0084	.0156	.0240	.0331	.0422	.0511
4-methyl-2-pentyne	.8467	.8434	.6644	.5190	.4172	.3468	.2967	.2598	.2317
3,3-dimethyl-1-butyne	.0005	.0005	.0011	.0017	.0023	.0028	.0033	.0038	.0043
C7H12									
1-heptyne	.0000	.0000	.0002	.0008	.0024	.0051	.0090	.0138	.0193
2-heptyne	.0221	.0227	.0645	.1016	.1292	.1485	.1614	.1698	.1750
3-heptyne	.0245	.0253	.0773	.1261	.1629	.1889	.2063	.2175	.2243
2-methyl-3-hexyne	.2880	.2907	.3428	.3150	.2781	.2459	.2196	.1983	.1808
5-methyl-2-hexyne	.0649	.0660	.1019	.1113	.1108	.1072	.1026	.0979	.0934
5-methyl-1-hexyne	.0000	.0000	.0002	.0009	.0021	.0037	.0057	.0079	.0103
3(RS)-methyl-1-hexyne	.0000	.0000	.0005	.0018	.0042	.0075	.0116	.0161	.0208
4(RS)-methyl-2-hexyne	.1344	.1365	.2090	.2271	.2254	.2175	.2078	.1980	.1886
4(RS)-methyl-1-hexyne	.0000	.0000	.0005	.0018	.0041	.0074	.0114	.0159	.0206
4,4-dimethyl-2-pentyne	.4647	.4573	.1978	.1031	.0639	.0449	.0343	.0278	.0236
4,4-dimethyl-1-pentyne	.0004	.0004	.0010	.0015	.0020	.0024	.0028	.0031	.0035
3(RS),4-dimethyl-1-pentyne	.0005	.0005	.0021	.0045	.0071	.0097	.0122	.0145	.0166
3,3-dimethyl-1-pentyne	.0004	.0004	.0014	.0025	.0036	.0047	.0057	.0068	.0078
3-ethyl-1-pentyne	.0001	.0001	.0007	.0020	.0041	.0067	.0096	.0126	.0155
C8H14									
1-octyne	.0000	.0000	.0000	.0002	.0007	.0018	.0033	.0054	.0079
2-octyne	.0029	.0030	.0127	.0263	.0395	.0507	.0597	.0665	.0717
3-octyne	.0032	.0033	.0153	.0326	.0498	.0645	.0763	.0852	.0919
4-octyne	.0016	.0017	.0076	.0163	.0249	.0323	.0381	.0426	.0459
2-methyl-3-heptyne	.0373	.0380	.0677	.0814	.0850	.0840	.0812	.0777	.0740
6-methyl-3-heptyne	.0094	.0096	.0241	.0356	.0427	.0466	.0485	.0491	.0490
6-methyl-2-heptyne	.0084	.0086	.0201	.0287	.0339	.0366	.0379	.0383	.0382
6-methyl-1-heptyne	.0000	.0000	.0000	.0002	.0006	.0013	.0021	.0031	.0042
3(RS)-methyl-1-heptyne	.0000	.0000	.0003	.0011	.0025	.0046	.0071	.0098	.0127
5(RS)-methyl-3-heptyne	.0747	.0760	.1354	.1627	.1700	.1680	.1623	.1553	.1481
5(RS)-methyl-2-heptyne	.0168	.0173	.0403	.0575	.0678	.0733	.0758	.0767	.0765
5(RS)-methyl-1-heptyne	.0000	.0000	.0001	.0005	.0013	.0025	.0042	.0062	.0084
4(RS)-methyl-1-heptyne	.0000	.0000	.0001	.0005	.0013	.0025	.0042	.0062	.0084
4(RS)-methyl-2-heptyne	.0672	.0683	.1130	.1312	.1348	.1321	.1270	.1213	.1155
2,2-dimethyl-3-hexyne	.0670	.0666	.0469	.0330	.0246	.0195	.0162	.0140	.0124
5,5-dimethyl-2-hexyne	.1643	.1620	.0822	.0482	.0320	.0234	.0183	.0151	.0128
5,5-dimethyl-1-hexyne	.0000	.0000	.0000	.0001	.0002	.0003	.0004	.0005	.0006
4(RS),5-dimethyl-2-hexyne	.0513	.0518	.0652	.0642	.0591	.0537	.0488	.0447	.0412
4(RS),5-dimethyl-1-hexyne	.0000	.0000	.0002	.0005	.0011	.0018	.0027	.0036	.0045
3(RS),5-dimethyl-1-hexyne	.0000	.0000	.0002	.0005	.0011	.0019	.0027	.0036	.0045
3,3-dimethyl-1-hexyne	.0000	.0000	.0001	.0003	.0006	.0009	.0013	.0017	.0021
4,4-dimethyl-2-hexyne	.0469	.0469	.0429	.0357	.0300	.0259	.0230	.0209	.0194
4,4-dimethyl-1-hexyne	.0000	.0000	.0001	.0002	.0005	.0008	.0011	.0015	.0019
2,5-dimethyl-3-hexyne	.4390	.4365	.3002	.2033	.1450	.1094	.0864	.0708	.0597
3(RS),4(RS)-dimethyl-1-hexyne	.0005	.0005	.0023	.0052	.0085	.0118	.0149	.0178	.0203
4-ethyl-1-hexyne	.0000	.0000	.0000	.0002	.0006	.0013	.0021	.0031	.0042
4-ethyl-2-hexyne	.0087	.0089	.0206	.0293	.0345	.0372	.0384	.0388	.0386
3(RS)-ethyl-1-hexyne	.0000	.0000	.0003	.0011	.0025	.0046	.0071	.0098	.0127
3(RS),4,4-trimethyl-1-pentyne	.0001	.0001	.0002	.0004	.0005	.0007	.0008	.0009	.0010
3(RS)-ethyl-4-methyl-1-pentyne	.0001	.0001	.0004	.0012	.0022	.0033	.0045	.0057	.0068
3-ethyl-3-methyl-1-pentyne	.0000	.0000	.0001	.0003	.0006	.0009	.0013	.0017	.0021
3,3,4-trimethyl-1-pentyne	.0006	.0006	.0012	.0016	.0018	.0020	.0022	.0024	.0025

Table 10. Standard heat capacity at constant pressure for alkynes in J/K mol

T/K	298.15	300	400	500	600	700	800	900	1000
C2H2									
ethyne	43.93	44.06	50.08	54.27	58.45	60.12	62.47	64.64	66.61
C3H4									
propyne	60.67	60.88	72.51	82.59	91.21	98.66	105.19	110.92	115.94
C4H6									
1-butyne	81.42	81.76	99.87	115.60	128.99	140.46	150.41	159.08	166.69
2-butyne	77.95	78.24	94.64	110.29	124.18	136.36	147.03	156.31	164.39
C5H8									
1-pentyne	106.69	107.32	130.12	151.04	169.03	184.10	197.07	208.36	218.40
2-pentyne	98.70	99.12	122.17	143.51	161.92	178.24	192.05	204.60	215.06
3-methyl-1-butyne	104.68	105.14	130.12	151.46	169.87	184.93	198.32	209.62	219.24
C6H10									
1-hexyne	127.85	128.42	157.65	183.86	207.04	227.18	244.29	258.37	269.42
2-hexyne	121.38	121.95	151.29	177.76	201.37	222.10	239.97	254.96	267.09
3-hexyne	119.18	119.76	149.53	176.36	200.25	221.20	239.21	254.28	266.41
4-methyl-1-pentyne	126.79	127.37	157.32	184.08	207.64	228.01	245.19	259.17	269.96
3(RS)-methyl-1-pentyne	126.79	127.37	157.32	184.08	207.64	228.01	245.19	259.17	269.96
4-methyl-2-pentyne	120.32	120.90	150.96	177.98	201.97	222.93	240.86	255.76	267.63
3,3-dimethyl-1-butyne	129.58	130.18	161.22	189.06	213.69	235.11	253.33	268.34	280.15
C7H12									
1-heptyne	150.8	151.5	186.7	218.2	246.1	270.3	290.8	307.7	321.0
2-heptyne	144.4	145.1	180.3	212.1	240.4	265.2	286.5	304.3	318.6
3-heptyne	142.2	142.9	178.6	210.7	239.3	264.3	285.8	303.6	317.9
2-methyl-3-hexyne	141.1	141.8	178.3	210.9	239.9	265.2	286.7	304.4	318.5
5-methyl-2-hexyne	143.3	144.0	180.0	212.3	241.0	266.1	287.4	305.1	319.2
5-methyl-1-hexyne	149.8	150.5	186.4	218.4	246.7	271.1	291.7	308.5	321.5
3(RS)-methyl-1-hexyne	149.8	150.5	186.4	218.4	246.7	271.1	291.7	308.5	321.5
4(RS)-methyl-2-hexyne	143.3	144.0	180.0	212.3	241.0	266.1	287.4	305.1	319.2
4(RS)-methyl-1-hexyne	149.8	150.5	186.4	218.4	246.7	271.1	291.7	308.5	321.5
4,4-dimethyl-2-pentyne	146.1	146.8	183.9	217.3	247.1	273.2	295.6	314.3	329.4
4,4-dimethyl-1-pentyne	152.1	152.9	190.5	223.8	252.9	277.6	298.1	314.2	326.1
3(RS),4-dimethyl-1-pentyne	148.7	149.4	186.0	218.7	247.3	272.0	292.6	309.3	322.0
3,3-dimethyl-1-pentyne	152.6	153.3	190.3	223.4	252.7	278.2	299.9	317.7	331.7
3-ethyl-1-pentyne	149.8	150.5	186.4	218.4	246.7	271.1	291.7	308.5	321.5
C8H14									
1-octyne	173.8	174.6	215.8	252.6	285.2	313.4	337.4	357.1	372.5
2-octyne	167.4	168.2	209.4	246.5	279.5	308.3	333.1	353.7	370.2
3-octyne	165.2	166.0	207.6	245.1	278.4	307.4	332.3	353.0	369.5
4-octyne	165.2	166.0	207.6	245.1	278.4	307.4	332.3	353.0	369.5
2-methyl-3-heptyne	164.1	164.9	207.3	245.3	279.0	308.3	333.2	353.8	370.0
6-methyl-3-heptyne	164.1	164.9	207.3	245.3	279.0	308.3	333.2	353.8	370.0
6-methyl-2-heptyne	166.3	167.1	209.1	246.7	280.1	309.2	334.0	354.5	370.7
6-methyl-1-heptyne	172.8	173.6	215.4	252.8	285.8	314.3	338.3	357.9	373.0
3(RS)-methyl-1-heptyne	172.8	173.6	215.4	252.8	285.8	314.3	338.3	357.9	373.0
5(RS)-methyl-3-heptyne	164.1	164.9	207.3	245.3	279.0	308.3	333.2	353.8	370.0
5(RS)-methyl-2-heptyne	166.3	167.1	209.1	246.7	280.1	309.2	334.0	354.5	370.7
5(RS)-methyl-1-heptyne	172.8	173.6	215.4	252.8	285.8	314.3	338.3	357.9	373.0
4(RS)-methyl-1-heptyne	172.8	173.6	215.4	252.8	285.8	314.3	338.3	357.9	373.0
4(RS)-methyl-2-heptyne	166.3	167.1	209.1	246.7	280.1	309.2	334.0	354.5	370.7
2,2-dimethyl-3-hexyne	166.9	167.7	211.2	250.3	285.0	315.4	341.4	363.0	380.2
5,5-dimethyl-2-hexyne	168.7	169.5	213.2	252.1	286.3	315.7	340.3	360.2	375.3
5,5-dimethyl-1-hexyne	175.1	176.0	219.6	258.2	291.9	320.8	344.6	363.6	377.6
4(RS),5-dimethyl-2-hexyne	165.2	166.1	208.7	246.9	280.7	310.0	334.9	355.3	371.2
4(RS),5-dimethyl-1-hexyne	171.7	172.5	215.1	253.0	286.4	315.1	339.2	358.7	373.6
3(RS),5-dimethyl-1-hexyne	171.7	172.5	215.1	253.0	286.4	315.1	339.2	358.7	373.6
3,3-dimethyl-1-hexyne	175.6	176.4	219.3	257.8	291.8	321.4	346.4	367.1	383.2
4,4-dimethyl-2-hexyne	169.1	169.9	213.0	251.7	286.1	316.3	342.1	363.6	380.9
4,4-dimethyl-1-hexyne	175.1	176.0	219.6	258.2	291.9	320.8	344.6	363.6	377.6
2,5-dimethyl-3-hexyne	163.0	163.9	207.0	245.5	279.6	309.1	334.1	354.6	370.6
3(RS),4(RS)-dimethyl-1-hexyne	171.7	172.5	215.1	253.0	286.4	315.1	339.2	358.7	373.6
4-ethyl-1-hexyne	172.8	173.6	215.4	252.8	285.8	314.3	338.3	357.9	373.0
4-ethyl-2-hexyne	166.3	167.1	209.1	246.7	280.1	309.2	334.0	354.5	370.7
3(RS)-ethyl-1-hexyne	172.8	173.6	215.4	252.8	285.8	314.3	338.3	357.9	373.0
3(RS),4,4-trimethyl-1-pentyne	174.1	174.9	219.2	258.4	292.6	321.6	345.5	364.4	378.2
3(RS)-ethyl-4-methyl-1-pentyne	171.7	172.5	215.1	253.0	286.4	315.1	339.2	358.7	373.6
3-ethyl-3-methyl-1-pentyne	175.6	176.4	219.3	257.8	291.8	321.4	346.4	367.1	383.2
3,3,4-trimethyl-1-pentyne	174.5	175.3	219.0	258.0	292.4	322.2	347.3	367.9	383.8

Table 11. Standard entropy of alkynes in J/K mol

T/K	298.15	300	400	500	600	700	800	900	1000
C2H2									
ethyne	200.94	201.23	214.79	226.42	236.59	245.67	253.87	261.32	268.26
C3H4									
propyne	248.22	248.60	267.76	285.04	300.90	315.54	329.14	341.86	353.83
C4H6									
1-butyne	290.94	291.48	317.51	341.52	363.83	384.58	404.03	422.23	439.39
2-butyne	283.41	283.91	308.68	331.52	352.86	372.95	391.86	409.72	426.63
C5H8									
1-pentyne	329.89	330.56	364.62	395.96	425.12	452.36	477.80	501.65	524.16
2-pentyne	331.90	332.53	364.24	393.87	421.69	447.88	472.61	496.00	518.09
3-methyl-1-butyne	319.06	319.73	353.49	384.87	414.16	441.48	467.09	491.10	513.70
C6H10									
1-hexyne	370.05	370.84	411.86	449.91	485.53	518.99	550.48	580.09	607.92
2-hexyne	371.96	372.71	411.88	448.54	483.08	515.71	546.57	575.72	603.24
3-hexyne	375.64	376.38	414.98	451.28	485.59	518.07	548.82	577.89	605.34
4-methyl-1-pentyne	358.82	359.61	400.43	438.46	474.16	507.74	539.34	569.06	596.95
3(RS)-methyl-1-pentyne	364.58	365.37	406.19	444.23	479.92	513.50	545.10	574.82	602.71
4-methyl-2-pentyne	360.73	361.48	400.45	437.09	471.71	504.45	535.43	564.69	592.28
3,3-dimethyl-1-butyne	332.10	332.90	374.68	413.71	450.40	484.99	517.61	548.35	577.26
C7H12									
1-heptyne	409.5	410.4	458.9	504.0	546.3	586.1	623.6	658.9	692.0
2-heptyne	411.4	412.3	458.9	502.6	543.9	582.8	619.7	654.5	687.3
3-heptyne	415.1	415.9	462.0	505.4	546.4	585.2	621.9	656.7	689.4
2-methyl-3-hexyne	403.8	404.7	450.6	493.9	535.0	573.9	610.8	645.6	678.5
5-methyl-2-hexyne	400.1	401.0	447.5	491.2	532.5	571.6	608.5	643.5	676.4
5-methyl-1-hexyne	398.2	399.2	447.5	492.6	534.9	574.9	612.5	647.8	681.0
3(RS)-methyl-1-hexyne	404.0	404.9	453.2	498.3	540.7	580.6	618.2	653.6	686.8
4(RS)-methyl-2-hexyne	405.9	406.8	453.2	497.0	538.3	577.3	614.3	649.2	682.1
4(RS)-methyl-1-hexyne	404.0	404.9	453.2	498.3	540.7	580.6	618.2	653.6	686.8
4,4-dimethyl-2-pentyne	373.4	374.3	421.7	466.4	508.7	548.8	586.8	622.7	656.7
4,4-dimethyl-1-pentyne	371.4	372.4	421.6	467.8	511.2	552.1	590.6	626.7	660.4
3(RS),4-dimethyl-1-pentyne	392.8	393.7	441.8	486.9	529.3	569.4	607.1	642.5	675.8
3,3-dimethyl-1-pentyne	380.6	381.6	430.8	476.9	520.3	561.2	599.9	636.2	670.5
3-ethyl-1-pentyne	398.2	399.2	447.5	492.6	534.9	574.9	612.5	647.8	681.0
C8H14									
1-octyne	448.9	450.0	505.9	558.1	607.1	653.2	696.7	737.6	776.1
2-octyne	450.8	451.8	505.9	556.7	604.7	650.0	692.8	733.3	771.4
3-octyne	454.5	455.5	509.0	559.5	607.2	652.3	695.0	735.4	773.5
4-octyne	448.7	449.7	503.3	553.7	601.4	646.6	689.3	729.7	767.7
2-methyl-3-heptyne	443.2	444.3	497.6	548.0	595.8	641.1	683.9	724.4	762.5
6-methyl-3-heptyne	443.2	444.3	497.6	548.0	595.8	641.1	683.9	724.4	762.5
6-methyl-2-heptyne	439.6	440.6	494.5	545.3	593.3	638.7	681.7	722.2	760.4
6-methyl-1-heptyne	437.6	438.7	494.5	546.7	595.7	642.0	685.6	726.6	765.1
3(RS)-methyl-1-heptyne	443.4	444.5	500.3	552.4	601.5	647.7	691.3	732.3	770.9
5(RS)-methyl-3-heptyne	440.0	440.0	503.4	553.8	601.6	646.8	689.7	730.1	768.3
5(RS)-methyl-2-heptyne	445.3	446.4	500.3	551.1	599.0	644.5	687.4	728.0	766.2
5(RS)-methyl-1-heptyne	443.4	444.5	500.3	552.4	601.5	647.7	691.3	732.3	770.9
4(RS)-methyl-1-heptyne	443.4	444.5	500.3	552.4	601.5	647.7	691.3	732.3	770.9
4(RS)-methyl-2-heptyne	445.3	446.4	500.3	551.1	599.0	644.5	687.4	728.0	766.2
2,2-dimethyl-3-hexyne	416.5	417.6	471.9	523.3	572.0	618.3	662.2	703.7	742.8
5,5-dimethyl-2-hexyne	412.8	413.8	468.7	520.5	569.6	616.0	659.8	701.1	739.8
5,5-dimethyl-1-hexyne	410.8	411.9	468.6	521.9	572.0	619.2	663.7	705.4	744.5
4(RS),5-dimethyl-2-hexyne	434.1	435.1	488.8	539.6	587.7	633.2	676.3	716.9	755.2
4(RS),5-dimethyl-1-hexyne	432.2	433.2	488.8	541.0	590.1	636.5	680.2	721.3	759.9
3(RS),5-dimethyl-1-hexyne	432.2	433.2	488.8	541.0	590.1	636.5	680.2	721.3	759.9
3,3-dimethyl-1-hexyne	420.1	421.1	477.9	531.0	581.1	628.4	673.0	715.0	754.6
4,4-dimethyl-2-hexyne	422.0	423.0	477.9	529.7	578.7	625.1	669.1	710.6	749.9
4,4-dimethyl-1-hexyne	420.0	421.1	477.8	531.0	581.1	628.4	672.8	714.6	753.6
2,5-dimethyl-3-hexyne	432.0	433.0	486.2	536.6	584.4	629.8	672.8	713.3	751.6
3(RS),4(RS)-dimethyl-1-hexyne	437.9	439.0	494.6	546.7	595.9	642.3	686.0	727.1	765.7
4-ethyl-1-hexyne	437.6	438.7	494.5	546.7	595.7	642.0	685.6	726.6	765.1
4-ethyl-2-hexyne	439.6	440.6	494.5	545.3	593.3	638.7	681.7	722.2	760.4
3(RS)-ethyl-1-hexyne	443.4	444.5	500.3	552.4	601.5	647.7	691.3	732.3	770.9
3(RS),4,4-trimethyl-1-pentyne	405.4	406.5	463.0	516.2	566.4	613.7	658.3	700.1	739.3
3(RS)-ethyl-4-methyl-1-pentyne	432.2	433.2	488.8	541.0	590.1	636.5	680.2	721.3	759.9
3-ethyl-3-methyl-1-pentyne	420.1	421.1	477.9	531.0	581.1	628.4	673.0	715.0	754.6
3,3,4-trimethyl-1-pentyne	408.8	409.9	466.4	519.6	569.7	617.1	661.8	704.0	743.6

Table 12. Standard enthalpy of formation for alkynes in kJ/mol

T/K	298.15	300	400	500	600	700	800	900	1000
C2H2									
ethyne	226.73	226.73	226.48	226.10	225.60	225.02	224.35	223.63	222.97
C3H4									
propyne	185.43	185.39	183.18	181.08	179.20	177.49	176.02	174.77	173.76
C4H6									
1-butyne	165.18	165.10	161.38	158.07	155.18	152.80	150.79	149.20	148.03
2-butyne	146.31	146.23	142.05	138.20	134.81	131.96	129.58	127.70	126.27
C5H8									
1-pentyne	144.35	144.26	139.37	135.10	131.50	128.57	126.19	124.39	123.14
2-pentyne	128.87	128.74	123.05	117.99	113.68	110.08	107.19	104.93	103.34
3-methyl-1-butyne	136.40	136.27	131.29	127.07	123.51	120.67	118.41	116.73	115.60
C6H10									
1-hexyne	124.22	124.09	117.77	112.29	107.75	104.16	101.47	99.53	98.19
2-hexyne	104.77	104.62	97.66	91.56	86.43	82.30	79.13	76.80	75.18
3-hexyne	105.60	105.45	98.30	92.04	86.78	82.55	79.30	76.90	75.21
4-methyl-1-pentyne	114.85	114.71	108.33	102.85	98.35	94.63	92.22	90.37	89.10
3(RS)-methyl-1-pentyne	114.77	114.63	108.25	102.76	98.27	94.75	92.14	90.29	89.02
4-methyl-2-pentyne	95.31	95.16	88.14	82.03	76.94	72.88	69.81	67.56	66.01
3,3-dimethyl-1-butyne	105.35	105.22	99.17	94.13	90.19	87.33	85.48	84.49	84.20
C7H12									
1-heptyne	103.6	103.4	95.8	89.3	83.9	79.7	76.6	74.5	73.1
2-heptyne	84.1	84.0	75.7	68.5	62.6	57.8	54.3	51.7	50.0
3-heptyne	85.0	84.8	76.3	69.0	62.9	58.1	54.4	51.8	50.1
2-methyl-3-hexyne	75.5	75.3	66.8	59.5	53.4	48.7	45.1	42.6	40.9
5-methyl-2-hexyne	78.1	77.9	69.6	62.4	56.5	51.8	48.4	45.9	44.3
5-methyl-1-hexyne	97.6	97.4	89.7	83.2	77.8	73.7	70.7	68.7	67.3
3(RS)-methyl-1-hexyne	97.5	97.3	89.6	83.1	77.7	73.6	70.6	68.6	67.2
4(RS)-methyl-2-hexyne	78.0	77.9	69.5	62.3	56.4	51.8	48.3	45.8	44.2
4(RS)-methyl-1-hexyne	97.6	97.4	89.7	83.2	77.8	73.7	70.7	68.7	67.3
4,4-dimethyl-2-pentyne	65.3	65.1	57.1	50.4	45.0	41.0	38.3	36.7	36.0
4,4-dimethyl-1-pentyne	82.2	82.1	74.7	68.6	63.9	60.4	58.0	56.6	55.8
3(RS),4-dimethyl-1-pentyne	88.1	87.9	80.2	73.6	68.3	64.3	61.4	59.4	58.1
3,3-dimethyl-1-pentyne	84.7	84.6	77.2	71.1	66.3	62.9	60.6	59.4	59.1
3-ethyl-1-pentyne	94.1	94.0	86.3	79.7	74.4	70.3	67.3	65.2	63.9
C8H14									
1-octyne	83.0	82.8	73.8	66.2	60.0	55.2	51.8	49.4	47.9
2-octyne	63.5	63.3	53.7	45.5	38.7	33.4	29.4	26.7	24.9
3-octyne	64.3	64.1	54.4	46.0	39.0	33.6	29.6	26.8	24.9
4-octyne	64.3	64.1	54.4	46.0	39.0	33.6	29.6	26.8	24.9
2-methyl-3-heptyne	54.9	54.7	44.8	36.4	29.6	24.2	20.3	17.5	15.8
6-methyl-3-heptyne	58.3	58.1	48.3	39.9	33.0	27.6	23.7	21.0	19.2
6-methyl-2-heptyne	57.5	57.3	47.6	39.4	32.6	27.4	23.5	20.9	19.2
6-methyl-1-heptyne	76.9	76.7	67.7	60.1	54.0	49.2	45.9	43.6	42.2
3(RS)-methyl-1-heptyne	73.5	73.3	64.3	56.7	50.5	45.8	42.4	40.2	38.7
5(RS)-methyl-3-heptyne	54.9	54.7	44.8	36.4	29.6	24.2	20.3	17.5	15.8
5(RS)-methyl-2-heptyne	57.5	57.3	47.6	39.4	32.6	27.4	23.5	20.9	19.2
5(RS)-methyl-1-heptyne	76.9	76.7	67.7	60.1	54.0	49.2	45.9	43.6	42.2
4(RS)-methyl-1-heptyne	76.9	76.7	67.7	60.1	54.0	49.2	45.9	43.6	42.2
4(RS)-methyl-2-heptyne	54.1	53.9	44.2	35.9	29.2	23.9	20.1	17.4	15.7
2,2-dimethyl-3-hexyne	45.6	45.3	35.8	27.8	21.6	16.8	13.6	11.7	10.9
5,5-dimethyl-2-hexyne	42.1	41.9	32.6	24.8	18.7	14.1	10.9	8.8	7.6
5,5-dimethyl-1-hexyne	68.3	68.1	59.4	52.3	46.7	42.6	39.9	38.2	37.3
4(RS),5-dimethyl-2-hexyne	51.4	51.2	41.5	33.2	26.5	21.3	17.6	15.0	13.3
4(RS),5-dimethyl-1-hexyne	70.9	70.7	61.6	54.0	47.9	43.3	40.0	37.8	36.4
3(RS),5-dimethyl-1-hexyne	70.8	70.6	61.6	53.9	47.8	43.2	39.9	37.7	36.3
3,3-dimethyl-1-hexyne	67.4	67.3	58.6	51.4	45.8	41.7	39.1	37.7	37.3
4,4-dimethyl-2-hexyne	48.0	47.8	38.5	30.7	24.5	19.9	16.8	15.0	14.3
4,4-dimethyl-1-hexyne	68.3	68.1	59.4	52.3	46.7	42.6	39.9	38.2	37.3
2,5-dimethyl-3-hexyne	45.4	45.2	35.3	26.9	20.1	14.8	10.9	8.3	6.6
3(RS),4(RS)-dimethyl-1-hexyne	64.1	63.9	54.9	47.2	41.1	36.5	33.2	31.0	29.7
4-ethyl-1-hexyne	76.9	76.7	67.7	60.1	54.0	49.2	45.9	43.6	42.2
4-ethyl-2-hexyne	57.4	57.2	47.6	39.3	32.5	27.3	23.4	20.8	19.1
3(RS)-ethyl-1-hexyne	73.5	73.3	64.3	56.7	50.5	45.8	42.4	40.2	38.7
3(RS),4,4-trimethyl-1-pentyne	58.8	58.6	49.9	42.7	37.2	33.2	30.6	29.0	28.1
3(RS)-ethyl-4-methyl-1-pentyne	67.5	67.3	58.2	50.6	44.5	39.8	36.5	34.3	33.0
3-ethyl-3-methyl-1-pentyne	67.4	67.3	58.6	51.4	45.8	41.7	39.1	37.7	37.3
3,3,4-trimethyl-1-pentyne	54.7	54.5	45.8	38.6	33.0	29.1	26.5	25.2	24.8

Table 13. Standard Gibbs energy of formation for alkynes in kJ/mol

T/K	298.15	300	400	500	600	700	800	900	1000
C2H2									
ethyne	209.20	209.07	203.22	197.44	191.75	186.19	180.67	175.23	169.91
C3H4									
propyne	194.46	194.51	197.90	201.81	206.13	210.78	215.61	220.64	225.84
C4H6									
1-butyne	202.15	202.36	215.35	229.27	243.77	258.72	273.98	289.48	305.15
2-butyne	185.50	185.75	199.58	214.41	229.96	246.05	262.51	279.23	296.19
C5H8									
1-pentyne	210.34	210.76	233.68	257.77	282.66	308.09	333.89	359.95	386.26
2-pentyne	194.28	194.65	217.53	241.75	266.88	292.73	319.00	345.64	372.49
3-methyl-1-butyne	205.62	206.03	230.08	255.30	281.28	307.79	334.69	361.83	389.15
C6H10									
1-hexyne	218.97	219.56	252.38	286.66	321.99	357.98	394.45	431.16	468.08
2-hexyne	198.95	199.53	232.26	266.62	302.14	338.42	375.25	412.37	449.74
3-hexyne	198.69	199.26	231.65	265.72	300.98	337.02	373.62	410.52	447.68
4-methyl-1-pentyne	212.95	213.55	247.51	282.94	319.41	356.53	394.12	431.94	469.96
3(RS)-methyl-1-pentyne	211.15	211.74	245.12	279.97	315.87	352.41	389.43	426.67	464.11
4-methyl-2-pentyne	192.84	193.44	227.30	262.81	299.47	336.88	374.83	413.07	451.54
3,3-dimethyl-1-butyne	211.42	212.07	248.65	286.61	325.50	364.95	404.76	444.70	484.74
C7H12									
1-heptyne	227.3	228.0	270.8	315.3	361.0	407.5	454.6	502.0	549.5
2-heptyne	207.2	208.0	250.6	295.2	341.2	388.0	435.4	483.2	531.2
3-heptyne	207.0	207.7	250.0	294.3	340.0	386.6	433.8	481.3	529.1
2-methyl-3-hexyne	200.9	201.6	245.1	290.5	337.3	385.0	433.4	482.0	530.9
5-methyl-2-hexyne	204.6	205.3	249.1	294.8	341.9	389.9	438.4	487.3	536.4
5-methyl-1-hexyne	224.6	225.4	269.2	314.9	361.8	409.4	457.6	506.1	554.8
3(RS)-methyl-1-hexyne	222.8	223.6	266.9	311.9	358.2	405.3	452.9	500.8	548.9
4(RS)-methyl-2-hexyne	202.8	203.5	246.7	291.9	338.4	385.7	433.7	482.0	530.6
4(RS)-methyl-1-hexyne	222.9	223.6	266.9	312.0	358.3	405.4	453.0	500.9	549.0
4,4-dimethyl-2-pentyne	199.7	200.5	246.9	295.2	344.7	394.9	445.7	496.7	547.9
4,4-dimethyl-1-pentyne	217.2	218.1	264.6	312.7	362.1	412.0	462.5	513.1	563.8
3(RS),4-dimethyl-1-pentyne	216.8	217.6	262.0	308.2	355.7	403.9	452.6	501.6	550.8
3,3-dimethyl-1-pentyne	217.0	217.8	263.4	310.6	359.0	408.1	457.6	507.3	557.1
3-ethyl-1-pentyne	221.2	221.9	265.8	311.5	358.4	406.0	454.2	502.7	551.3
C8H14									
1-octyne	235.6	236.5	289.2	343.9	400.0	457.1	514.8	572.7	631.0
2-octyne	215.5	216.5	269.0	323.8	380.2	437.5	495.6	554.0	612.6
3-octyne	215.3	216.2	268.4	322.9	379.0	436.1	493.9	552.1	610.6
4-octyne	217.0	217.9	270.7	325.8	382.5	440.2	498.5	557.3	616.3
2-methyl-3-heptyne	209.2	210.1	263.5	319.1	376.4	434.6	493.5	552.8	612.4
6-methyl-3-heptyne	212.6	213.5	266.9	322.6	379.8	438.0	496.9	556.2	615.8
6-methyl-2-heptyne	212.9	213.8	267.5	323.5	380.9	439.4	498.6	558.1	617.9
6-methyl-1-heptyne	232.9	233.8	287.6	343.5	400.8	459.0	517.8	576.9	636.2
3(RS)-methyl-1-heptyne	227.7	228.7	281.9	337.2	393.9	451.5	509.7	568.3	627.0
5(RS)-methyl-3-heptyne	207.5	208.4	261.2	316.2	372.9	430.6	488.9	547.6	606.6
5(RS)-methyl-2-heptyne	211.1	212.1	265.2	320.6	377.5	435.4	494.0	552.9	612.1
5(RS)-methyl-1-heptyne	231.2	232.1	285.3	340.6	397.3	454.9	513.2	571.7	630.4
4(RS)-methyl-1-heptyne	231.2	232.1	285.3	340.6	397.3	454.9	513.2	571.7	630.4
4(RS)-methyl-2-heptyne	207.7	208.7	261.8	317.1	374.1	432.0	490.5	549.5	608.7
2,2-dimethyl-3-hexyne	207.7	208.7	264.7	322.9	382.5	443.1	504.2	565.6	627.2
5,5-dimethyl-2-hexyne	205.5	206.5	262.8	321.3	381.2	442.0	503.4	565.1	626.9
5,5-dimethyl-1-hexyne	232.2	233.2	289.7	348.1	407.8	468.3	529.3	590.5	652.0
4(RS),5-dimethyl-2-hexyne	208.4	209.3	263.6	320.1	378.2	437.2	496.9	556.9	617.2
4(RS),5-dimethyl-1-hexyne	228.5	229.5	283.8	340.2	398.1	456.8	516.2	575.8	635.7
3(RS),5-dimethyl-1-hexyne	228.4	229.4	283.7	340.2	398.0	456.8	516.1	575.7	635.6
3,3-dimethyl-1-hexyne	228.6	229.6	285.1	342.6	401.4	461.0	521.1	581.4	641.8
4,4-dimethyl-2-hexyne	208.6	209.6	265.0	322.6	381.6	441.4	501.9	562.6	623.5
4,4-dimethyl-1-hexyne	229.5	230.5	286.0	343.5	402.3	461.9	522.0	582.3	642.8
2,5-dimethyl-3-hexyne	203.1	204.0	258.5	315.3	373.7	433.1	493.1	553.5	614.2
3(RS),4(RS)-dimethyl-1-hexyne	220.0	221.0	274.7	330.6	387.9	446.0	504.8	563.8	623.1
4-ethyl-1-hexyne	232.9	233.8	287.6	343.5	400.8	459.0	517.8	576.9	636.2
4-ethyl-2-hexyne	212.8	213.7	267.4	323.4	380.9	439.3	498.5	558.0	617.8
3(RS)-ethyl-1-hexyne	227.7	228.7	281.9	337.2	393.9	451.5	509.7	568.3	627.0
3(RS),4,4-trimethyl-1-pentyne	224.4	225.4	282.4	341.4	401.7	462.7	524.3	586.1	648.0
3(RS)-ethyl-4-methyl-1-pentyne	225.1	226.0	280.4	336.8	394.7	453.4	512.8	572.4	632.2
3-ethyl-3-methyl-1-pentyne	228.6	229.6	285.1	342.6	401.4	461.0	521.1	581.4	641.8
3,3,4-trimethyl-1-pentyne	219.3	220.3	276.9	335.5	395.5	456.2	517.4	578.8	640.4

crease with temperature. The usual equation for the propagation of variance indicates that the equilibrium mole fractions are uncertain by about 15% at the lower temperature and 10% at the higher temperatures. This makes it difficult to indicate the uncertainties in the table. It could be done by using exponential notation, but this makes it difficult to compare the mole fractions of various isomers.

Compounds are named in tables according to the IUPAC Revised and Collected Recommendations for the Nomenclature of Organic Chemistry, 1979.[13]

6. Standard Thermodynamic Properties of Individual Alkyne Species

The values of C_P°, S°, $\Delta_f H^\circ$, and $\Delta_f G^\circ$ for all the alkyne species through C_8H_{14} are given in Tables 10–13 in SI units for a standard state pressure of 1 bar. The values for C_2H_2 through C_5H_8 have been converted from the tables of Stull, Westrum, and Sinke[6] and the values for C_6H_{10}, C_7H_{12}, and C_8H_{14} have been calculated using the Benson method.[7] The values for chiral forms are for the racemates.

7. Discussion

The values of standard thermodynamic properties of isomer groups given here may be used in predicting equilibrium compositions of organic systems at temperature-catalyst conditions where species in an isomer group are in equilibrium. The chemical thermodynamic properties of alkylacetylenes are of interest in calculating equilibrium compositions in C/H systems at high temperatures.[14]

8. Nomenclature

C_{Pi}° = standard heat capacity at constant pressure of isomer i, J K^{-1} mol^{-1}

$C_P^\circ(I)$ = standard heat capacity at constant pressure of isomer group I, J K^{-1} mol^{-1}

$\Delta_f G_i^\circ$ = standard Gibbs energy of formation of isomer i, kJ mol^{-1}

$\Delta_f G^\circ(I)$ = standard Gibbs energy of formation of isomer group I, kJ mol^{-1}

$H^\circ(I,T) - H^\circ(I,298.15\ K)$ = standard enthalpy for isomer groups relative to isomer groups at 298.15 K, kJ mol^{-1}

$H^\circ(I,T) - H^\circ(I,298.15\ K) + \Delta_f H^\circ(I,298.15\ K)$ = standard enthalpy of formation for isomer groups relative to elements at 298.15 K, kJ mol^{-1}

$\Delta_f H_i^\circ$ = standard enthalpy of formation of isomer i, kJ mol^{-1}

$\Delta_f H^\circ(I)$ = standard enthalpy of formation of isomer group I, kJ mol^{-1}

n = number of carbon atoms in a molecule

N_I = number of isomers in an isomer group

OPT = number of optical isomers

r_i = equilibrium mole fraction of species i in an isomer group

S_i° = standard entropy of isomer i, J K^{-1} mol^{-1}

$S^\circ(I)$ = standard entropy of isomer group I, J K^{-1} mol^{-1}

TSN = total symmetry number

y_i = mole fraction of isomer i within the isomer group

y_I = mole fraction of isomer group I in a mixture

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