

Standard enthalpies of formation of 2-thenoyltrifluoroacetone and monothio-2-thenoyltrifluoroacetone by rotating-bomb calorimetry

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The standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation of crystalline 1,1,1-trifluoro-4-(2-thienyl)-4-hydroxy-3-buten-2-one, HTTFA, and 1,1,1-trifluoro-4-(2-thienyl)-4-mercapto-3-buten-2-one, HTTFAS, at $T = 298.15$ K were measured by rotating-bomb calorimetry and the standard molar enthalpies of sublimation at $T = 298.15$ K were measured by microcalorimetry, with the following results:

	$\Delta_f H_m^\circ(\text{cr})$ $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_{\text{cr}}^\circ H_m^\circ$ $\text{kJ}\cdot\text{mol}^{-1}$
HTTFA	-948.6 ± 4.1	86.18 ± 0.64
HTTFAS	-725.4 ± 3.9	95.1 ± 3.7

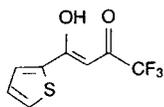
The results demonstrate an increase in stabilization energy of $\approx (38.7 \pm 5.0)$ $\text{kJ}\cdot\text{mol}^{-1}$ in HTTFA compared with thiophene and that in these molecules, the intramolecular hydrogen bond energy ($\text{O}-\text{H}\cdots\text{O}$), appears ≈ 20 $\text{kJ}\cdot\text{mol}^{-1}$ larger than for ($\text{S}-\text{H}\cdots\text{O}$). © 1997 Academic Press Limited

KEYWORDS: enthalpy of formation; 2-thenoyltrifluoroacetone; monothio-2-thenoyltrifluoroacetone; rotating-bomb calorimetry

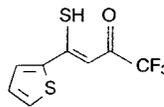
1. Introduction

The compound 1,1,1-trifluoro-4-(2-thienyl)-4-hydroxy-3-buten-2-one, HTTFA, and 1,1,1-trifluoro-4-(2-thienyl)-4-mercapto-3-buten-2-one, HTTFAS, are a β -diketone and a monothio- β -diketone, respectively, which can form bidentate complexes with a wide variety of metals.

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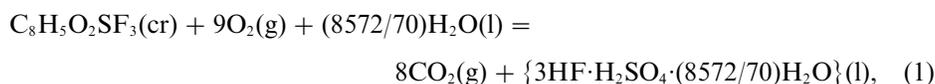


HTTFA

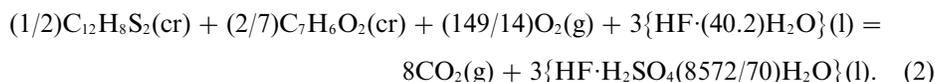


HTTFAS

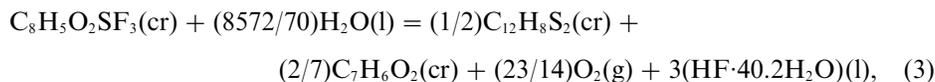
To derive the enthalpies of formation of such metal complexes from reaction-calorimetry studies, the enthalpies of formation of the ligands are required. In this paper we report the determination of the standard molar enthalpies of formation $\Delta_f H_m^\circ$ of these ligands by rotating-bomb calorimetry. Combustion of these compounds results in a final bomb solution of a mixture of sulphuric and hydrofluoric acids for which the thermodynamic properties are unknown. The procedure adopted was to design comparison experiments using standardized samples of benzoic acid and thianthrene, in such amounts to ensure that the chemical composition of the final states of the combustion reactions in the combustion of the compound and in the comparison experiments were as close as possible. Corrections to the standard state were required for the initial states, but were unnecessary for the final states, except for a minor correction because the amounts of gas in the final states were slightly different. The combustion reaction for HTTFA was:



and the reaction for the comparison experiment was:

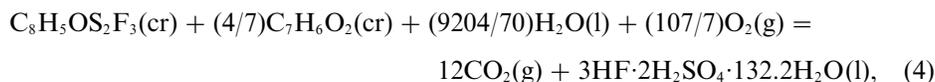


Subtracting (2) from (1) gives:

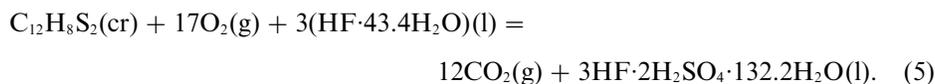


so that $\Delta_f H_m^\circ(\text{HTTFA}, \text{cr})$ may be derived from the standard enthalpy of reaction (3).

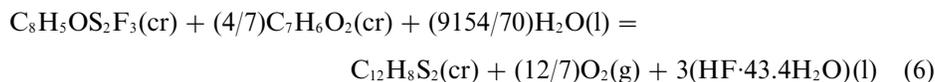
HTTFAS was burned together with benzoic acid according to the reaction,



and the reaction for the comparison experiment was:



Subtracting (5) from (4) gives:



and $\Delta_f H_m^\circ(\text{HTTFAS}, \text{cr})$ may be derived from the standard enthalpy of reaction (6).

The enthalpy of sublimation of HTTFA has been reported,⁽¹⁾ determined by the Knudsen technique, and that of HTTFAS, in this work by microcalorimetry. These results enable the standard enthalpies of formation in the gaseous state to be derived.

2. Experimental

Two samples of 2-thenoyltrifluoroacetone (HTTFA) were examined, from Carlo Erba and from Aldrich. They were purified by repeated sublimation in vacuum to give white crystals and microanalysis results were in accord with the empirical formula $\text{C}_8\text{H}_5\text{O}_2\text{SF}_3$. Monothio-2-thenoyltrifluoroacetone (HTTFAS), was prepared as described by Das *et al.*⁽²⁾ The sample was purified by crystallization from light petroleum ($T = 313 \text{ K}$ to $T = 333 \text{ K}$) and repeated sublimation in vacuum to give red crystals. Thianthrene (NBS SRM 1659) was used in the comparison experiments and benzoic acid (NBS SRM 39i) as a combustion auxiliary to ensure the correct stoichiometry of the combustion reaction of HTTFAS. The hydrofluoric acid solutions were made by dilution of HF(aq) (mass fraction, 0.60) from Fison and the concentrations were monitored by titration.

The rotating-bomb calorimeter was that used formerly at the National Physical Laboratory, Teddington, U.K.,⁽³⁾ with a platinum-lined bomb of internal volume 0.337 dm^3 . Water was added to the calorimeter from a weighed glass vessel, and for each experiment a correction to the energy equivalent was made for the deviation from 4063.3 g of the mass of water added. Calorimetric temperatures were measured to $1 \cdot 10^{-4} \text{ K}$ with a quartz thermometer (Hewlett Packard HP 2804) interfaced to a microcomputer programmed to compute the adiabatic temperature change. Ignition temperatures were chosen so that the final temperatures were very close to 298.15 K . The frictional work of bomb rotation was automatically included in the corrections for heat exchange and work of stirring by using the procedure described by Good *et al.*⁽⁴⁾

The energy equivalent of the calorimeter was determined from the combustion of benzoic acid (NBS SRM 39i), as described previously.⁽⁵⁾ The electrical energy for the ignition was determined from the change in potential difference across a capacitor when 40 V was discharged through the platinum ignition wire. For the cotton thread fuse, empirical formula $\text{CH}_{1.686}\text{O}_{0.843}$, the massic energy of combustion $-\Delta_c u^\circ = 16\,250 \text{ J} \cdot \text{g}^{-1}$.⁽⁶⁾ Corrections for nitric acid formation were based on $-59.7 \text{ kJ} \cdot \text{mol}^{-1}$ for the molar energy of formation of $0.1 \text{ mol} \cdot \text{dm}^{-3}$ $\text{HNO}_3(\text{aq})$ from O_2 , N_2 , and $\text{H}_2\text{O}(\text{l})$.⁽⁷⁾ From 12 calibrations, done with bomb rotation, $\varepsilon(\text{calor}) = (20\,691.58 \pm 0.30) \text{ J} \cdot \text{K}^{-1}$ where the uncertainty quoted is the standard deviation of the mean.

HTTFA, in pellet form, was ignited in oxygen at $p = 3.04 \text{ MPa}$ with 10.00 cm^3 of water added to the bomb. For the comparison experiments, pellets of thianthrene with benzoic acid auxiliary were ignited in oxygen at $p = 3.04 \text{ MPa}$ with 10.00 cm^3 of $1.352 \text{ mol} \cdot \text{dm}^{-3}$ HF(aq) added to the bomb. HTTFAS in pellet form with benzoic acid auxiliary was ignited in oxygen at $p = 3.04 \text{ MPa}$ with 10.00 cm^3 of water added

to the bomb: for the comparison experiments, thianthrene was ignited in oxygen at $p = 3.04$ MPa with 10.00 cm³ of 1.252 mol·dm⁻³ HF(aq) added to the bomb. The masses of the pellets were carefully adjusted so that the chemical compositions of the final bomb contents for the measurement and comparison experiments were similar. The mean final compositions with standard deviations are given in table 1. The amount of nitric acid was determined using the Devarda alloy method, Densities of HTTFA and HTTFAS were assumed to be 1.3 g·cm⁻³; for benzoic acid $\rho = 1.32$ g·cm⁻³, and for thianthrene $\rho = 1.44$ g·cm⁻³. For each compound, $(\partial u/\partial p)_T$ at $T = 298.15$ K was assumed to be -0.1 J·g⁻¹·MPa⁻¹.

Standard state corrections were calculated for the initial states by the procedures given by Hubbard *et al.*⁽⁶⁾ and by Good and Scott:⁽⁸⁾ the only term included for the final state was for the compression of the gaseous phase. The heat capacities of the final bomb contents were calculated assuming the acidic aqueous phase to be entirely HF(aq), but because the final temperatures were so close to 298.15 K, any error arising from uncertainty in the heat capacity of the final bomb contents was calculated to be negligible. The energy of dilution of the nitric acid to $c = 0.1$ mol·dm⁻³ was calculated assuming the final solution to be water, but because the concentration of nitric acid in the measurement and comparison experiments were so close, no systematic error arises from this assumption. The relative atomic masses used were those recommended by the IUPAC Commission.⁽⁹⁾

The enthalpies of sublimation of HTTFA and of dibenzoylmethane, (86.18 ± 0.64) kJ·mol⁻¹ and (115.7 ± 0.9) kJ·mol⁻¹, respectively, were determined from vapour pressure measured as a function of temperature by the Knudsen technique.⁽¹⁾ The enthalpies of sublimation of HTTFA, of monothiodibenzoylmethane, and of HTTFAS were measured using the ‘‘Vacuum Sublimation’’ drop-microcalorimetric method.⁽¹⁰⁾ Samples of about 5 mg contained in thin glass capillary tubes sealed at one end were dropped from room temperature into the hot reaction vessel in the Calvet High-Temperature Microcalorimeter and then removed from the hot-zone by vacuum sublimation. The observed enthalpies of sublimation $\{H_m^\circ(g, T) - H_m^\circ(g, 298.15)\}$ were corrected to $T = 298.15$ K using $\Delta_{298.15\text{ K}}^T H_m^\circ(g)$ estimated by a group method based on the values of Stull *et al.*⁽¹¹⁾ The calorimeter was calibrated *in situ*, making use of the reported enthalpy of sublimation of naphthalene (72.513 ± 0.071) kJ·mol⁻¹.⁽¹²⁾

TABLE 1. Molar compositions of the final combustion states, HTTFA is 1,1,1-trifluoro-4-(2-thienyl)-4-hydroxy-3-buten-2-one and HTTFAS is 1,1,1-trifluoro-4-(2-thienyl)-4-mercapto-3-buten-2-one

	HTTFA		HTTFAS	
	Measurement reaction (1)	Comparison reaction (2)	Measurement reaction (4)	Comparison reaction (5)
$n(\text{CO}_2)/\text{mol}$	0.0360 ± 0.0001	0.0362 ± 0.0001	0.0505 ± 0.0001	0.0503 ± 0.0002
$n(\text{H}_2\text{O})/\text{mol}$	0.5535 ± 0.0008	0.5541 ± 0.0015	0.5565 ± 0.0008	0.5551 ± 0.0015
$n(\text{H}_2\text{SO}_4)/\text{mol}$	0.0045 ± 0.0001	0.0045 ± 0.0001	0.0084 ± 0.0001	0.0084 ± 0.0001
$n(\text{HF})/\text{mol}$	0.0135 ± 0.0001	0.0135 ± 0.0001	0.0125 ± 0.0001	0.0125 ± 0.0001

3. Results

Table 2 lists typical combustion results for each compound and the corresponding comparison experiment where the terms are as previously defined:⁽⁶⁾ $\Delta m(\text{H}_2\text{O})$ is the deviation of the mass of water added to the calorimeter from 4063.3 g; $\Delta U(\text{BA}, \text{corr})$ is to correct for the fact that the mass of benzoic acid used was not the precisely correct stoichiometric amount required for the reaction, calculated using the massic energy of combustion of benzoic acid with 10.00 cm³ of water added to the bomb. For each compound, the products of combustion in both the measurement and comparison experiments consist of gaseous phase and an aqueous mixture of hydrofluoric and sulphuric acids for which the thermodynamics properties are unknown. Consequently, the thermodynamic correction to convert the final real state to the final standard state cannot be calculated. The experiments have been designed, however, to make this particular correction irrelevant, by the subtraction of the enthalpy of the comparison reaction from that of the measurement reaction. The only corrections needed to convert the real state to the standard state are those for the bomb contents before combustion and because the amounts of gas in the final states are slightly different, correction for the compression of this gas phase was made. The corrections were calculated using the procedures given by Hubbard *et al.*⁽⁶⁾ and by Good and Scott.⁽⁸⁾ The sum of the corrections is listed as ΔU_Σ^* , and because the individual massic energies of combustion are not fully corrected to the standard state, these are listed as $\Delta_c u^*$. Table 3 lists the individual values of $-\Delta_c u^*$ together

TABLE 2. Typical combustion results at $T = 298.15 \text{ K}$ ($p^\circ = 0.1 \text{ MPa}$), where HTTFA is 1,1,1-trifluoro-4-(2-thienyl)-4-hydroxy-3-buten-2-one and HTTFAS is 1,1,1-trifluoro-4-(2-thienyl)-4-mercapto-3-buten-2-one

	HTTFA		HTTFAS	
	Measurement reaction (1)	Comparison reaction (2)	Measurement reaction (4)	Comparison reaction (5)
$m(\text{cpd.})/\text{g}$	0.998193		0.998328	
$m(\text{thianthrene})/\text{g}$		0.489933		0.904341
$m(\text{benzoic acid})/\text{g}$		0.158060	0.293817	
$m(\text{fuse})/\text{g}$	0.003113	0.002912	0.003117	0.002995
T_i/K	298.147067	298.185152	298.152307	298.171556
T_f/K	297.236454	297.160181	296.757739	296.677106
$\Delta T_{\text{ad}}/\text{K}$	0.883816	0.996793	1.365151	1.466598
$\varepsilon_i(\text{cont.})/\text{J}\cdot\text{K}^{-1}$	53.35	52.85	53.69	53.02
$\varepsilon_f(\text{cont.})/\text{J}\cdot\text{K}^{-1}$	53.48	53.35	54.48	53.88
$\Delta m(\text{H}_2\text{O})/\text{g}$	-7.3	-4.4	-9.0	-8.4
$-\Delta U(\text{IBP})/\text{J}$	18306.64	20658.47	28269.14	30371.01
$\Delta U(\text{HNO}_3)/\text{J}$	23.92	29.53	37.74	39.44
$\Delta U(\text{ignition})/\text{J}$	1.09	1.11	1.04	1.09
$\Delta U(\text{BA, corr})/\text{J}$		0.12	37.55	
$\Delta U_\Sigma^*/\text{J}$	22.51	19.18	24.06	20.70
$-m\Delta_c u$ (fuse)/J	50.56	47.29	50.62	48.64
$-\Delta_c u^*/\{\text{J}\cdot\text{g}^{-1}(\text{cpd.})\}$	18242.61		28166.26	
$-\Delta_c u^*/\{\text{J}\cdot\text{g}^{-1}(\text{thianthrene})\}$		41969.72		33463.30

TABLE 3. Individual values of $\Delta_c u^*$ at $T = 298.15$ K, where $\Delta_c u^*$ denotes the massic energies of combustion defined in table 1, where HTTFA is 1,1,1-trifluoro-4-(2-thienyl)-4-hydroxy-3-buten-2-one and HTTFAS is 1,1,1-trifluoro-4-(2-thienyl)-4-mercapto-3-buten-2-one

HTTFA		HTTFAS	
Measurement reaction (1)	Comparison reaction (2)	Measurement reaction (4)	Comparison reaction (5)
$-\Delta_c u^*/(\text{J}\cdot\text{g}^{-1})$			
18 228.19	41 978.69	28 164.77	33 469.24
18 242.61	41 963.47	28 180.73	33 454.45
18 241.30	41 981.00	28 166.26	33 463.30
18 216.22	41 969.72	28 176.07	33 473.97
18 214.21	41 984.18	28 178.93	33 469.19
18 201.24	41 974.34	28 169.04	33 457.55
$-\langle\Delta_c u^*\rangle/(\text{J}\cdot\text{g}^{-1})$			
$18\,223.98 \pm 6.67$	$41\,975.23 \pm 3.13$	$28\,172.63 \pm 2.78$	$33\,464.62 \pm 3.08$

with the mean and its standard deviation. Table 4 lists the derived molar values for the energies of combustion, the standard molar values for the energies and enthalpies of reactions (3) and (6), and the standard molar enthalpy of formation of the crystalline solids.

To derive $\Delta_r H_m^\circ(\text{cr})$ from $\Delta_r H_m^\circ$ for reactions (3) and (6), the following standard molar enthalpies of formation were used: for $\text{H}_2\text{O}(\text{l})$, $-(285.83 \pm 0.04)$ $\text{kJ}\cdot\text{mol}^{-1}$; ⁽¹³⁾ for benzoic acid(cr), $-(385.11 \pm 0.99)$ $\text{kJ}\cdot\text{mol}^{-1}$; for thianthrene(cr) (185.1 ± 2.5) $\text{kJ}\cdot\text{mol}^{-1}$; for $\{\text{HF}\cdot 40.4\text{H}_2\text{O}(\text{l}) - 40.4\text{H}_2\text{O}(\text{l})\}$, $-(322.27 \pm 0.65)$ $\text{kJ}\cdot\text{mol}^{-1}$; ⁽¹⁴⁾ for $\{\text{HF}\cdot 43.4\text{H}_2\text{O}(\text{l}) - 43.4\text{H}_2\text{O}(\text{l})\}$, $-(322.28 \pm 0.65)$ $\text{kJ}\cdot\text{mol}^{-1}$. ⁽¹⁴⁾ The values for benzoic acid and thianthrene were calculated from the NBS certificate values. In accordance with normal thermochemical practice the uncertainties assigned to the standard molar quantities are twice the overall standard deviations of the mean and include the uncertainties in calibration and in the values of the auxiliary quantities.

4. Discussion

From the enthalpies of sublimation at $T = 298.15$ K, for HTTFA, (86.18 ± 0.64) $\text{kJ}\cdot\text{mol}^{-1}$, and for HTTFAS, (95.1 ± 3.7) $\text{kJ}\cdot\text{mol}^{-1}$, the standard

TABLE 4. Derived molar values at $T = 298.15$ K ($p^\circ = 0.1$ MPa), where HTTFA is 1,1,1-trifluoro-4-(2-thienyl)-4-hydroxy-3-buten-2-one and HTTFAS is 1,1,1-trifluoro-4-(2-thienyl)-4-mercapto-3-buten-2-one

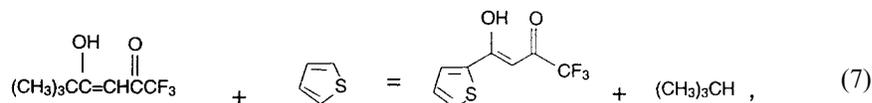
	$-\Delta_c U_m^*$ (Measurement) $\text{kJ}\cdot\text{mol}^{-1}$	$-\Delta_c U_m^*$ (Comparison) $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_r U_m^\circ$ $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_r H_m^\circ$ $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_r H_m^\circ(\text{cr})$ $\text{kJ}\cdot\text{mol}^{-1}$
HTTFA	4049.0 ± 3.0 ^a	9079.9 ± 1.7 ^b	491.0 ± 3.4 ^c	495.1 ± 3.4 ^c	-948.6 ± 4.1
HTTFAS	6711.9 ± 1.5 ^d	7238.9 ± 1.6 ^e	527.0 ± 2.2 ^f	531.2 ± 2.2 ^f	-725.4 ± 3.9

For HTTFA, $\Delta_r U_m^\circ(3) = \Delta_c U_m^* \{\text{Reaction (1)}\} - 0.5 \Delta_c U_m^* \{\text{Reaction (2)}\}$; for HTTFAS $\Delta_r U_m^\circ(6) = \Delta_c U_m^* \{\text{Reaction (4)}\} - \Delta_c U_m^* \{\text{Reaction (5)}\}$.

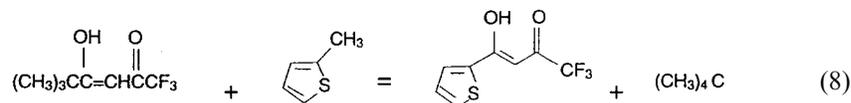
^a Reaction (1). ^b Reaction (2). ^c Reaction (3). ^d Reaction (4). ^e Reaction (5). ^f Reaction (6).

molar enthalpies of formation in gaseous state were derived: $\Delta_f H_m^\circ(\text{HTTFA}, \text{g}) = -(862.4 \pm 4.2) \text{ kJ}\cdot\text{mol}^{-1}$; $\Delta_f H_m^\circ(\text{HTTFAS}, \text{g}) = -(630.3 \pm 5.4) \text{ kJ}\cdot\text{mol}^{-1}$.

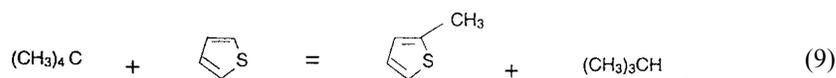
The enthalpies of the gas phase isodesmic reactions,



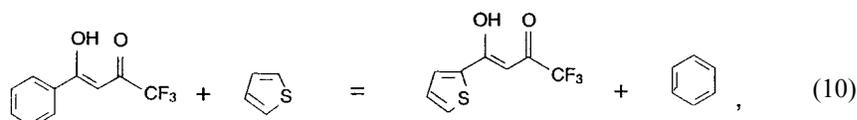
where $\Delta_r H_m^\circ(\text{g}) = -(37.4 \pm 7.1) \text{ kJ}\cdot\text{mol}^{-1}$, and



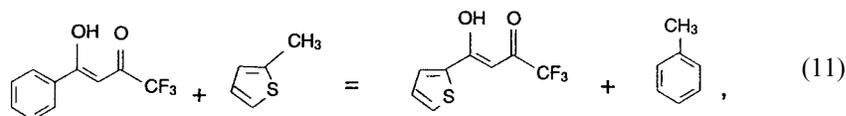
where $\Delta_r H_m^\circ(\text{g}) = -(39.9 \pm 7.2) \text{ kJ}\cdot\text{mol}^{-1}$, demonstrate an increase in stabilization of $(38.7 \pm 5.0) \text{ kJ}\cdot\text{mol}^{-1}$ of the products over the reactants because of the thermoneutrality of the following gaseous reaction:



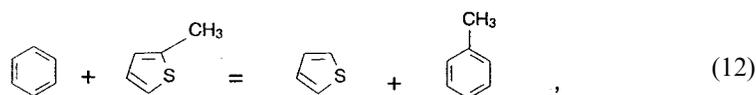
where $\Delta_r H_m^\circ(\text{g}) = -(1.4 \pm 1.2) \text{ kJ}\cdot\text{mol}^{-1}$. Moreover, for the isodesmic gas phase reactions,



where $\Delta_r H_m^\circ(\text{g}) = -(19.5 \pm 7.8) \text{ kJ}\cdot\text{mol}^{-1}$, and

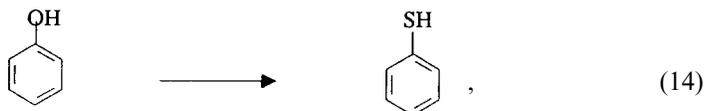
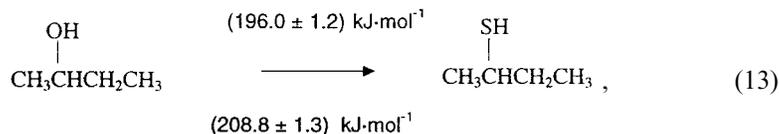


where $\Delta_r H_m^\circ(\text{g}) = -(20.3 \pm 7.8) \text{ kJ}\cdot\text{mol}^{-1}$, demonstrating an increase in stabilization energy $(19.9 \pm 5.5) \text{ kJ}\cdot\text{mol}^{-1}$ of the products over the reactants because the following reaction is thermoneutral,

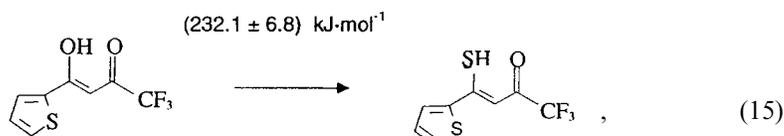


where $\Delta_r H_m^\circ(\text{g}) = -(0.8 \pm 1.4) \text{ kJ}\cdot\text{mol}^{-1}$. Thus, these results indicate an increase in delocalization energy of $(38.7 \pm 5.0) \text{ kJ}\cdot\text{mol}^{-1}$ in thenoyltrifluoroacetone compared with thiophene, and of $(19.9 \pm 5.5) \text{ kJ}\cdot\text{mol}^{-1}$ in the benzoyltrifluoroacetone compared with benzene. The above enthalpies of reaction were calculated using $\Delta_f H_m^\circ(\text{g})$ values from Pedley *et al.*⁽¹⁵⁾ except for 1,1,1-trifluoro-5,5-dimethyl-hexan-2,4-dione⁽¹⁶⁾ and benzoyltrifluoroacetone.⁽¹⁷⁾ Lack of subsidiary data precludes a similar analysis of the result for the monothio-2-thenoyltrifluoroacetone. Consideration,

however, of the following increments in $\Delta_f H_m^\circ(\text{g})$ for:



and



shows that for this case the intramolecular hydrogen bond energy in the monothio- β -diketone appears to be $\approx 20 \text{ kJ}\cdot\text{mol}^{-1}$ less than for the hydrogen bond energy in the β -diketone.

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