Supporting information

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Thermodynamic Analysis of Strain in Heteroatom Derivatives of Indene.

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TABLE S1. Results from typical combustion experiments for 2,3-benzofuran at T = 298.15 K[a]

	1	2	3	4	5
m (substance) /g [b]	0.843701	1.009884	0.729292	0.977412	0.860188
m' (cotton) /g [b,e]	0.001232	0.001190	0.001135	0.001092	0.001007
m'' (polyethene) /g [b,f]	0.271921	0.284273	0.274483	0.283479	0.274185
ΔT_c /K[c]	1.62972	1.87497	1.48126	1.82988	1.65638
$(\varepsilon_{calor})\cdot(-\Delta T_c)$ /J	-40949.83	-47112.28	-37219.53	-45979.07	-41619.63
$(\varepsilon_{cont})\cdot(-\Delta T_c)$ /J	-23.01	-27.02	-20.63	-26.21	-23.47
$\Delta U_{corr.}$ /J[d]	24.77	29.99	21.56	28.98	25.29
$-m'\cdot\Delta_c u'$ /J[d]	20.87	20.16	19.23	18.50	17.06
$-m''\cdot\Delta_c u''$ /J[d]	12606.53	13179.15	12725.30	13142.34	12711.47
$\Delta_c u^\circ$ (sub) /(J·g^{-1})	-33574.4	-33589.2	-33587.4	-33585.1	-33598.1
$\Delta_c H^\circ$ (sub) /(kJ·mol^{-1})	-3968.7	-3970.5	-3970.2	-3970.0	-3971.5

[a] For the definition of the symbols see reference 12;: T_h = 298.15 K; V(bomb) = 0.2664 dm^3; p^i(gas) = 3.04 MPa; $m^i(H_2O)$ = 0.78 g; ΔU(ign) = 1.5 J; m(Pt) = 8.61 g; [b] Masses obtained from apparent masses. [c] $\Delta T_c = T^f - T^i + \Delta T_{corr}$; $(\varepsilon_{cont})\cdot(-\Delta T_c) = (\varepsilon^i_{cont})\cdot(T^i - 298.15\ K) + (\varepsilon^f_{cont})\cdot(298.15\ K - T^f + \Delta T_{corr.})$. ε_{calor} = (25112.6 ± 1.9) J·K^{-1}, [d] ΔU_{corr}, the correction to standard states, is the sum of items 81 to 85, 87 to 90, 93, and 94 in reference 12. [e] We used cotton $CH_{1.774}O_{0.887}$ with $\Delta_c u^\circ$ = -(16945.2±4.2) J·g^{-1}. [f] We used polyethene $CH_{1.930}$ with $\Delta_c u^\circ$ = -(46361.0±3.1) J·g^{-1}.

TABLE S2. Results from typical combustion experiments for indole at T = 298.15 K

	1	2	3	4	5
m (substance) /g [b]	0.568896	0.675011	0.548595	0.6665813	0.722099
m' (cotton) /g [b,e]	0.001058	0.001133	0.001028	0.001102	0.001097
m'' (polyethene) /g [b,f]	0.263286	0.267948	0.274855	0.264411	0.266624
ΔT_c /K[c]	1.30728	1.46842	1.29921	1.44880	1.53386
$(\varepsilon_{calor})\cdot(-\Delta T_c)$ /J	-32829.12	-36875.81	-32626.45	-36376.33	-38519.25
$(\varepsilon_{cont})\cdot(-\Delta T_c)$ /J	-18.14	-20.69	-17.89	-20.11	-21.57
$\Delta U_{corr.}$ /J[d]	15.11	17.72	14.86	17.11	18.83
$-m'\cdot\Delta_c u'$ /J[d]	17.92	19.19	17.41	18.67	18.58
$-m''\cdot\Delta_c u''$ /J[d]	12206.19	12422.35	12742.57	12258.35	12360.94
ΔU (dec) /J	38.51	45.38	37.02	44.11	48.36
$\Delta_c u^\circ$ (sub) /(J·g^{-1})	-36146.3	-36126.7	-36140.5	-36124.7	-36128.8
$\Delta_c H^\circ$ (sub) /(kJ·mol^{-1})	-4236.3	-4234.0	-4235.6	-4233.7	-4234.2

TABLE S3. G3MP2 Total Energies at 0 K and Enthalpies at 298 K (in Hartree) of the Molecules Studied in This Work

Compounds	G3MP2 [a]		$\Delta_f H_m^\circ$(g) exp,
	E_0	H_{298}	kJ·mol^{-1}
cyclopentane	-196.158809	-196.152506	-76.4±0.7
cyclopentene	-194.951894	-194.946862	34.0±1.4
2,3-dihydro-1H-indene	-348.351342	-348.343308	60.9±2.1
1H-indene	-347.147953	-347.140409	161.2±2.3
9H-fluorene	-500.547122	-500.536941	175.0±1.5
tetrahydrofurane	-232.056169	-232.050200	-184.1±0.7
2,3-dihydrofurane	-230.850929	-230.845347	-72.3±0.4
2,3-dihydrobenzofuran	-384.250423	-384.242610	-46.5±0.8
benzofuran	-383.060395	-383.053327	13.6±0.7
dibenzo[b,d]furan	-536.454948	-536.445219	47.3±4.8
pyrrolidine	-212.190026	-212.183921	-3.4±0.8
2,3-dihydro-1H-pyrrole	-210.987445	-210.981919	---
indoline	-364.387822	-364.379918	---
1H-indole	-363.206064	-363.198551	---
9H-carbazole	-516.598758	-516.633113	205.0±3.0
1-methylpyrrolidine	-251.421688	-251.414240	---
1-methyl-2,3-dihydro-1H-pyrrole	-250.217123	-250.210165	---
1-methylindoline	-403.618525	-403.609070	---
1-methyl-1H-indole	-402.436234	-402.427094	155.8±2.8
9-methyl-9H-carbazole	-555.829384	-555.817495	199.1±0.5

[a] 1 Hartree = 2625.46 kJ/mol

TABLE S4. Correction of the enthalpies of formation calculated with the G3MP2 (using the atomization procedure), kJ·mol^{-1} (Data from [2])

Compounds	AT	AT (corr)	exp	Exp-AT(corr)
cyclopentane	-74.3	-63.4	-76.4±0.7	-13.0
cyclopentene	32.4	42.4	34.0±1.4	-8.4
2,3-dihydro-1H-indene	53.1	63.0	60.9±2.1	-2.1
1H-indene	152.5	161.6	161.2±2.3	-0.4
9H-fluorene	173.0	181.9	175.0±1.5	-6.9
tetrahydrofurane	-180.4	-168.7	-184.1±0.7	-15.4
2,3-dihydrofurane	-75.8	-64.9	-72.3±0.4	-7.4
2,3-dihydrobenzofuran	-57.3	-46.5	-46.5±0.8	0.0
benzofuran	6.4	16.6	13.6±0.7	-3.0
dibenzo[b,d]furan	39.1	49.1	47.3±4.8	-1.8
pyrrolidine	2.2	12.5	-3.4±0.8	-15.9
2,3-dihydro-1H-pyrrole	99.3	108.8	---	---
indoline	115.9	125.3	---	---
1H-indole	158.8	167.8	---	---
9H-carbazole	196.7	205.4	205.0±3.0	-0.4
1-methylpyrrolidine	-12.2	-1.8	---	---
1-methyl-2,3-dihydro-1H-pyrrole	90.4	100.0	---	---
1-methylindoline	104.6	114.1	---	---
1-methyl-1H-indole	149.1	158.2	155.8±2.8	-2.4
9-methyl-9H-carbazole	185.7	194.5	199.1±0.5	4.6

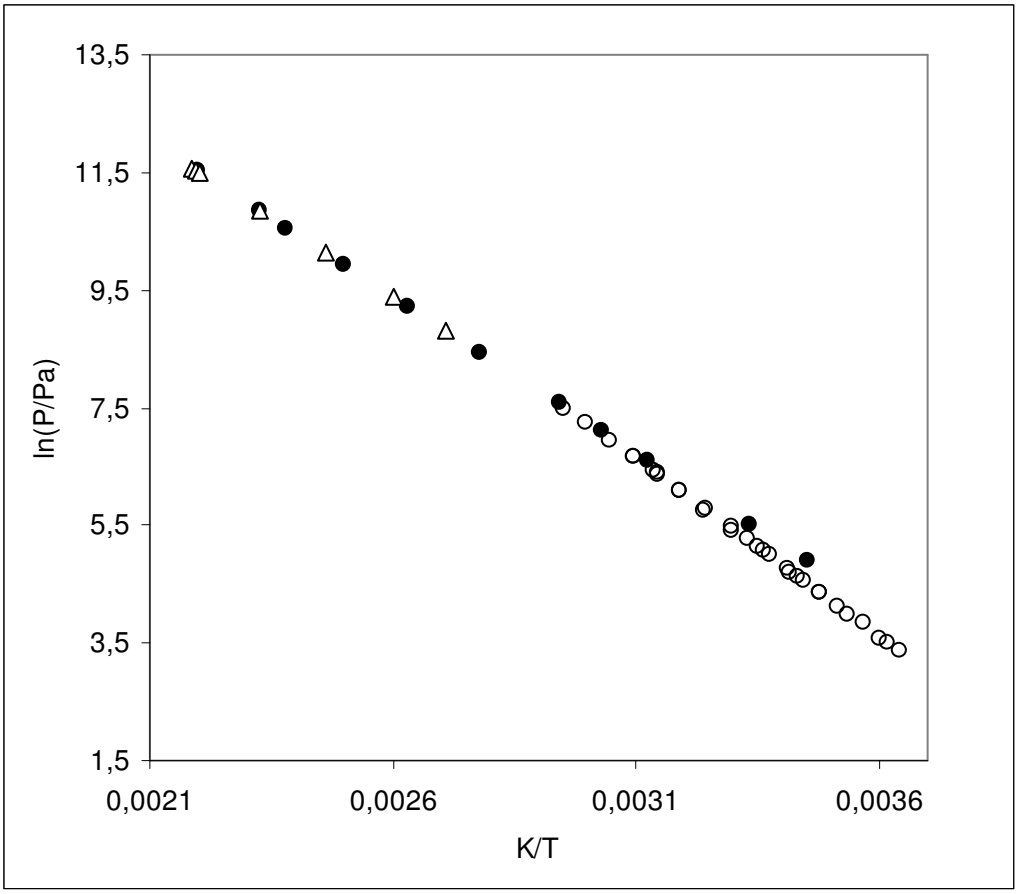

Figure S1. Plot of vapor pressure against reciprocal temperature for indene
∆ -Stull 1961 [20]; ●Stull 1947 [21]; ○ this work

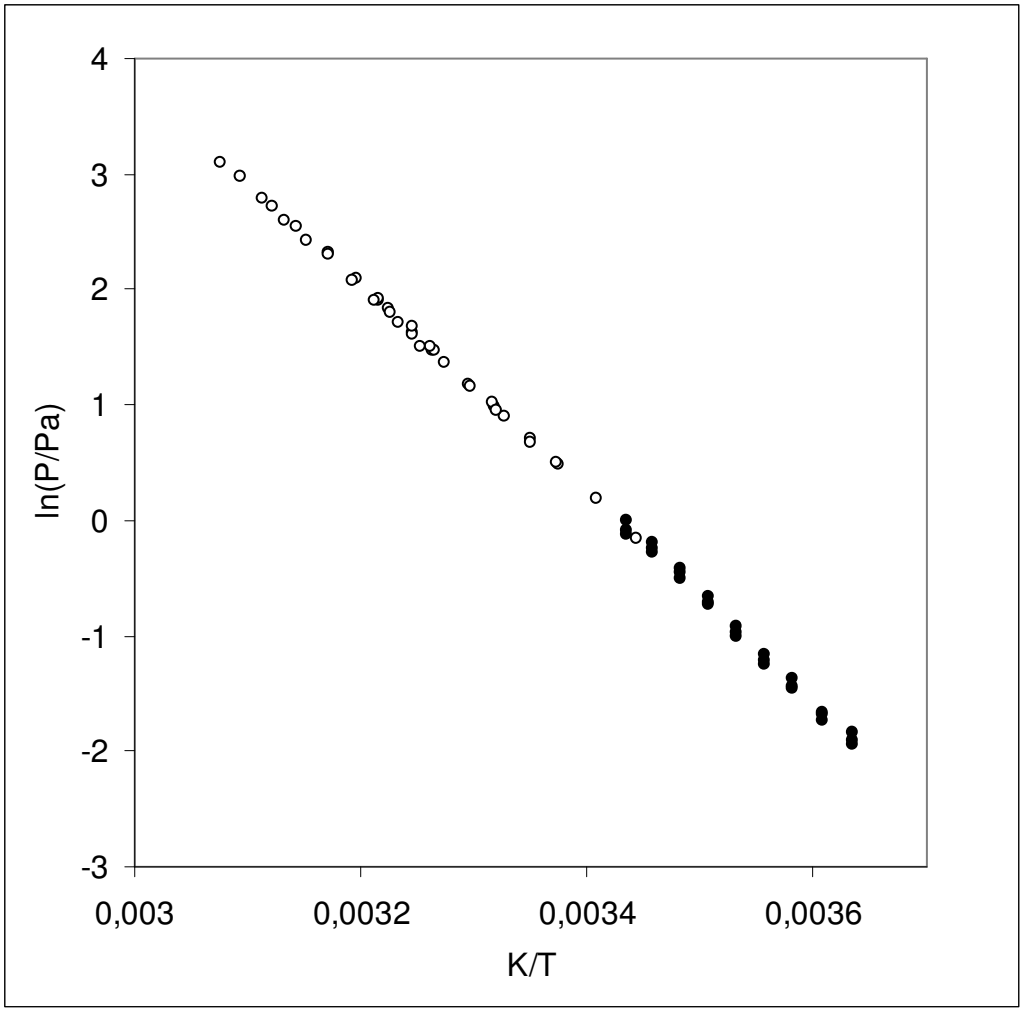

Figure S2. Plot of vapor pressure against reciprocal temperature for indole ● [6]; ○ this work