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1 October 1981 - 30 September 1982

THERMODYNAMICS OF ORGANIC COMPOUNDS

Bartlesville Energy Technology Center
Department of Energy
Bartlesville, Oklahoma

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This research program consisted of an integrated and interrelated effort of basic and applied research in chemical thermodynamics and thermochemistry. Knowledge of variation of physical and thermodynamic properties with molecular structure was used to select compounds for study that because of high ring strain or unusual steric effects may have good energy characteristics per unit volume or per unit mass and thus be useful in the synthesis of high energy fuels. These materials were synthesized, and their

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thermodynamic properties were evaluated. In cooperation with researchers at Wright-Patterson Air Force Base, ramjet fuels currently in use were subjected to careful thermodynamic evaluation by measurements of heat capacity, enthalpy of combustion and vapor pressure. During the last year of this effort, seven kerosene-type fuels produced by British Petroleum and seven jet fuels produced from shale oil were studied.

FINAL TECHNICAL SUMMARY REPORT

THERMODYNAMICS OF ORGANIC COMPOUNDS

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Bartlesville Energy Technology Center
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FOREWORD

This research program consists of an integrated and interrelated effort of basic and applied research in chemical thermodynamics and thermochemistry. Knowledge of variation of physical and thermodynamic properties with molecular structure is used to select compounds for study that because of high ring strain or unusual steric effects may have good energy characteristics per unit volume or per unit mass and thus be useful in the synthesis of high energy fuels. These materials are synthesized, and their thermodynamic properties are evaluated. In cooperation with researchers at Wright-Patterson Air Force Base, ramjet fuels currently in use are subjected to careful thermodynamic evaluation by measurements of heat capacity, enthalpy of combustion and vapor pressure.

ABSTRACT

The research effort continues to be focused on high-density/high-energy hydrocarbons. In cooperation with researchers at Wright-Patterson Air Force Base, heats of combustion are measured for constituents of current ramjet fuels and for finished fuels; meanwhile, pure hydrocarbons were synthesized for heat-of-combustion measurements to determine unusual steric or strain energies which may contribute to design of high-energy/high-density fuels of the future.

Seven kerosene-type fuels produced by British Petroleum and seven jet fuels produced from shale oil were studied during the current reporting period. Synthesis and purification of hydrocarbons were continued at Oklahoma State University; two ethylindans have been received and are being prepared for study.

RESEARCH PROGRESS

1. ENTHALPY OF COMBUSTION OF FUELS

A set of seven kerosene-type fuels produced by British Petroleum, designated BP···, and a set of seven jet fuels produced from shale oil, designated JP···, were studied by bomb calorimetry at the request of researchers at Wright-Patterson Air Force Base. The procedures used and the results from these studies are given below. The letters BP were added to the prefix for the so-designated samples to be consistent with designations received by phone from Don Potter in the spring of 1982 when he gave the 15° C densities and the hydrogen and sulfur analysis for these materials. Otherwise the designations were taken from the labels on the sample bottles from Wright-Patterson Air Force Base dated January 1982.

Experimental procedures used for the combustion calorimetry of hydrocarbons by this laboratory have been described;[1,2] although the fuels used in these experiments are not hydrocarbons, essentially the same procedures were used. Rotating-bomb calorimeter BMR II[3] and platinum-lined bomb Pt-3b[4] were used, without bomb rotation. Fragile, flexible borosilicate glass ampoules[2,5] were used to confine the volatile samples. For each experiment, 1 cm^3 of water was added to the bomb. In one experiment on each sample, the air was flushed from the bomb before charging with pure oxygen; in all the other experiments the bomb was charged with oxygen without flushing. After one of the combustion experiments for each sample, the CO_2 was recovered in weighing tubes to provide missing information and independent checks on the elemental analyses. After the bomb was discharged, the liquid content was quantitatively transferred to an Erlenmeyer flask, and it was then titrated with standard sodium hydroxide solution to determine the total acid formed in the combustion reaction (either sulfuric acid, nitric acid, or a mixture of these two acids). The relative amounts of sulfuric and nitric acids were determined by subtracting the calculated amount of sulfuric acid from the measured total amount of acid; the amount of sulfuric acid was calculated from the empirical formula of the sample and the sample mass.

Results of all of the experiments are given in Tables 1 through 7. Values of $\Delta E\overset{\circ}{c}/m$ in these tables refer to the reaction of unit mass of sample according to the following equation:

$$C_aH_bS_e(liq) + [a + b/4 + 3e/2]\ O_2(g) + (ne + e - b/2)\ H_2O(liq) =$$
$$a\ CO_2(g) + e(H_2SO_4 \cdot nH_2O)(liq). \qquad (1)$$

A more useful value computed from the combustion experiments may be the value of the energy of the reaction in which water appears in the combustion products in the gaseous state, and sulfur, if present, appears as gaseous sulfur dioxide:

$$C_aH_bS_e(liq) + [a + b/4 + e]\ O_2(g) =$$
$$a\ CO_2(g) + b/2\ H_2O(g) + e\ SO_2(g). \qquad (2)$$

Values of the enthalpies of formation of gaseous SO_2, aqueous H_2SO_4, gaseous H_2O and liquid H_2O[6] were used to convert the average values of the energy of reaction (Tables 1 through 7, Equation 1) to the energy of reaction (Table 8, Equation 2).

The empirical formulas shown in Table 8 were derived from the analysis for sulfur and the ASTM wide-line NMR analysis for hydrogen from Don Potter at Wright-Patterson Air Force Base and from our analysis for carbon. The percentages of elements usually summed to 100 to within 0.1 percent for each compound; one noted exception was sample JP-4-S-A (UN-81-141) which had a sum of 0.45 percent low. In Table 8 the densities at 15° C were supplied by Don Potter, and the values at 25° C were determined as auxiliary information to the bomb calorimetry.

A simple correlation of the values of $\Delta E\overset{\circ}{c}/m$ in column five of Table 8 was made as follows:

$$\Delta E\overset{\circ}{c}/m = A + B(\text{pct H}) \qquad (3)$$

$$A = -8400.24 \pm 61.83$$

B = [illegible]36.047 ± 4.437

where the weight percent hydrogen (pct H) can be determined from the empirical formulas of Table 8. The deviations from the equation are shown in column six of Table 8 where the largest value is 0.25 percent too positive.

TABLE 1. Summary of combustion experiments for BP-IP-1 and BP-IP-2 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-1			BP-IP-2		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.668625	0.675561	0.675463	0.679541	0.679461	0.679908
m''(auxiliary oil)/g	0.054757	0.048261	0.053966	0.053499	0.045640	0.050006
m'''(fuse)/g	0.000997	0.000932	0.001071	0.000761	0.000901	0.000990
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.99784	2.00272	2.01882	2.02150	2.00293	2.01697
ϵ(calor)$(-\Delta t_c)/cal_{th}$	-8005.89	-8025.43	-8089.95	-8100.69	-8026.28	-8082.54
ϵ(cont)$(-\Delta t_c)/cal_{th}$[b]	-8.69	-8.69	-8.84	-8.77	-8.76	-8.74
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	13.43	13.77	0.00	14.78	13.92
ΔE(corr to std states)$/cal_{th}$[c]	2.47	2.39	2.42	2.52	2.39	2.42
$\{-m''(\Delta E_c^\circ/m)$(auxiliary oil)$\}/cal_{th}$	602.56	531.09	593.87	588.72	502.24	550.29
$\{-m'''(\Delta E_c^\circ/m)$(fuse)$\}/cal_{th}$	4.04	3.77	4.34	3.08	3.65	4.01
$\{m'(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}$	-7405.33	-7483.26	-7484.21	-7514.96	-7511.80	-7520.46
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11075.45	-11077.10	-11080.13	-11058.88	-11055.52	-11060.99
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11077.56 ± 1.37 (mean and standard deviation of the mean)			-11058.46 ± 1.59		

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[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\epsilon^i(\text{cont})(t_i - 298.15\ K) + \epsilon^f(\text{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 2. Summary of combustion experiments for BP-IP-3 and BP-IP-4 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-3			BP-IP-4		
Experiment number	1	2	3	1	2	3
$m'(\text{fuel})/g$	0.667804	0.666184	0.663254	0.667251	0.664744	0.660514
$m''(\text{auxiliary oil})/g$	0.053619	0.060042	0.065139	0.060106	0.061745	0.060458
$m'''(\text{fuse})/g$	0.001007	0.000826	0.000942	0.001083	0.000801	0.001049
$n^i(H_2O)/mol$	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.98547	2.00253	2.00862	2.00254	2.00319	1.98846
$\varepsilon(\text{calor})(-\Delta t_c)/cal_{th}$	-7956.31	-8024.68	-8049.08	-8024.72	-8027.33	-7968.32
$\varepsilon(\text{cont})(-\Delta t_c)/cal_{th}$[b]	-8.55	-8.78	-8.73	-8.70	-8.70	-8.69
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.62	14.27	0.00	13.14	12.93
$\Delta E_{(\text{corr to std states})}/cal_{th}$[c]	2.47	2.40	2.42	2.51	2.43	2.41
$\{-m''(\Delta E_c^\circ/m)(\text{auxiliary oil})\}/cal_{th}$	590.05	660.72	716.81	661.43	679.47	665.30
$\{-m'''(\Delta E_c^\circ/m)(\text{fuse})\}/cal_{th}$	4.08	3.34	3.81	4.38	3.24	4.25
$\{m'(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}$	-7368.08	-7352.20	-7320.32	-7364.92	-7337.57	-7291.94
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11033.29	-11036.30	-11036.96	-11037.71	-11038.19	-11039.81
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11035.52 ± 1.13 (mean and standard deviation of the mean)			-11038.57 ± 0.64		

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[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(\text{cont})(t_i - 298.15\ K) + \varepsilon^f(\text{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 3. Summary of combustion experiments for BP-IP-5 and BP-IP-6 fuels[a]

($cal_{th} = 4.184$ J)

Sample	BP-IP-5			BP-IP-6		
Experiment number	1	2	3	1	2	3
$m'(\text{fuel})/g$	0.648128	0.645746	0.608922	0.644414	0.611948	0.609626
$m''(\text{auxiliary oil})/g$	0.061152	0.081022	0.131735	0.069067	0.121556	0.118052
$m'''(\text{fuse})/g$	0.000952	0.001063	0.001104	0.000980	0.001356	0.001128
$n^i(H_2O)/\text{mol}$	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.94828	2.00115	2.03850	1.94755	2.00696	1.99156
$\varepsilon(\text{calor})(-\Delta t_c)/cal_{th}$	-7807.28	-8019.15	-8168.84	-7804.38	-8042.45	-7980.72
$\varepsilon(\text{cont})(-\Delta t_c)/cal_{th}$[b]	-8.49	-8.76	-8.88	-8.41	-8.81	-8.66
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	12.51	13.55	0.00	13.03	13.98
$\Delta E_{(\text{corr to std states})}/cal_{th}$[c]	2.48	2.48	2.53	2.55	2.55	2.52
$\{-m''(\Delta E_c^\circ/m)(\text{auxiliary oil})\}/cal_{th}$	672.94	891.60	1449.67	760.04	1337.65	1299.09
$\{-m'''(\Delta E_c^\circ/m)(\text{fuse})\}/cal_{th}$	3.85	4.30	4.47	3.97	5.49	4.57
$\{m'(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}$	-7136.32	-7116.84	-6707.32	-7046.05	-6692.36	-6669.04
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11010.66	-11021.10	-11015.08	-10934.04	-10936.16	-10939.56
$\langle(\Delta E_c^\circ/m)(\text{fuel})\rangle/cal_{th}\ g^{-1}$	-11015.61 ± 3.02 (mean and standard deviation of the mean)			-10936.58 ± 1.61		

---

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(\text{cont})(t_i - 298.15\ K) + \varepsilon^f(\text{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 4. Summary of combustion experiments for BP-IP-7 and BP-IP-9 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-7		BP-IP-6		
Experiment number	1	2	1	2	3
$m'(\text{fuel})/g$	0.607569	0.676230	0.639897	0.689602	0.610359
$m''(\text{auxiliary oil})/g$	0.066801	0.054959	0.083057	0.050499	0.130568
$m'''(\text{fuse})/g$	0.000796	0.001023	0.000919	0.001108	0.001101
$n^i(H_2O)/mol$	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.84351	2.00214	1.96109	2.01002	2.01545
$\varepsilon(\text{calor})(-\Delta t_c)/cal_{th}$	-7387.46	-8023.14	-7858.61	-8054.69	-8076.45
$\varepsilon(\text{cont})(-\Delta t_c)/cal_{th}$[b]	-7.93	-8.73	-8.51	-8.70	-8.86
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	12.50	0.00	12.77	13.24
$\Delta E_{(\text{corr to std states})}/cal_{th}$[c]	2.37	2.55	2.68	2.69	2.66
$\{-m''(\Delta E_c^\circ/m)(\text{auxiliary oil})\}/cal_{th}$	735.11	604.79	913.99	555.71	1436.82
$\{-m'''(\Delta E_c^\circ/m)(\text{fuse})\}/cal_{th}$	3.22	4.14	3.72	4.49	4.46
$\{m'(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}$	-6654.51	-7407.71	-6946.55	-7487.55	-6627.95
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-10952.69	-10954.42	-10855.74	-10857.79	-10859.08
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-10953.55 ± 0.86 (mean and standard deviation of the mean)		-10857.54 ± 0.97		

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[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(\text{cont})(t_i - 298.15\ K) + \varepsilon^f(\text{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 5. Summary of combustion experiments for JP-10 and JP-7P-TK-WA-10 fuels[a]

(cal_{th} = 4.184 J)

Sample	JP-10			JP-7P-TK-WA-10		
Experiment number	1	2	3	1	2	3
$m'(\mathrm{fuel})/g$	0.579676	0.572309	0.629061	0.663507	0.662551	0.672399
$m''(\mathrm{auxiliary\ oil})/g$	0.069644	0.171760	0.116740	0.054313	0.056088	0.046723
$m'''(\mathrm{fuse})/g$	0.000838	0.001095	0.001116	0.000999	0.001033	0.001243
$n^i(H_2O)/mol$	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.74082	2.00553	2.00572	1.99218	1.99749	1.99972
$\varepsilon(\mathrm{calor})(-\Delta t_c)/cal_{th}$	-6975.96	-8036.71	-8037.46	-7983.22	-8004.51	-8013.42
$\varepsilon(\mathrm{cont})(-\Delta t_c)/cal_{th}$[b]	-7.40	-8.75	-8.80	-8.61	-8.75	-8.64
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.63	12.42	0.00	12.40	12.39
$\Delta E_{(\mathrm{corr\ to\ std\ states})}/cal_{th}$[c]	2.45	2.76	2.81	2.39	2.32	2.32
$\{-m''(\Delta E_c^\circ/m)(\mathrm{auxiliary\ oil})\}/cal_{th}$	766.39	1890.11	1284.66	597.69	617.21	514.16
$\{-m'''(\Delta E_c^\circ/m)(\mathrm{fuse})\}/cal_{th}$	3.39	4.43	4.52	4.04	4.18	5.03
$\{m'(\Delta E_c^\circ/m)(\mathrm{fuel})\}/cal_{th}$	-6210.95	-6133.35	-6741.67	-7387.53	-7376.97	-7487.98
$\{(\Delta E_c^\circ/m)(\mathrm{fuel})\}/cal_{th}\ g^{-1}$	-10714.51	-10716.84	-10717.05	-11134.06	-11134.19	-11136.20
$\{(\Delta E_c^\circ/m)(\mathrm{fuel})\}/cal_{th}\ g^{-1}$	-10716.13 ± 0.82 (mean and standard deviation of the mean)			-11134.82 ± 0.69		

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[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(\mathrm{cont})(t_i - 298.15\ K) + \varepsilon^f(\mathrm{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 6. Summary of Combustion Experiments for JP-4-S-A(UN-81-141) and JP-4-S-U(UN-81-149) fuels[a]

(cal_{th} = 4.184 J)

Sample	JP-4-S-A(UN-81-141)			JP-4-S-U(UN-81-149)		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.667500	0.673418	0.671975	0.660780	0.680387	0.653276
m''(auxiliary oil)/g	0.053899	0.050716	0.053975	0.069630	0.039719	0.071866
m'''(fuse)/g	0.001055	0.001046	0.001010	0.000799	0.001193	0.001109
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.98881	2.00023	2.00481	2.02651	2.00216	2.01577
$\varepsilon(\text{calor})(-\Delta t_c)/cal_{th}$	-7969.70	-8015.47	-8033.84	-8120.78	-8023.21	-8077.76
$\varepsilon(\text{cont})(-\Delta t_c)/cal_{th}$[b]	-8.67	-8.71	-8.75	-8.90	-8.65	-8.73
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.33	14.96	0.00	12.53	14.66
$\Delta E_{(\text{corr to std states})}/cal_{th}$[c]	2.47	2.39	2.40	2.44	2.32	2.33
$\{-m''(\Delta E_c^\circ/m)(\text{auxiliary oil})\}/cal_{th}$	593.13	558.10	593.96	766.23	437.08	790.84
$\{-m'''(\Delta E_c^\circ/m)(\text{fuse})\}/cal_{th}$	4.27	4.23	4.09	3.23	4.83	4.49
$\{m'(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}$	-7378.32	-7444.95	-7427.00	-7357.60	-7574.92	-7273.99
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11053.66	-11055.46	-11052.50	-11134.70	-11133.24	-11134.65
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11053.87 ± 0.86 (mean and standard deviation of the mean)			-11134.20 ± 0.48		

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[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(\text{cont})(t_i - 298.15\ K) + \varepsilon^f(\text{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 7. Summary of combustion experiments for JP-4-S-S(UN-81-155) and JP-4P-TK-F2 fuels[a]

(cal_{th} = 4.184 J)

Sample	JP-4-S-S(UN-81-155)				JP-4P-TK-F2		
Experiment number	1	2	3	4	1	2	3
$m'(\text{fuel})/g$	0.635793	0.651134	0.623469	0.594547	0.633889	0.644861	0.651471
$m''(\text{auxiliary oil})/g$	0.067031	0.068983	0.096102	0.124989	0.051761	0.081177	0.070461
$m'''(\text{fuse})/g$	0.000928	0.001206	0.001209	0.001014	0.000987	0.001081	0.001008
$n^i(H_2O)/\text{mol}$	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.95521	2.00736	2.00441	2.00304	1.90235	2.01664	2.00617
$\epsilon(\text{calor})(-\Delta t_c)/cal_{th}$	-7835.07	-8044.06	-8032.20	-8026.71	-7623.23	-8081.23	-8039.27
$\epsilon(\text{cont})(-\Delta t_c)/cal_{th}$[b]	-8.50	-8.71	-8.72	-8.75	-8.18	-8.82	-8.70
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.89	14.71	13.56	0.00	13.95	12.52
$\Delta E_{(\text{corr to std states})}/cal_{th}$[c]	2.30	2.28	2.28	2.29	2.23	2.32	2.31
$\{-m''(\Delta E_c^\circ/m)(\text{auxiliary oil})\}/cal_{th}$	737.63	759.12	1057.55	1375.43	569.59	893.31	775.38
$\{-m'''(\Delta E_c^\circ/m)(\text{fuse})\}/cal_{th}$	3.76	4.88	4.90	4.11	4.00	4.38	4.08
$\{m'(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}$	-7099.70	-7271.42	-6961.30	-6639.89	-7055.41	-7175.91	-7253.50
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11166.68	-11167.33	-11165.44	-11167.99	-11130.35	-11127.86	-11134.04
$\{(\Delta E_c^\circ/m)(\text{fuel})\}/cal_{th}\ g^{-1}$	-11166.86 ± 0.54 (mean and standard deviation of the mean)				-11130.75 ± 1.89		

---

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\epsilon^i(\text{cont})(t_i - 298.15\ K) + \epsilon^f(\text{cont})(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

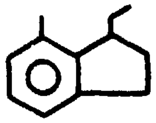
TABLE 8. Properties summary

Sample designation	Empirical formula [a]	Density g cm^{-3} 15°C [b]	Density g cm^{-3} 25°C	$\Delta E_c^\circ/m$ Eq. 2 cal g^{-1} [c]	Deviation Eq. 3[d] cal g^{-1} [c]
BP-IP-1	$CH_{1.9696}$	0.7989	0.795	-10337.4	-6.6
BP-IP-2	$CH_{1.9589}S_{0.0006}$	0.7888	0.785	-10319.6	-1.1
BP-IP-3	$CH_{1.9487}S_{0.0011}$	0.7948	0.791	-10298.2	-8.1
BP-IP-4	$CH_{1.9397}S_{0.0009}$	0.8002	0.797	-10304.9	-4.1
BP-IP-5	$CH_{1.9089}$	0.7990	0.791	-10295.1	-14.7
BP-IP-6	$CH_{1.8604}S_{0.0001}$	0.8293	0.826	-10231.6	5.3
BP-IP-7	$CH_{1.8675}$	0.8180	0.814	-10246.6	-2.9
BP-IP-9	$CH_{1.7784}S_{0.0001}$	0.8309	0.824	-10179.6	-8.0
JP-10	$CH_{1.6806}$[e]	0.9193	0.918	-10071.2	10.6
JP-7P-TK-WA-10	$CH_{2.0258}$[e]	0.7994	0.793	-10376.7	0.3
JP-4-S-A(UN-81-141)	$CH_{1.9630}$	0.7825	0.780	-10315.9	-0.1
JP-4-S-U(UN-81-149)	$CH_{2.0188}S_{0.0004}$	0.7801	0.779	-10376.9	-5.3
JP-4-S-S(UN-81-155)	$CH_{2.0475}$[e]	------	0.758	-10401.7	-7.0
JP-4P-TK-F2	$CH_{2.0444}S_{0.0001}$	------	0.759	-10366.3	25.7

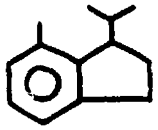
[a] From analysis for each element.
[b] From Wright-Patterson Air Force Base.
[c] 1 cal = 4.184 J.
[d] Deviation of $\Delta E_c^\circ/m$ from equation 3.
[e] From analysis for carbon only.

2. MODEL COMPOUND STUDIES

No model compounds were studied this year; however, samples of 1-isopropyl-7-methylindan and 1-ethyl-7-methylindan were recently received from the laboratories of E. J. Eisenbraun at Oklahoma State University where the compounds were synthesized and purified.



1-Ethyl-7-methylindan



1-Isopropyl-7-methylindan

Preparations are being made to study these compounds to further delineate the steric interaction energies of the 1-7-substituted indans in relation to other results for the 1-6-substituted indans and the 1-8-substituted naphthalenes.[7-10]

3. PUBLICATION AND PRESENTATION

Chemical Thermodynamic Properties of Molecules Which Undergo Inversion: I. Aniline, Methylamine, Cyclopropylamine, and Cyclopentene by J. A. Draeger, R. H. Harrison and W. D. Good. Accepted for publication by the *Journal of Chemical Thermodynamics*.

Thermodynamics of Organic Compounds by W. D. Good and N. K. Smith was presented at the AFOSR meeting on Airbreathing Combustion Dynamics at Clearwater, Florida, November 16-20, 1981.

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