# **Estimated Gas-Phase Standard State Enthalpies of Formation for Organic Compounds Using the Gaussian-4 (G4) and W1BD Theoretical Methods**

# Sierra Rayne\*,<sup>‡</sup> and Kaya Forest<sup>†</sup>

Ecologica Research, Penticton, British Columbia, Canada V1Y 1R9, and Department of Chemistry, Okanagan College, Penticton, British Columbia, Canada V2A 8E1

Gas-phase standard state (298.15 K, 1.01325 bar [1 atm]) enthalpies of formation ( $\Delta_{f}H^{\circ}_{(g)}$ ) were calculated using the atomization approach for 313 organic compounds with the Gaussian-4 (G4) composite method and for 54 molecules with the W1BD level of theory. The functional group types considered span a range of mono- and polyfunctionalized halogenated, saturated and unsaturated, cyclic and acyclic, and heteroatom (N, O, S) substituted moieties without substantial conformational complexity. Good agreement was found using both computational methods against available experimental data.

# Introduction

Improvements in software development, theoretical approaches, and computing power have led to recent widespread advances in computational thermodynamics over the past several decades.<sup>1</sup> These trends come during a period over which experimental thermochemistry has generally received correspondingly less attention. The apparent inverse temporal correlation between interest in theoretical and experimental thermochemistry is unfortunate, as advancements in instrumental methods now allow the determination of molecular properties such as enthalpies of formation to accuracies not previously accessible.<sup>2</sup> Ideally, the intersection of broadly structured and coupled studies into computational and experimental thermochemistry jointly using the best available methods would facilitate ongoing progress in both fields. This is particularly the situation for some "classic" organic compounds, whose theoretical and experimental prominence came in previous eras, and for which reconsiderations with modern technologies are warranted.

The high level Gaussian-*n* ( $n \le 3$ ) suite of composite methods (G1, G2, and G3 and their derivatives [e.g., G2MP2, G3MP2, G3MP2B3])<sup>3-9</sup> has been widely benchmarked and employed in the thermochemical study of various compounds, 4,10-23 with less emphasis on the latest G4 and G4MP2 versions<sup>24,25</sup> due to their more recent release.<sup>26-31</sup> Similarly, the W1 methods,<sup>32,33</sup> such as W1BD,34 have also been introduced for high level calculations. Collectively, these levels of theory appear to offer effective chemical accuracy (< 4.2 kJ·mol<sup>-1</sup> error) when estimating enthalpies of formation for organic compounds using atomization, isodesmic, and homodesmic approaches, particularly where conformational effects are accounted for using correction factors. In the current work, we examine the gasphase standard state (298.15 K, 1.01325 bar [1 atm]) enthalpy of formation  $(\Delta_{\rm f} H^{\circ}_{(g)})$  prediction capacity of the G4 and W1BD methods via the atomization approach on a suite of small- to medium-sized organic compounds having diverse mono- and polyfunctionalization. Our focus is on moieties and larger molecules without substantial conformational complexity that

<sup>‡</sup> Ecologica Research.

are not often included in benchmarking efforts, as well as the use of the G4 level of theory to estimate  $\Delta_f H^{\circ}_{(g)}$  (and optimized gas-phase geometries) for a number of compounds of broad interest in organic chemistry that lack experimental data.

#### **Experimental Section**

Compound structures and experimental data were obtained from the online National Institute of Standards and Technology (NIST) Chemistry WebBook (http://webbook.nist.gov/chemistry/).<sup>35</sup> Where applicable, two-dimensional structures from this reference database were converted to three-dimensional geometries using Avogadro v.1.0.1 (http://avogadro.openmolecules.net/). All compounds were subjected to a systematic rotor search which identified the lowest energy MMFF94<sup>36-40</sup> conformation followed by a 500 step geometry optimization using the steepest descent algorithm and a convergence criterion of  $10^{-7}$  within the Avogadro software environment. The resulting geometries were used as inputs for Gaussian-4  $(G4)^{24}$  and  $W1BD^{32,34}$ composite method calculations with Gaussian 09.41 All molecular enthalpies include zero-point and thermal corrections, and no compounds have imaginary frequencies at the final optimized geometry. Only the lowest energy conformation of each compound was considered. Gabedit v.2.2.12 (http://gabedit. sourceforge.net/) was used for geometry visualization.<sup>42</sup> Brief descriptions of the G4 and W1BD methodologies are provided in the Supporting Information (SI).

Enthalpies of formation were calculated using the atomization approach<sup>43,44</sup> with the following experimental atomic  $\Delta_t H^{\circ}_{(g)}$ (values in kJ·mol<sup>-1</sup>):<sup>35,45</sup> H, 217.998 ± 0.006; C, 716.68 ± 0.45; N, 472.68 ± 0.40; O, 249.18 ± 0.10; S, 277.17 ± 0.15; F, 79.38 ± 0.30; and Cl, 121.301 ± 0.008. Corresponding atomic enthalpies at the G4 and W1BD levels of theory are as follows (values in hartrees): G4, H (-0.499060), C (-37.831808), N (-54.571306), O (-75.043141), S (-397.977818), F (-99.702622), and Cl (-460.012692); W1BD, H (-0.497634), C (-37.850525), N (-54.608843), O (-75.108897), S (-399.062789), F (-99.809076), and Cl (-461.431267). Optimized geometries, energies at each step of the calculation process, and frequency coordinates for all compounds are provided in the SI. A conversion factor of 1 hartree = 2625.4997 kJ·mol<sup>-1</sup> was used for all calculations.

<sup>\*</sup> Corresponding author. E-mail: rayne.sierra@gmail.com.

<sup>&</sup>lt;sup>†</sup> Okanagan College.

Table 1.	Experimental and G4/V	W1BD Calculated	Gas Phase Stan	dard State (298.)	15 K, 1.01325 bar	) Enthalpies of Formation	$(\Delta_{\mathbf{f}} H^{\circ}_{(\mathbf{g})})$ for
Various S	Small Organic Compour	nds <sup>a</sup>					_

	$\Delta_{\rm f} H^{ m o}{}_{ m (g)}/({ m kJ}{ m \cdot}{ m mol}^{-1})$			$\Delta_{\rm f} H^{\rm o}{}_{\rm (g)}/({\rm kJ} \cdot {\rm mol}^{-1})$			
compound	expt.	G4	W1BD	compound	expt.	G4	W1BD
1-methylcyclopropene	244.0	241.5	235.7	dimethylamine	-19.0 to -23.8	-15.3	-21.0
1,1-dichloroethene	2.0 to 2.2	2.8	-5.1	ethane	-84.7 to -83.8	-82.9	-88.6
1,1-difluoroethene	-344.0 to -325.0	-348.1	-357.2	ethanol	-235.3 to -232.4	-233.1	-240.7
2-methyl-1-propene	-17.9	-15.3	-22.7	ethylene	52.4 to 52.5	52.6	50.0
acetaldehyde	-170.7	-165.3	-168.6	ethylene oxide	-52.6 to -70.2	-53.1	-55.9
acetic acid	-435.4 to -431.9	-428.8	-435.3	fluoroethene	-136.0	-140.7	-147.0
acetone	-218.5 to -216.4	-214.9	-221.2	formaldehyde	-108.6	-111.2	-110.5
acetonitrile	65.9 to 74.0	73.3	73.8	formic acid	-379.2 to -378.3	-377.6	-381.0
acetylene	226.7 to 227.4	229.1	228.3	furan	-27.7 to $-34.7$	-32.6	-39.6
bicyclo[1.1.0]butane	217.0	224.6	219.3	hydrogen cyanide	135.1	128.5	131.2
carbon dioxide	-393.5	-396.0	-394.6	methane	-74.8 to -73.4	-74.4	-76.4
carbon disulfide	116.9 to 117.1	105.8	114.4	methanethiol	-22.8	-21.6	-28.2
carbon monoxide	-110.5	-113.7	-110.1	methanol	-214.0 to -200.6	-200.3	-205.1
carbonic difluoride	$-640.6 \pm 5.9$ to $-638.9$	-606.0	-612.3	methylamine	-23.5 to -12.2	-19.3	-24.6
chloroethene	21.0 to 38.1	22.8	16.3	methylenecyclopropane	201.0	193.8	188.6
chloromethane	-85.9 to -81.9	-81.1	-88.3	oxetane	$-80.5 \pm 0.6$	-78.7	-84.9
chlorotrifluoromethane	-739.5 to -699.0	-707.6	-720.9	phosgene	-220.1 to -209.5	-220.7	-226.6
cis-1,2-dichloroethene	-3.0 to $4.3$	0.6	-8.6	propene	20.4	21.1	15.6
cis-2-butene	-7.7	-3.6	-12.0	propylene oxide	-94.7 to -117.1	-93.8	-98.9
cyanogen chloride	138.0	129.3	132.7	propyne	185.4	186.2	183.3
cyclobutene	157.0	163.9	155.8	pyrrole	108.3 to 143.2	109.7	102.6
cyclopropane	39.3 to 53.3	55.2	49.3	tetrafluoromethane	-953.4 to -908.8 (-678.0)	-931.7	-944.5
cyclopropanecarbonitrile	180.6 to 182.7	186.3	184.7	trans-1,2-dichloroethene	-1.0 to 1.7	3.2	-6.0
cyclopropene	277.0	285.1	280.6	trans-2-butene	-10.8	-9.0	-16.9
dichloromethane	-95.7 to -95.1	-92.5	-102.5	trichloromethane	-103.2 to $-102.9$	-100.4	-110.6
difluoromethane	-452.2 to $-450.7$	-450.3	-457.5	trifluoromethane	-697.1 to $-690.8$	-695.2	-705.4
dimethyl sulfoxide	-150.5	-146.7	-157.4	trimethylamine	-23.7 to $-30.7$	-24.4	-30.4

<sup>a</sup> Experimental values are the lower and upper boundaries of multiple individual data points with likely outlying experimental data given in parentheses. Experimental data taken from ref 35 with full referencing for all individual data points provided in the SI.

#### **Results and Discussion**

The gas-phase standard state (298.15 K, 1.01325 bar [1 atm]) enthalpies of formation  $(\Delta_{\rm f} H^{\circ}_{\rm (g)})$  were initially calculated at both the G4 and W1BD levels of theory for a set of 54 organic compounds also having experimental  $\Delta_{\rm f} H^{\circ}{}_{({\rm g})}$  data for comparison (Table 1). The compounds were chosen to span a range of mono- and polyfunctionalized halogenated, saturated and unsaturated, cyclic and acyclic, and heteroatom (N, O, S) substituted moieties without substantial conformational complexity. As previously noted,<sup>44</sup> where conformationally complex compounds have multiple low-energy conformations that can collectively and significantly contribute to the composite  $\Delta_{\rm f} H^{\circ}{}_{\rm (g)}$ measured experimentally, computational approaches that only consider the global minimum conformation will underestimate the conformationally weighted  $\Delta_{f}H^{\circ}_{(g)}$ . Thus, omitting conformational analyses during theoretical  $\Delta_{\rm f} H^{\circ}{}_{\rm (g)}$  studies can lead to spurious benchmarking conclusions, such as finding apparent excellent agreement with experimental  $\Delta_{\rm f} H^{\circ}{}_{({\rm g})}$  when—if low energy conformations were included in the analysis-the computational approach would overestimate the conformationally averaged experimental  $\Delta_f H^{\circ}_{(g)}$  it is being compared to. Similarly, an apparent  $\Delta_{\rm f} H^{\circ}{}_{\rm (g)}$  underestimation by a global minimum theoretical treatment may not be a result of any fundamental inaccuracies in the computational method, but rather the failure to fully account for significant enthalpic contributions from other low-lying conformers.

For broader benchmarking efforts on small- and mediumsized organic compounds, such as those presented herein, full conformational studies on each compound are impractical. Instead, data sets having compounds with higher symmetry and/ or rigidity potentially reduce errors from a global minimum theoretical treatment. However, rigid molecules are often strained, and these compounds are difficult to synthesize, purify, and accurately determine their experimental  $\Delta_f H^{\circ}_{(g)}$ . Consequently, a paradox arises in computational thermodynamics: either conduct expensive full conformational studies for benchmarking investigations of conformationally complex compounds having more reliable experimental  $\Delta_t H^{\circ}_{(g)}$  data, or use global minimum approaches on more symmetrical and rigid molecules likely to have less reliable experimental  $\Delta_t H^{\circ}_{(g)}$  data. In the first case, it is likely that the experimental  $\Delta_t H^{\circ}_{(g)}$  data will be as accurate as the theoretical estimate. In the second case (particularly where non-C/H functional groups are present that can cause difficulties in ensuring complete experimental combustion), the experimental  $\Delta_t H^{\circ}_{(g)}$  data may be less accurate than that obtained theoretically.

For these reasons, it is difficult to present rigorous error metrics (e.g., mean signed deviation [MSD], mean absolute deviation [MAD], root mean squared deviation [rmsd]) for comparison between the experimental and the G4/W1BD calculated  $\Delta_{\rm f} H^{\circ}_{\rm (g)}$  data. As evident in Table 1, many compounds (e.g., tetrafluoromethane, pyrrole, etc.) contain wide ranges of individual experimental  $\Delta_{\rm f} H^{\circ}{}_{\rm (g)}$  reports (up to  $\approx 50 \text{ kJ} \cdot \text{mol}^{-1}$ after screening of clear outliers and up to  $\approx 300 \text{ kJ} \cdot \text{mol}^{-1}$ including all available data points), and it is not clear which (if any) of the primary data points are accurate. Furthermore,  $\Delta_{\rm f} H^{\circ}{}_{\rm (g)}$  assessments in various standard source compendia and reviews do not generally explain how a final single value was obtained. In some cases, unsatisfying methods such as simply averaging all available experimental data points are used. Even simple compounds such as furan, acetonitrile, and methylamine have experimental  $\Delta_{\rm f} H^{\circ}_{(\rm g)}$  ranges of (7.0, 8.1, and 11.0) kJ·mol<sup>-1</sup>, respectively, outside the boundaries of experimental accuracy (4.2 kJ·mol<sup>-1</sup>) and the error bounds given for each data point. However, with few exceptions, the G4 and W1BD estimates are within the ranges of experimental data (or within several  $kJ \cdot mol^{-1}$  where only a single data point is available). The W1BD  $\Delta_{f} {H^{\circ}}_{(g)}$  are also systematically lower than the G4

Table 2. Experimental and G4 Calculated Gas-Phase Standard State (298.15 K, 1.01325 bar) Enthalpies of Formation  $(\Delta_f H^{\circ}_{(g)})$  for Various Organic Compounds<sup>*a*</sup>

$\Delta_{\rm f} H^{\circ}{}_{ m (g)}/({ m kJ}{ m \cdot mol}^{-1})$		-1)		$\Delta_{\rm f} H^{\circ}{}_{({\rm g})}/({\rm kJ} \cdot {\rm mol}^{-1})$	
compound	expt.	G4	compound	expt.	G4
$(1\alpha, 2\alpha, 4\alpha, 5\alpha)$ -tricyclo $[3.2.1.0^{2,4}]$ oct-6-ene	239.0 to 247.0	233.7	bicyclo[4.2.0]octa-1,3,5-triene	199.4	200.9
(E)-hexa-1,5-diyne-3-ene	538.1	526.6	butane	-127.1 to -125.6	-123.6
(Z)-3-penten-1-yne	258.0	255.0	carbon suboxide	-97.8 to -93.6	-89.9
(Z)-hexa-1,5-diyne-3-ene	541.8	527.3	chlorobenzene	54.4	52.4
1-buten-3-yne	295.0	290.3	chlorotrifluoroethene	-564.8 to -505.5	-505.6
1-cyclopropylpenta-1,3-diyne	484.7	481.6	cis-2,3,4-hexatriene	265.0	261.0
1-propynylbenzene	268.2	279.5	cis-bicyclo[4.3.0]nona-3,7-diene	109.2	113.1
1,1-dimethylcyclopropane	-8.2	-8.8	cyclobutane, 1,2-bis(methylene)-	204.0	211.4
1,1,1-trichloroethane	-145.0 to $-142.3$	-146.1	cyclopropane, 1,1-diethynyl-	538.5	547.1
1,1,1-trifluoroethane	-749.0 to -748.7	-750.3	cyclopropanone	16.0	20.4
1,2-bis(methylene)cyclobutane	204.0	211.4	cyclopropylacetylene	292.0	297.1
1,2,3-trichlorobenzene	3.8 to 8.2	5.5	cyclopropylbenzene	150.4 to 150.7	160.9
1,2,4-trichlorobenzene	-8.0 to 4.9	-0.1	difluorodichloromethane	-491.6 to $-469.0$	-492.2
1,3-cyclopentadiene	133.4 to 139.0	137.1	diketene	-190.2	-190.4
1,3-cyclopentadiene, 5-(1-methylethylidene)-	144.0	145.5	dispiro[2.0.2.1]heptane	302.8	312.5
1,3-dioxol-2-one	-418.6	-396.2	fluorotrichloromethane	-290.0 to $-268.3$	-288.3
1,3,5-triazine	224.7 to 225.9	224.1	fulvene	224.0	216.6
1,3,5-trichlorobenzene	-2.6 to $-13.4$	-5.8	hexafluorobenzene	-956.0	-949.3
1,3,5-trioxane	-489.5 to $-464.0$	-468.3	hexane	-167.2 to $-167.1$	-165.2
1 <i>H</i> -imidazole	128.0 to 139.3	131.4	isobutane	-134.2 to -135.6	-132.0
1 <i>H</i> -pyrazole	177.4 to 181.0	177.3	isopentane	-154.5 to $-153.7$	-150.6
2-butynedinitrile	529.3	530.1	<i>m</i> -dichlorobenzene	28.1	22.0
2-methyl-1-buten-3-yne	259.0	254.8	<i>m</i> -difluorobenzene	-309.2	-302.9
2-methyl-1 <i>H</i> -imidazole	89.8 ± 1.1	88.8	neopentane	-168.5 to $-166.0$	-166.6
2-methylpyridine	(-26.5) 87.7 to 102.0	99.5	norbornan-/-one	-134.0	-142.2
2-norbornene	63.3 to 90.6 (121.0)	82.0	nortricyclene	62.0 to 99.6	71.5
2-propenenitrile	1/2.6 to 1/9.7	186.3	o-dichlorobenzene	33.0	28.0
2,2-dimethylbutane	-185.6	-182.3	o-difluorobenzene	-283.0	-28/.1
2,3-bis(methylene)bicyclo[2.2.0]nexane	315.0	307.6	octanydrodicyclopropa[cd,gn]pentalene	180.0	1/5.8
2,3-diazabicyclo[2.2.1]-nept-2-ene	196.0	205.8	<i>p</i> -dichlorobenzene	24.0	22.7
2,3-dimydrotniopnene	90.7	82.2	p-diluorobenzene	-300.7	-299.0
2,5-dimethylbutane	-1/7.8	-1/4.4	pentane	-14/.1 to $-140.4$	-144.5
2, (ais athylidana) 1 avalanantana	211.7 10 247.0	239.7	phenol mbanyla astylana	-90.4 10 -94.2	220.1
2 mathylana 1.4 avalahavadiana	04.J 150.0	160.9	preniolonitrile	254.0	272.0
2 mathylenegyelopentane	130.0	109.4	propioloinume	106.1	205.2
2.4 dimethylenegyelobut 1 and	226.0	220.7	pyrazine	278.4	205.5
2.6 bis(mathylana) 1.4 avalabavadiana	210.0	222.7	pyridazine	(110, 1) 140.2 to 140.7	140.8
4 methylene 2 ovetanone	-190.2	-190.4	pyrimidine	(110.1) 140.2 to 140.7	140.0
5.5 dimethyl 1.2 evalopentadiona	86.6	81.6	guadrigualana	(252.2) 225.0 to 220.1	224.5
6 mathylfulyana	185.0	182.1	spire[2.4]hopta 4.6 diana	223.3) 323.0 10 339.1	227.5
7 methylenebicyclo[2,2,1] hentane	60.0	102.1	spiro[cyclopropage(1.5')bicyclo[2.1.0]pentage]	288.0	227.5
aniline	81.0 to 87.0	89.7	spiropentane	185.1	185.2
antitricyclo[ $3200^{2,4}$ ]hept-6-ene	383.9	374.2	styrene	(-15.1) 131.5 to 151.5	150.3
antitricyclo[ $3.2.0.0^{-1}$ ]hept o che	235.0	238.7	tetrachloroethene	-240  to  -124	-24.6
antitricyclo[4,1,0,0 <sup>2,4</sup> ]heptane	154.0	155.9	tetrachloromethane	-1250 to $-940$	-98.0
antitricyclo[4 2 0 0 <sup>2,5</sup> ]octane	211.0	217.4	tetracyclo[4 1 0 $0^{2,4}$ $0^{3,5}$ ]heptane	370.0	368.1
benzene	79.9 to 82.9	85.6	tetrafluoroethene	-686.0 to $-658.6$	-670.2
benzyne	440.0 to 490.0	459.6	tetrahydrofuran	-184.2	-178.9
bicyclo[1,1,0]but-1(3)-ene	544.0	567.8	thiophene	115.0 to 116.7 (218.4)	112.7
bicyclo[1,1,0]butane-1-carbonitrile	304.5	352.1	thiophene. 2.5-dihydro-	87.3	84.5
bicyclo[2.1.0]pent-2-ene	333.0	329.6	toluene	48.0 to 50.1	52.6
bicyclo[2.1.0]pentane	158.0	157.8	trans-2,3,4-hexatriene	265.0	261.0
bicyclo[2.1.0]pentane-1-carbonitrile	272.0	278.4	trans-bicyclo[6.1.0]nona-2.4.6-triene	372.0	344.7
bicyclo[2.1.1]hex-2-ene	251.0	230.3	trichloroethene	-19.1 to -5.9	-14.1
bicyclo[2.2.0]hex-1(4)-ene	304.0	383.1	tricyclo[4.1.0.0 <sup>2,4</sup> ]-heptane	149.0	155.9
bicyclo[2.2.0]hexane	125.0	131.7	tricyclo[4.1.0.0 <sup>2,7</sup> ]heptane	191.0	196.4
bicyclo[3.2.0]hept-1-ene	167.0	171.9	trifluoroacetonitrile	-496.6 to -460.0	-498.5
bicyclo[3.2.0]hept-1(5)-ene	173.0	184.3	trifluoroethene	-474.0	-495.4
bicyclo[3.2.0]hepta-2,6-diene	264.0	263.1	tris(methylene)cyclopropane	396.0	441.3
hicyclo[3 2 1]octa-2 6-diene	158 0 to 159 0	148 3			

<sup>a</sup> Experimental values are the lower and upper boundaries of multiple individual data points with likely outlying experimental data given in parentheses. Experimental data taken from ref 35 with full referencing for all individual data points provided in the SI.

level of theory, with MSD, MAD, and rmsd values of  $(-5.3, 6.0, \text{ and } 6.7) \text{ kJ} \cdot \text{mol}^{-1}$ , respectively, between the two methods.

Two sets of error metrics against the experimental data were developed. For each compound, the lowest and highest deviations between the theoretical data point and experimental data point(s) were determined, giving MSD<sub>best</sub>/MAD<sub>best</sub>/rmsd<sub>best</sub> and MSD<sub>worst</sub>/MAD<sub>worst</sub>/rmsd<sub>worst</sub>. For the G4 calculations on the G4/W1BD common 54 compound data set, the MSD<sub>best</sub>/MAD<sub>best</sub>/rmsd<sub>best</sub> of (-1.1, 3.2, and 5.8) kJ·mol<sup>-1</sup>, respectively, were obtained, compared to the MSD<sub>worst</sub>/MAD<sub>worst</sub>/rmsd<sub>worst</sub> of (-1.6, 8.2, and

12.2) kJ·mol<sup>-1</sup>, respectively. At the W1BD level of theory, the MSD<sub>best</sub>/MAD<sub>best</sub>/rmsd<sub>best</sub> of (4.2, 5.6, and 7.1) kJ·mol<sup>-1</sup>, respectively, were obtained, compared to the MSD<sub>worst</sub>/MAD<sub>worst</sub>/rmsd<sub>worst</sub> of (3.6, 8.9, and 12.9) kJ·mol, respectively. In both cases, the anomalously high experimental  $\Delta_{\rm f} H^{\circ}_{\rm (g)}$  of  $-678.0 \pm 8.0$  kJ·mol<sup>-1</sup> for tetrafluoromethane was omitted as an outlier.

Because of computational expense, W1BD calculations were not practical for larger compounds that also have experimental  $\Delta_{\rm f} H^{\rm o}_{\rm (g)}$  values. For these additional 121 molecules, only G4 calculations were completed (Table 2). A generally strong \_

# Table 3. G4 Calculated Gas-Phase Standard State (298.15 K, 1.01325 bar) Enthalpies of Formation ( $\Delta_f H^{\circ}_{(g)}$ ) for Various Organic Compounds Which Lack Experimental $\Delta_f H^{\circ}_{(g)}$ Data

$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$		G4 $\Delta_{\rm f} H^{\circ}{}_{\rm (g)}$		G4 $\Delta_{\rm f} H^{\rm o}{}_{\rm (g)}$
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	compound	$kJ \cdot mol^{-1}$	compound	$kJ \cdot mol^{-1}$
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	(1α,2α,5α,6α)-tricyclo[4.2.0.0 <sup>2,5</sup> ]octa-3,7-diene	502.6	4-methylpyrazole	148.0
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$(1\alpha, 2\beta, 5\beta, 6\alpha)$ -tricyclo[4.2.0.0 <sup>2,5</sup> ]octa-3,7-diene	475.6	5-(dimethylamino)tetrazole	327.5
	$(1\alpha, 4\alpha, 5\beta)$ -5-methyl-2-methylenebicyclo[2.1.0]pentane	259.6	5-ethenylidene-1,3-cyclopentadiene	354.1
Function         123.7         5-methylenebicyclo[2.2.0]hex-2-ene         134.6           1-methyl-1.2-propadienylcyclopropane         236.2         5-methylenebicyclo[2.1.0]hex-2-ene         187.1           1-methyl-1.2-yclopentaldiene         101.1         5.5-dimethylbicyclo[2.1.0]hex-2-ene         187.1           1-methyl-1.2-ininopyrazole         165.9         6-methyl-1.2-linebicyclo[2.1.0]her-2-ene         264.9           1-methyl-5-aninopyrazole         165.9         6-methyl-1.2-linebicyclo[3.2.0]hept-3-ene         273.0           1-methyl-5-aninopyrazole         165.9         6-methyl-1.2-linebicyclo[3.2.0]hept-3-ene         265.7           1-methyl-cyclopropanecarbonitrile         125.5         7-thiabicyclo[4.1.0.0 <sup>2+</sup> ]hept-3e         170.9           1-methyl-cyclopropanecarbonitrile         175.3         berozolithiet         242.0           1-methyl-cyclopropanecarbonitrile         275.3         berozolithiet         242.0           1-methyl-2-methyleneyclopropane         252.0         bicyclo[1.1]pentane         291.6           1-prazoline         181.5         bicyclo[2.2.0]hex-2-2.7         50.16           1-dicyancethane         225.2         bicyclo[2.2.0]hex-2.5-diene         404.8           1,1-discuptyl-2-methylenecyclopropane         225.2         bicyclo[2.2.0]hex-2.5-diene         404.6	[1.1.1]-propellane	360.2	5-methyl-1,3-cyclopentadiene	113.1
1. cmityl 1. C pop/10/2004 population         236.2         5. mityl indicipation 2.2.1 [hpt 2.cme         257.3           1mittyl 1. Jsyckopentadiene         101.1         5.5. dimethyl bicyclol 2.2.1 [hpt 2.cme         264.9           1mittyl 1. Jsyckopentadiene         101.1         5.5. dimethyl bicyclol 2.2.1 [hpt 2.cme         264.9           1mittyl 1. Jmittyl 2.5. dimethyl bicyclol 2.1.1 [hpt 2.cme         264.9         273.0           1mittyl 2.7. (mittyl 2.5. dimethyl bicyclol 2.2.1 [hpt 2.cme         273.0         273.0           1mittyl 2.7. (Job 2.2.1 [hpt 2.5. dimethyl 2.5	1-azeune	193.7 507.1	5-methylenebicyclo[2,2,0]hex-2-ene	354.6
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	1-methyl-1.2-propadienylcyclopropane	236.2	5-methylenebicyclo[2.2.1]hept-2-ene	187.1
$\begin{split} \begin{array}{llllllllllllllllllllllllllllllllllll$	1-methyl-1,3-cyclopentadiene	101.1	5,5-dimethylbicyclo[2.1.0]pent-2-ene	264.9
$\begin{split} &  -\text{methy}  3-\text{aminopyrazole} &   165.9 & 6-\text{methyltricyclo}  1.0.0^{21} [hept-3-ene & 273.0 \\  -\text{methyl-axindine} &   121.6 & 7-\text{methylenebicyclo}  3.2.0 [hept-1-ene & 265.7 \\  -\text{methyl-cyclopropanecarbonitrile} &   121.6 & 7-\text{methylenebicyclo}  3.2.0 [hept-1-ene & 265.7 \\  -\text{methyl-cyclopropanecarbonitrile} &   122.5 & 7-\text{thiabicyclo}  3.2.0 [hept-1-ene & 265.7 \\  -\text{methyl-cyclopropanecarbonitrile} &   152.5 & 7-\text{thiabicyclo}  3.2.0 [heptane &   101.4 \\  -\text{methyl-cyclopropanecarbonitrile} &   30.9 \\  -\text{methyl-cyclopropanecarbonitrile} &   202.8 & henzodithiete &   242.0 \\  -\text{methyl-cyclopropanecarbonitrile} &   202.8 & henzodithiete &   202.1 \\  -\text{methyl-cyclopropanecarbonitrile} &   202.5 & henzodithiete &   202.6 \\  -\text{pertens-3-yne} &   250.0 & hicyclo  1.1.1 [hentane &   201.6 \\  -prazoline &   181.5 & hicyclo  2.2.0 [hexa-2-ene &   261.6 \\  .1-dimethyl-2-methylenecyclopropane &   128.5 & hicyclo  2.2.0 [hexa-2-5.6 diene &   311.4 \\  .2-cyclobutanedione & -166.6 & hicyclo  3.2.0 [heptane + 2.5.5 diene &   404.8 \\  .2-dimethylcyclopropene &   199.8 & bicyclo  3.2.0 [heptane + 2.5.5 diene &   311.4 \\  .2.3-butartice &   335.2 & cyanoallene &   335.4 \\  .2.3-butartice &   335.2 & cyanoallene &   408.5 \\  .2.3-butartice &   335.2 & cyanoallene &   430.4 \\  .2.3-butartice &   335.2 & cyanoallene &   430.4 \\  .2.4-triazine &   405.5 & bicyclo  4.2.0 [hetan-1.3.5.7-tetrane &   409.4 \\  .3-dimethylbylcyclop1.0 [hetane + 1.3-dione & -180.2 \\  .3-dimethylbylcyclo  1.0 [hutane &   154.6 & cyclobutane + 1.3-dine & -180.2 \\  .3-dimethylbylcyclo  1.0 [hutane &   154.6 & cyclobutane + 0.5 \\  .3-dimethylbylcyclo  1.0 [hutane &   415.6 & cyclobutane + 0.5 \\  .4-dixin & -81.1 & cyclocata-1.5-diene-5-yne &   436.7 \\  .4-dixin & -81.1 & cyclocata-1.5-diene-5-yne &   436.7 \\  .4-dixin & -81.1 & cyclocata-1.5-diene-5-yne &   436.7 \\  .4-dixin & -81.1 & cyclocata-1.5-diene-5-yne &   401.9 \\  .4-dixin & -81.1 & cyclocata-1.5-diene-5-yne &   401.9 \\  .4-dixin & -81.1 & cyclocata-1.5-diene-5-yne &   401.9 \\  .4$	1-methyl-1H-imidazole	123.6	6-methyl-1,2,4-triazine	290.9
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	1-methyl-3-aminopyrazole	165.9	6-methyltricyclo[4.1.0.0 <sup>2,7</sup> ]hept-3-ene	273.0
1-methylexploated121.67-methylexploated205.71-methylexploated121.17-oxabicycloj 2.2.1 [heptane-176.61-methylexplopropene-3-carbonitrile152.57-thiabicycloj 2.2.1 [heptane101.41-methylexplopropene-3-carbonitrile378.9azetidine101.41-methylexplopropene-3-carbonitrile378.9azetidine202.81-methylexplopropene-3-carbonitrile202.8benzvalene385.91-penten-3-yne250.0bicycloj 1.1.1 [pentane201.61-pyrazoline181.5bicycloj 2.2.0 [hex-2-ene261.61,1-dirganoethane225.2bicycloj 2.2.0 [hex-2-ene261.61,1-dinethyl-2-methylenecyclopropane128.5bicycloj 2.2.0 [hex-2-ene296.01,2-vyclobutanedione-166.6bicycloj 2.2.0 [hex-2-ene380.31,2-3-bitaritine400.5bicycloj 3.0 [octa-2.6-diene131.41,2-3-bitaritine335.2cyanollene_1.3.5.triene490.41,2-3-bitaritine335.2cyanollene436.71,3-bigmethylencycloplatane154.6cyclobutadiene430.41,3-dimethylencyclojlutane154.6cyclobutadiene430.71,3-bigmethylencyclojl_1.0.0 [butane154.6cyclopropanie335.72,1-dimethylencyclojl_1.0.0 [butane154.6cyclopropanie335.72,1-dimethylencyclojl_1.0.0 [betnate24.6cyclopropanie335.72,1-dimethylencyclojl_1.0.0 [betnate24.6cyclopropanie335.72,1-dimethylencyclojl_1.0.0 [betnate2	1-methyl-5-aminopyrazole	174.7	7-methylenebicyclo[2.2.1]hepta-2,5-diene	344.0
$\begin{aligned} 1-\text{nethylycyclonicale} & 121.1 \\ 1-\text{nethylycyclopropanecarbonitrile} & 152.5 \\ 1-\text{nethylycyclopropanecarbonitrile} & 378.9 \\ 1-\text{nethylycyclopropanecarbonitrile} & 378.9 \\ 1-\text{nethylnoronadiene} & 202.8 \\ \text{benzvalene} & 385.9 \\ 1-\text{penten-3-yne} & 250.0 \\ \text{bicyclo[1.1.1]pentane} & 201.6 \\ 1-\text{pyrazoline} & 181.5 \\ \text{bicyclo[2.1.1]pexane} & 59.8 \\ 1,1-\text{dicyanocthane} & 225.2 \\ \text{bicyclo[2.1.1]pexane} & 59.8 \\ 1,1-\text{dicyanocthane} & 225.2 \\ \text{bicyclo[2.2.0]pex-2-ene} & 261.6 \\ 1,2-\text{cyclobutanedione} & 128.5 \\ \text{bicyclo[2.3.0]pex-2-S-dime} & 404.8 \\ 1,1^{-hinitryl-2-methylencyclopropane} & 128.5 \\ \text{bicyclo[2.3.0]pex-2-S-dime} & 404.8 \\ 1,2^{-hinitryl-2-methylencyclopropane} & 128.5 \\ \text{bicyclo[2.3.0]pex-2-S-dime} & 406.8 \\ 1,2-\text{cyclobutanedione} & -166.6 \\ \text{bicyclo[3.3.0]peta-3.5.4 \\ 1.2-\text{cyclobutanedione} & -166.6 \\ \text{bicyclo[3.3.0]peta-3.5.7 \\ 1.3.2-\text{tiratine} & 400.5 \\ \text{bicyclo[3.3.0]peta-3.5.7 \\ 1.3.2-\text{tiratine} & 400.5 \\ 1.2.3.4 \\ 1.2.3.4 \\ 1.2.3.4 \\ 1.2.3.4 \\ 1.2.3.4 \\ 1.2.3.4 \\ 1.2.4.4 \\ 1.2.4.4 \\ 1.3$	1-methylaziridine	121.6	7-methylenebicyclo[3.2.0]hept-1-ene	265.7
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1-methylcyclobulene	121.1	7-oxabicyclo[2.2.1]heptane	130.9
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	1-methylcyclopropene-3-carbonitrile	378.9	azetidine	101.4
1-methyltricyclo[ $4.1.0.0^{27}$ ]hept-3-ene275.3berzvalene385.91-penten-3-yne250.0bicyclo[ $1.1.1$ ]pentane201.61-pyrazoline181.5bicyclo[ $2.1.1$ ]hexane59.81.1-dicyanoethane225.2bicyclo[ $2.2.0$ ]hex-2-ene261.61.1-dimethylenecyclopropane128.5bicyclo[ $2.2.0$ ]hex- $2.5.7$ -triene296.01.2-cyclobutanedione-166.6bicyclo[ $3.2.0$ ]hepta- $1.4.6$ -triene446.81.2-dimethyleyclopropene199.8bicyclo[ $3.3.0$ ]hepta- $1.4.5$ -triene480.31.2.3-butatriene322.6bicyclo[ $4.2.0$ ]hepta- $1.3.5$ -triene380.31.2.3-butatriene448.7cirs1- $2.5.7$ -triene490.41.2.3-butatriene335.2cyanoallene618.71.3-bis(methylene)cyclobutane322.6cyclobutanelione430.41.3-bis(methylene)cyclobutane154.6cyclobutane- $1.3.4$ -dione-180.21.3-bis(methylene)cyclobutane154.6cyclobutane- $1.3.4$ -dione-180.21.3-bis(methylene)cyclobutane415.6cyclopurphylene400.51.4-dioxin-41.1cycloprophylene424.01.5-dimethyl-1-cxomethylenetricyclo[ $2.1.0.0$ ]pentane234.8cycloprophylene430.41.5-dimethyl-1-sexomethylenetricyclo[ $2.1.0.0$ ]pentane234.8cycloprophylene234.01.5-dimethyl-1-prene-43.8cycloprophylene306.82-aziridinecarbonitrile269.5dihlydro- $2(3/P)$ -hiopenthione65.62-methyl-1dimethylethylthitrane-45.5endo- $2-methylene-5-met$	1-methylnorbornadiene	202.8	benzodithiete	242.0
1-perten-3-yne250.0bicyclo[1.1]pentane201.61-pyrazoline181.5bicyclo[2.1]hexane59.81.1-dicyanoethane225.2bicyclo[2.2.0]hexa-2.5-diene404.81.1-bizzirdine335.9bicyclo[2.2.0]hexa-2.5-diene296.01.2-cyclobutanedione-166.6bicyclo[3.2.0]heta-1.4,6-triene446.81.2-dimethylcyclopropene199.8bicyclo[3.3.0]heta-1.4,6-triene446.81.2.3-butatriene322.6bicyclo[4.1.0]hepta-1.3,5-Trietane409.41.2.3-triazine400.5bicyclo[4.2.0]octa-1.3,5,7-tetraene409.41.2.3-triazine335.2cyanollene618.71.3-bis(methylene)cyclobutane322.2bicyclol[4.1.0]hepta-1.3,6-triene436.61.3-triazine415.6cyclobutane-180.21.3-bis(methylene)cyclobutane222.0cyclobutane-180.21.3-pentadiyne415.6cyclopropaine436.71.4-dioxin-81.1cyclocta-1.3-dien-6-yne436.71.4-dioxin-81.1cyclopropaine234.81.5-dimethyl-1-penten-3-yne214.7dimethylerol/2/H-hiophenthione65.62-methyl-1-penten-3-yne214.7dimethylerol/2/H-hiophenthione65.62-methyl-1-preten-3-yne214.7dimethylerol/2/H-pentane206.82-methyl-1-preten-3-yne214.7dimethylerol/2/H-hiophenthione65.62-methyl-1-preten-3-yne214.7dimethylerol/2/H-hiophenthione65.62-methyl-1-preten-3-yne214.7dimethylerol/2/H-hiophenthione	1-methyltricyclo[4.1.0.0 <sup>2,7</sup> ]hept-3-ene	275.3	benzvalene	385.9
1-pyrazoline181.5bicyclo[2.1.1]hexane59.81.1-dixportance225.2bicyclo[2.2.0]hex-2-ene261.61.1-dimethyl-2-methylenccyclopropane128.5bicyclo[2.2.0]hex-2.5,7-triene296.01.2-cyclobutanedione-166.6bicyclo[3.3.0]octa-2,6-diene131.41.2-cyclobutanedione199.8bicyclo[3.3.0]octa-2,6-diene131.41.2.3-triazine322.6bicyclo[3.1.0]heta-1,4,6-triene446.81.2.3-triazine400.5bicyclo[4.1.0]hepta-1,3,5-triene380.31.2.3-triazine400.5bicyclo[4.1.0]hepta-1,3,5-triene409.41.2.3-triazine448.7cis-1.2-diethynylcyclopropane618.71.3-bis(methylene)cyclobutane222.0cyclobutaneine430.41.3-dimethylbicyclo[1.1.0]butane154.6cyclobutane-1,3-diene401.91.4-dioxin-81.1cycloocta-1,5-dien-3-yne401.91.4-dioxin-81.1cycloopropidiene234.01.5-dimethyl-sexomethylenetricyclo[2.1.0.0]pentane421.5cyclopropidiene cyclopropane2-(1.1-dimethyl-thyl)thirane-43.8cyclopropylidene cyclopropane337.52-(1.1-dimethyl-thyl)thirane-44.5endo-2-methylense106.82-methyl-1.3-dithiacyclopentane26.2dipthylca-2(3/3)-thiopenthibiceclo[2.1.0]pentane21.12-methyl-1.3-dithiacyclopentane-45.5endo-2-methylca-5-methylbicyclo[2.1.0]pentane221.02-didimethyl-1.3-dithiacyclopentane-45.5endo-2-methylca-5-methylbicyclo[2.1.0]pentane266.52-methyl-1.3-dith	1-penten-3-yne	250.0	bicyclo[1.1.1]pentane	201.6
1,1-dicyanoethane225.2bicyclo[2.2.0]nex-2-sene261.61,1-dimethylencyclopropane128.5bicyclo[2.2.2]octa-2,5,7-triene404.81,1-binethylencyclopropane128.5bicyclo[3.2.0]nexa-2,5diene414.61,2-dimethyleyclopropene199.8bicyclo[3.2.0]nexa-1,5-diene131.41,2.3-butatriene322.6bicyclo[4.1.0]nepta-1,3,5-triene380.31,2.3-triazine400.5bicyclo[4.2.0]octa-1,5,6diene131.41,2.3-triazine400.5bicyclo[4.2.0]octa-1,3,5,7-tetraene409.41,2.3-tyentatertaene448.7cis-1,2-diethynylcyclopropane544.61,2.4-triazine335.2cyanoallene618.71,3-bis(methylene)cyclobutane154.6cyclobutadiene-180.21,3-pentadiyne415.0cyclobutal-1,3-dien-6-yne436.71,4-hexadiyne415.0cyclopcat-1,3-dien-3-yne401.91,5-diinethyl-3-exomethylenetricyclo[2.1.0.0]pentane421.5cyclopropaliane224.01,5-diinethyl-1-propen-1-one-86.5dihory-2(3P)-pildenemethanone108.02-aritdinecarbonitrile269.5dihydro-2(3P)-thiophenthione65.62-methyl-1,3-ditinacyclopentane-45.5endo-2-methylenes-methylbicyclo[2.1.0]pentane221.12-methyl-1,3-ditinacyclopentane-45.5endo-2-methylenes-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]pentane216.7ethylenexclopropane306.82-methyl-1,5-diazabicyclo[3.1.0]pentane216.7ethylidenexclopropane306.82-me	1-pyrazoline	181.5	bicyclo[2.1.1]hexane	59.8
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	1,1-dicyanoethane	225.2	bicyclo[2.2.0]hex-2-ene	261.6
$\begin{aligned} 1,1-\text{order} & 353.5 & \text{obsychol} 22.5, 0, \text{childer} & 290.0 \\ 1,2-\text{cyclobutanedione} & -166.6 & \text{bicyclo} 3.2, 0, \text{betar} 1.4, 6-\text{triene} & 446.8 \\ 1,2-\text{dimethylcyclopropene} & 199.8 & \text{bicyclo} 3.3, 0, \text{betar} 1.4, 6-\text{triene} & 380.3 \\ 1,2.3-\text{triazine} & 222.6 & \text{bicyclo} 4.1, 0, \text{heptar} 1.3, 5, 7-\text{tetraene} & 499.4 \\ 1,2.3+\text{triazine} & 305.2 & \text{cyclobutane} & 544.6 \\ 1,2.4-\text{triazine} & 335.2 & \text{cyclobutane} & 544.6 \\ 1,2.4-\text{triazine} & 335.2 & \text{cyclobutane} & 544.6 \\ 1,2.4-\text{triazine} & 335.2 & \text{cyclobutane} & 618.7 \\ 1,3-\text{bigmelyleocyclobutane} & 222.0 & \text{cyclobutane} & -180.2 \\ 1,3-\text{bigmelyleocyclobutane} & 154.6 & \text{cyclobutane} & -180.2 \\ 1,3-\text{gentadyne} & 415.0 & \text{cyclobutane} & -180.2 \\ 1,4-\text{dioxin} & -81.1 & \text{cycloocta-} 1,5-\text{dien-} 5-\text{yne} & 430.7 \\ 1,4-\text{dioxin} & -81.1 & \text{cycloota-} 1,5-\text{dien-} 5-\text{yne} & 400.9 \\ 1,5-\text{dinethyleoteyclo} [2,1.0,0]\text{pentane} & 234.8 & \text{cyclopropane} & 337.5 \\ 2-(1,1-\text{dimethylenetricyclo} [2,1.0,0]\text{pentane} & 415.6 & \text{cyclopropane} & 337.5 \\ 2-(1,1-\text{dimethylenetricyclo} [2,1.0,0]\text{pentane} & -43.8 & \text{cyclopropylidene cyclopropane} & 108.0 \\ 2-\text{azirdinecarbonitrile} & 269.5 & \text{dithydro-2(3H)-thiophenthione} & 65.6 \\ 2-\text{methyl-1-penten-3-yne} & 214.7 & \text{dimethyleycananide} & 140.7 \\ 2-\text{methyl-1-penten-3-yne} & 214.7 & \text{dimethyle} (\text{syclopropane} & 306.8 \\ 2-\text{methyl-1-penten-3-yne} & 214.7 & \text{dimethyle} (\text{syclopropane} & 216.7 \\ 2-\text{methyl-1-penten-3-yne} & 216.7 & \text{ethyliene-5-methyleine-5-methyleocyclo} (3.1,0)\text{lexane} & 266.7 \\ 2-\text{methyl-1-penten-3-yne} & 216.7 & \text{ethyliene-5-methyleocyclo} (2.1,0)\text{gentane} & 216.7 \\ 2-\text{methyl-1-penten-3-yne} & 216.7 & \text{dimethyleycananide} & 140.7 \\ 2-\text{methyl-1-penten-3-yne} & 216.7 & \text{dimethyleycananide} & 266.8 \\ 2-\text{methyl-1-penten-3-yne} & 216.7 & \text{thyliene-5-methylbicyclo} (2.1,0)\text{gentane} & 266.8 \\ 2-\text{methyl-1-propen-1-one} & -86.5 & \text{dithio-p-benzoquinone} & 266.8 \\ 2-\text{methyl-1-penten-3-yne} & 216.7 & \text{thyliene-5-methylbicyclo} (2.1,0)\text{gentane} & 266.8 \\ 2-m$	1,1-dimethyl-2-methylenecyclopropane	128.5	bicyclo[2.2.0]nexa-2,5-diene	404.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1,1 -orazinane 1 2-cyclobutanedione	-166.6	bicyclo[2.2.2]0cta-2,3,7-thene bicyclo[3.2.0]hepta-1.4.6-triene	446.8
1,2,3-butariene322.6bicyclo[4.1.0]hepta-1,3,5-triene380.31,2,3-triazine400.5bicyclo[4.2.0]octa-1,3,5,7-tetraene409.41,2,3-triazine400.5bicyclo[4.2.0]octa-1,3,5,7-tetraene409.41,2,3-triazine335.2cyanoallene544.61,2,4-triazine335.2cyanoallene618.71,3-bis(methylencyclobutane222.0cyclobutane-1,3-dione-180.21,3-pentadiyne415.0cyclootar-1,3-dien-6-yne436.71,4-dioxin-81.1cyclootar-1,5-dien-3-yne401.91,4-hexadiyne15.6cyclootar-1,5-dien-3-yne401.91,5-dihydropentalene234.8cyclopropanimine224.01,5-dihydropentalene-43.8cyclopropanimine224.01,5-diinydropentalene24.8cyclopropanimine108.02-aziridinearbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyannide140.72-methyl-1-propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,5-diazbicyclo[3.1.0]hexane216.7ethylidenecyclopropane221.12-methyl-1,5-diazbicyclo[3.1.0]hexane26.2heptaduvene266.82-oxaspiro[3,3]heptane29.5hex-3-en-1,5-diyne221.12-oxaspiro[3,3]heptane25.5hex-3-en-1,5-diyne256.62-pyrazoline17.3methylencyclopropane264.52,4-diindrylthirinane2.5hex-3-en-1,5-diyne256.62-pyrazoline17.3	1.2-dimethylcyclopropene	199.8	bicyclo[3.3.0]octa-2.6-diene	131.4
1,2,3-triazine400.5bicyclo[4.2.0]octa-1,3,5,7-tetraene409.41,2,3-triazine448.7 $cis-1,2-diethynylcyclopropane544.61,2,4-triazine335.2cyanoallene618.71,3-bis(methylene)cyclobutane222.0cyclobutadiene430.41,3-dimethylbicyclo[1,1.0]butane154.6cyclobutane-1,3-dione-180.21,3-pentadiyne415.0cycloocta-1,3-dien-6-yne401.91,4-dioxin-81.1cycloocta-1,5-dien-3-yne401.91,4-dioxin-81.1cycloocta-1,5-dien-3-yne401.91,5-dimydropentalene234.8cyclopropylidenemethanone108.02-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-perten-3-yne214.7dimethylcyanamide140.72-methyl-1-perten-3-yne214.7dimethylcyanamide140.72-methyl-1-perten-3-yne214.7dimethylcyanamide140.72-methyl-1-perten-3-yne214.7dimethylcyanamide140.72-methyl-1-perten-3-yne214.7dimethylcyanamide140.72-methyl-1-perten-3-yne214.7dimethylcyanamide21.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylacecyclopropane366.82-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylacecyclopropane266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne266.62-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne28.82,2-dimethylthiriane2.5methylcyclopropane38.9$	1,2,3-butatriene	322.6	bicyclo[4.1.0]hepta-1,3,5-triene	380.3
1.2.3.4-pentatetraene448.7 $cis-1.2$ -diethynylcyclopropane544.61.2.4-triazine335.2cyanoallene618.71.3-bis(methylenc)cyclobutane222.0cyclobutaliene430.41.3-dimethylencyclo[1.1.0]butane154.6cyclobutane-1,3-dione-180.21.3-pentadiyne415.0cycloocta-1,3-dien-6-yne436.71.4-kaxadiyne-81.1cycloocta-1,5-dien-3-yne401.91.4-kaxadiyne415.6cyclopropanimine224.01.5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane234.8cyclopropylidene cyclopropane375.52-(1,1-dimethylethyl)thiarane-43.8cyclopropylidene methanone108.62-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1.s-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane306.82-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane267.72-methylhitrane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,-dimethylthitrane2.5methylcycloptane267.42-dimethylthitrane2.5methylcyclopropane26.42-cotaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,-dimethylthitrane2.5methylcyclopropane26.42,4.6-octatriyne597.2methylenecyclopropane1	1,2,3-triazine	400.5	bicyclo[4.2.0]octa-1,3,5,7-tetraene	409.4
$1,2-4$ -triazine $335.2$ cyanollene $618.7$ $1,3-dimethylbicyclo[1.1.0]$ butane $222.0$ cyclobutadiene $430.4$ $1,3-dimethylbicyclo[1.1.0]$ butane $154.6$ cyclobutadiene $-180.2$ $1,3-pentadiyne$ $415.0$ cycloocta- $1,3$ -diene- $5$ -yne $436.7$ $1,4$ -dioxin $-81.1$ cycloocta- $1,5$ -dien- $3$ -yne $401.9$ $1,4$ -hexadiyne $415.6$ cycloopentyl acetylene $169.4$ $1,5$ -dihydropentalene $234.8$ cyclopropanimine $224.0$ $1,5$ -dimethyl- $3$ -exomethylenetricyclo[ $2.1.0.0$ ]pentane $421.5$ cyclopropylidene cyclopropane $337.5$ $2^{-}(1,1-dimethyl-thylpthiirane-43.8cyclopropylidenemethanone108.02-aratirdinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1-porpen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane216.7ethylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane266.82-oxaspiro[3.3]heptane2.5methylcylop256.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthitiane2.5methylcyclopropane264.82,2-dimethylthitiane2.5methylcyclopropane26.42,3-dihydro-1H-pyrrole117.3methylmethylenecyclopropane26.4$	1,2,3,4-pentatetraene	448.7	cis-1,2-diethynylcyclopropane	544.6
1,3-bis(methylene)cyclobutane222.0cyclobutadnene430.41,3-dimethylbicyclo[1.1.0]butane154.6cyclobutane-1,3-dione-180.21,3-pentadiyne415.0cycloocta-1,3-diene-6-yne436.71,4-dioxin-81.1cycloocta-1,5-dien-3-yne401.91,4-hexadiyne415.6cyclopropaliane-3-yne401.91,4-hexadiyne234.8cyclopropaliane224.01,5-dihydropentalene234.8cyclopropylidene cyclopropane337.52-(1,1-dimethylethyl)thirane-43.8cyclopropylidene methanone108.02-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1.5-ditazabicyclo[2.1.0]pentane-86.5dithio-p-benzoquinone306.82-methyl-1.5-ditazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methyl-1.5-ditazabicyclo[3.1.0]hexane26.2heptafulvene266.82-methylhitriane26.2heptafulvene266.82-methylhitriane26.2heptafulvene266.82-oxaspiro[3.3]heptane76.9isopropyl isocyanide28.82,2-dimethylthitriane2.5methylenecyclopropane388.92,2-dihydro-1H-pyrole117.3methylencyclopropane164.52,5-dihydrofuran-60.9methylenecyclopropane66.8	1,2,4-triazine	335.2	cyanoallene	618.7
1,3-dimension production15.6cyclobutane 1,3-dime-180.21,3-pentadiyne415.0cycloocta-1,3-dine-1,3-dine436.71,4-dioxin-81.1cycloocta-1,5-dien-3-yne401.91,4-hexadiyne415.6cyclopropanimine224.01,5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane234.8cyclopropanimine224.02-(1,1-dimethylethyl)thiirane-43.8cyclopropyliden cyclopropane337.52-(1,1-dimethylethyl)thiirane-43.8cyclopropyliden explopropane108.02-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-ditinacyclopentane216.7ethylidenecyclopropane163.02-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane266.82-methylthitane26.2heptafulvene266.8266.82-waspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylencyclopropane38.92,5-dihydro-1H-pyrole117.3methylencyclopropane164.52,5-dihydrofuran-60.9methylexirane-93.82,5-dihydrofuran-60.9Methylencyclopropane64.5	1,3-bis(methylene)cyclobutane	222.0	cyclobutadiene	430.4
1,3-bentadryne410.0Cycloocta-1,5-dien-3-yne430.71,4-dioxin-81.1cycloocta-1,5-dien-3-yne401.91,4-kexadiyne415.6cyclopentyl acetylene169.41,5-dihydropentalene234.8cyclopropanimine224.01,5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane421.5cyclopropylidene cyclopropane337.52-(1,1-dimethylethyl)thirane-43.8cyclopropylidene methanone108.02-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-proten-3-yne214.7dimethylcyanamide140.72-methyl-1.propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylickene267.72-methylhiretane26.2heptafulvene266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylorecyclopropane164.52,5-dihydrofuran-60.9methylonetylenecyclopropane26.42,5-dihydrofuran-748.3N-methylaretridine93.8	1,3-dimethylbicyclo[1.1.0]butane	154.6	cyclobutane-1,3-dione	-180.2
1,4-hexadiyne15.6cyclopentyl acetylene169.41,5-dihydropentalene234.8cyclopentyl acetylene224.01,5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane421.5cyclopropylidene cyclopropane337.52-(1,1-dimethylethyl)thiirane-43.8cyclopropylidenemethanone108.02-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcynamide140.72-methyl-1,3-dithiacyclopentane-86.5dithio-p-benzoquinone306.82-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane267.72-methylhiteane26.2heptafulvene267.72-methylhiteane26.2heptafulvene266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne226.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylenecyclopropane164.52,5-dihydrofuran-60.9methylenethylenecyclopropane-93.8	1,5-pentadiyile	-81.1	cycloocta-1,5-dien-3-yne	430.7
1.5-dihydropentalene234.8cyclopropanimine224.01.5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane421.5cyclopropanimine224.01.5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane421.5cyclopropanimine337.52-(1,1-dimethylethyl)thiirane-43.8cyclopropylidene cyclopropane337.52-(1,1-dimethylethyl)thiirane269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1-propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methylhritetane26.2heptafulvene266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylenecyclopropane164.52,5-dihydrofuran-60.9methylenecyclopropane-93.82,5-dihydrofuran-60.9methylenethylenecyclopropane64.8	1.4-hexadivne	415.6	cyclopentyl acetylene	169.4
1,5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane421.5cyclopropylidene cyclopropane337.5 $2-(1,1-dimethylethyl)thiirane-43.8cyclopropylidenemethanone108.02-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1-propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methylhitetane26.2heptafulvene266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylenecyclopropane66.82,5-dihydrofuran-60.9methylenecyclopropane26.42,5-dihydrofuran-60.9methylenecyclopropane26.42,5-dihydrofuran-60.9methylenecyclopropane388.92,5-dihydrofuran-60.9methylenecyclopropane93.82,5-dihydrofuran-60.9methylenecyclopropane66.82,5-dihydrofuran-60.9methylenecyclopropane66.82,5-dihydrofuran-60.9methylenecyclopropane66.82,5-dihydrofuran-60.9methyla$	1,5-dihydropentalene	234.8	cyclopropanimine	224.0
2-(1,1-dimethylethyl)thiirane-43.8cyclopropylidenemethanone108.0 $2-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1-propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methylhinetane26.2heptafulvene266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylmetrane-60.92(3H)-furanone-248.3N-methylazetidine-93.8$	1,5-dimethyl-3-exomethylenetricyclo[2.1.0.0]pentane	421.5	cyclopropylidene cyclopropane	337.5
2-aziridinecarbonitrile269.5dihydro-2(3H)-thiophenthione65.62-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1-propen-1-one-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methylhorbornadiene199.7ethynlcyclobutane266.82-oxaspiro[3,3]heptane26.2heptafulvene266.82-oyrazoline176.9isopropyl isocyanide28.82,2-dimethylthirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylmetrane-68.82,5-dihydrofuran-60.9methylmetrane-93.8	2-(1,1-dimethylethyl)thiirane	-43.8	cyclopropylidenemethanone	108.0
2-methyl-1-penten-3-yne214.7dimethylcyanamide140.72-methyl-1-propen-1-one-86.5dimethylcyanamide140.72-methyl-1,3-dithiacyclopentane-86.5dithio-p-benzoquinone306.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methylhorbornadiene199.7ethynlcyclobutane266.82-oxaspiro[3,3]heptane26.2heptafulvene266.82-oyrazoline176.9isopropyl isocyanide28.82,2-dimethylthirane2.5methylcyclopropane26.42,4.6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylmethylenecyclopropane164.52,5-dihydrofuran-60.9methylusriane-93.8	2-aziridinecarbonitrile	269.5	dihydro-2(3H)-thiophenthione	65.6
2-inetryl-1-propert-1-one $-80.3$ $ditmo-p-berzodumone50.82-methyl-1,3-dithiacyclopentane-4.5endo-2-methylene-5-methylbicyclo[2.1.0]pentane221.12-methyl-1,5-diazabicyclo[3.1.0]hexane216.7ethylidenecyclopropane163.02-methylhorbornadiene199.7ethynlcyclobutane266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylmethylenecyclopropane164.52(3H)-furanone-248.3N-methylazetidine93.8$	2-methyl-1-penten-3-yne	214.7	dimethylcyanamide	140.7
2-methyl-1,5-diazabicyclo[3.1.0]hexane216.72-methyl-1,5-diazabicyclo[3.1.0]hexane216.72-methylhorbornadiene199.72-methylhietane26.22-oxaspiro[3,3]heptane-39.52-oxaspiro[3,3]heptane-39.52-yrazoline176.92,2-dimethylthirane26.42,2-dimethylthirane25.52,5-dihydrofuran597.22,5-dihydrofuran-60.92,5-dihydrofuran-60.92(3H)-furanone-248.3N-methylazetidine86.8	2-methyl-1-propen-1-one	-80.5	endo-2-methylene-5-methylbicyclo[2,1,0]pentane	221.1
2-methylnorbornadiene199.7ethynylcyclobutane267.72-methylhietane26.2heptafulvene266.82-oxaspiro[3,3]heptane-39.5hex-3-en-1,5-diyne526.62-pyrazoline176.9isopropyl isocyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4.6-octatriyne597.2methylenecyclopropane388.92,5-dihydrofuran-60.9methylmethylenecyclopropane164.52,5-dihydrofuran-248.3N-methylazetidine86.8	2-methyl-1,5-diazabicyclo[3,1,0]hexane	216.7	ethylidenecyclopropane	163.0
2-methylthietane $26.2$ heptafulvene $266.8$ 2-oxaspiro[3,3]heptane $-39.5$ hex-3-en-1,5-diyne $526.6$ 2-pyrazoline $176.9$ isopropyl isozyanide $28.8$ 2,2-dimethylthiirane $2.5$ methylcyclopropane $26.4$ 2,4,6-octatriyne $597.2$ methylenecyclopropene $388.9$ 2,5-dihydro-1H-pyrrole $117.3$ methylmethylenecyclopropane $164.5$ 2,5-dihydrofuran $-60.9$ methyloxirane $-93.8$ $2(3H)$ -furanone $-248.3$ N-methylazetidine $86.8$	2-methylnorbornadiene	199.7	ethynylcyclobutane	267.7
2-oxaspiro[3,3]heptane $-39.5$ hex-3-en-1,5-diyne $526.6$ 2-pyrazoline176.9isopropyl isozyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4,6-octatriyne597.2methylenecyclopropene388.92,5-dihydro-1H-pyrrole117.3methylmethylenecyclopropane164.52,5-dihydrofuran-60.9methyloxirane-93.8 $2(3H)$ -furanone-248.3N-methylazetidine86.8	2-methylthietane	26.2	heptafulvene	266.8
2-pyrazoline176.9isopropyl isozyanide28.82,2-dimethylthiirane2.5methylcyclopropane26.42,4.6-octatriyne597.2methylenecyclopropene388.92,5-dihydro-1H-pyrrole117.3methylmethylenecyclopropane164.52,5-dihydrofuran-60.9methyloxirane-93.82(3H)-furanone-248.3N-methylazetidine86.8	2-oxaspiro[3,3]heptane	-39.5	hex-3-en-1,5-diyne	526.6
2.2-dimethylthiirane2.5methylcyclopropane26.42.4,6-octatriyne597.2methylenecyclopropene388.92,5-dihydro-1H-pyrrole117.3methylmethylenecyclopropane164.52,5-dihydrofuran-60.9methyloxirane-93.82(3H)-furanone-248.3N-methylazetidine86.8	2-pyrazoline	176.9	isopropyl isocyanide	28.8
2,4,6-octatryne597.2methylenecyclopropete588.92,5-dihydro-1H-pyrrole117.3methylmethylenecyclopropane164.52,5-dihydrofuran-60.9methyloxirane-93.82(3H)-furanone-248.3N-methylazetidine86.8	2,2-dimethylthiirane	2.5	methylcyclopropane	26.4
2,5-dihydrofuran $-60.9$ methyloxirane $-93.8$ $2(3H)$ -furanone $-248.3$ N-methylozetidine $86.8$	2,4,0-0ctatriyile	397.2 117 3	methylmethylenecyclopropane	500.9 164 5
-2483 N-methylazetidine 868	2,5-dihydrofuran	-60.9	methyloxirane	-93.8
	2(3 <i>H</i> )-furanone	-248.3	<i>N</i> -methylazetidine	86.8
2a,2b,4a,4b-tetrahydrocyclopropa[cd]pentalene 303.7 penta-1,4-diyne 455.4	2a,2b,4a,4b-tetrahydrocyclopropa[cd]pentalene	303.7	penta-1,4-diyne	455.4
3-methyl-1,2-dithiolane -12.3 pentacyclo[3.3.0.0 <sup>2,4</sup> .0 <sup>3,7</sup> .0 <sup>6,8</sup> ]octane 445.6	3-methyl-1,2-dithiolane	-12.3	pentacyclo[3.3.0.0 <sup>2,4</sup> .0 <sup>3,7</sup> .0 <sup>6,8</sup> ]octane	445.6
3-methyl-1,2,4-triazine 286.9 pyrrole-2-carbonitrile 237.8	3-methyl-1,2,4-triazine	286.9	pyrrole-2-carbonitrile	237.8
3-methyleneoxetane 22.9 spiro[3.3]hepta-2,5-diene 365.8	3-methyleneoxetane $1 12 2 0 0^{27} 0^{461}$	22.9	spiro[3.3]hepta-2,5-diene	365.8
$\frac{1}{2}$ methyleneteracyclo[3.2.0.0 <sup></sup> .0 <sup></sup> ]neptane $\frac{1}{2}$ (3.2.0 <sup></sup> ) $\frac{1}{2}$ (3.2.0 <sup></sup>	3-methylenetetracycio[3.2.0.0 <sup>27</sup> .0 <sup>47</sup> .0 <sup>47</sup> .0 <sup>47</sup> .0 <sup>47</sup>	429.1	syn-tricyclo[3.2.0.0 <sup>2,4</sup> ]heptane	2/0.0
3 3-dimethylocylobutene 97 3 thieno(2 3-bliophene 214 1	3 3-dimethylcyclobutene	97.3	thieno[2 3-b]thionhene	214.1
3.3-dimethylevelopropene 220.7 thieno[3.2-b]thiphophene 20.1	3.3-dimethylcyclopropene	220.7	thieno[3,2-b]thiophene	206.1
3,3-dimethyldiaziridine 148.1 thiono[3,4-b]thiophene 225.0	3,3-dimethyldiaziridine	148.1	thieno[3,4-b]thiophene	225.0
3,3-dimethyldiazirine 231.3 <i>trans</i> -1,2-diethynylcyclopropane 540.7	3,3-dimethyldiazirine	231.3	trans-1,2-diethynylcyclopropane	540.7
3,3-dimethylthietane $-9.2$ tricyclo[3.1.0.0 <sup>2.6</sup> ]hexane 229.3	3,3-dimethylthietane	-9.2	tricyclo[3.1.0.0 <sup>2,6</sup> ]hexane	229.3
-205.9 tricyclo[3.1.1.0 <sup>5,0</sup> ]heptane 233.9	3(2 <i>H</i> )-furanone	-205.9	tricyclo $[3.1.1.0^{3,0}]$ heptane	233.9
4-aminopyrimidine $152.7$ tricyclo[4.1.0.0 <sup>1,2</sup> ]heptane 241.6 4-motbyl 1.2 dithiolone $-9.9$ tricyclo[4.1.0.0 <sup>2</sup> /lbort 2 and 212.5	4-aminopyrimidine	152.7	tricyclo[4.1.0.0 <sup>+,7</sup> ]heptane tricyclo[4.1.0.0 <sup>2,7</sup> ]hepta.2 are	241.6
-6.6 tricyclo[4.1.0.0 <sup>-7</sup> ] nept-5-ene 312.5 4-methyl-1.2.3-triazine $354.4$ tricyclo[4.1.0.0 <sup>-7</sup> ] nept-5-ene 305.0	4-methyl-1,2-utilioialle 4-methyl-1,2-3-triazine	-0.8 354 4	tricyclo[4.1.0.0 ] JIept-5-ene	312.3 305 Q
4-methyl-1.3-dithiolane $-2.7$ tricyclo[4.1.10 jpct-2-ene 303.9	4-methyl-1.3-dithiolane	-2.7	tricyclo[4.1.1.0 <sup>7,8</sup> ]oct-3-ene	307.1
4-methyl-3 <i>H</i> -1,2-dithiole-3-thione 149.4 tricvclo[4.1.1.0 <sup>7,8</sup> ]octa-2,4-diene 407.8	4-methyl-3 <i>H</i> -1,2-dithiole-3-thione	149.4	tricyclo[4.1.1.0 <sup>7,8</sup> ]octa-2,4-diene	407.8
4-methylene-1,3-dioxolane -222.9 trimethylthiirane -28.6	4-methylene-1,3-dioxolane	-222.9	trimethylthiirane	-28.6
4-methylimidazole 92.6 $\alpha$ -trimethylethylene oxide -173.6	4-methylimidazole	92.6	α-trimethylethylene oxide	-173.6

agreement between the G4 and the experimental  $\Delta_f H^{\circ}_{(g)}$  was observed, yielding the MSD<sub>best</sub>/MAD<sub>best</sub>/rmsd<sub>best</sub> of (-2.1, 6.8, and 12.1) kJ·mol<sup>-1</sup>, respectively, and the MSD<sub>worst</sub>/MAD<sub>worst</sub>/

rmsd<sub>worst</sub> of (-4.3, 14.0, and 27.5) kJ·mol, respectively. Molecular weight scaling errors in  $\Delta_t H^{o}_{(g)}$  estimates were not observed using either MSD<sub>best</sub>/MSD<sub>worst</sub> (SI, Figure S1a,b) or

MAD<sub>best</sub>/MAD<sub>worst</sub> (SI, Figure S2a,b) and the G4 method but are evident at the W1BD level of theory using MSD<sub>best</sub> (SI, Figure S1c) and MAD<sub>best</sub>/MAD<sub>worst</sub> (SI, Figure S2c,d), but not MSD<sub>worst</sub> (SI, Figure S1d). However, the large degree of scatter and poor quality of fit in the relationship between the minimum and the maximum signed and unsigned  $\Delta_{f}H^{\circ}_{(g)}$  errors and molecular weight for the W1BD method preclude the development of a reliable correction factor that can be applied to estimated  $\Delta_{f}H^{\circ}_{(g)}$  values.

Large numbers of conceptually interesting and/or industrially relevant organic compounds also have no experimental  $\Delta_f H^{\circ}_{(g)}$ reports nor any theoretical estimates (particularly at high levels of theory) in the literature. G4 calculations were also completed on 138 of these molecules (Table 3), which is intended to serve as a comparative database for researchers performing future experimental  $\Delta_f H^{\circ}_{(g)}$  determinations, as well as those interested in thermochemical modeling of various processes and fundamental structure—property studies such as molecular strain and geometry relationships.

#### Conclusions

The gas-phase standard state (298.15 K, 1.01325 bar) enthalpies of formation ( $\Delta_{\rm f}H^{\circ}_{\rm (g)}$ ) were calculated at the G4 and W1BD levels of theory for a set of 54 nonconformationally complex small organic compounds, as well as G4 calculations for an additional suite of 121 larger compounds. Good agreement with experimental data was obtained. For compounds having a broad range of experimental  $\Delta_{\rm f}H^{\circ}_{\rm (g)}$  reports, the high level  $\Delta_{\rm f}H^{\circ}_{\rm (g)}$  estimates may help resolve which experimental values are more accurate. G4 calculations were also completed on 138 molecules without experimental  $\Delta_{\rm f}H^{\circ}_{\rm (g)}$  measurements, thereby providing a theoretically rigorous thermochemical and structural database for future thermodynamic studies.

## **Supporting Information Available:**

Optimized geometries, energies at each stage of the optimization process, and frequency coordinates for all compounds investigated, as well as available experimental enthalpies of formation. This material is available free of charge via the Internet at http:// pubs.acs.org.

### Literature Cited

- Cramer, C. J. Essentials of computational chemistry: Theories and models; Wiley: New York, 2004.
- (2) Brown, M. E.; Gallagher, P. K. Handbook of thermal analysis and calorimetry: Recent advances, techniques and applications; Elsevier: New York, 2007.
- (3) Curtiss, L. A.; Jones, C.; Trucks, G. W.; Raghavachari, K.; Pople, J. A. Gaussian-1 theory of molecular energies for second-row compounds. J. Chem. Phys. **1990**, 93, 2537–2545.
- (4) Pople, J. A.; Head-Gordon, M.; Fox, D. J.; Raghavachari, K.; Curtiss, L. A. Gaussian-1 theory: A general procedure for prediction of molecular energies. J. Chem. Phys. 1989, 90, 5622–5629.
- (5) Curtiss, L. A.; Raghavachari, K.; Trucks, G. W.; Pople, J. A. Gaussian-2 theory for molecular energies of first- and second-row compounds. J. Chem. Phys. **1991**, 94, 7221–7230.
- (6) Curtiss, L. A.; Raghavachari, K.; Pople, J. A. Gaussian-2 theory using reduced Moller-Plesset orders. J. Chem. Phys. 1993, 98, 1293–1298.
- (7) Curtiss, L. A.; Raghavachari, K.; Redfern, P. C.; Rassolov, V.; Pople, J. A. Gaussian-3 (G3) theory for molecules containing first and secondrow atoms. J. Chem. Phys. **1998**, 109, 7764–7776.
- (8) Baboul, A. G.; Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Gaussian-3 theory using density functional geometries and zero-point energies. J. Chem. Phys. 1999, 110, 7650–7657.
- (9) Curtiss, L. A.; Redfern, P. C.; Raghavachari, K.; Rassolov, V.; Pople, J. A. Gaussian-3 theory using reduced Moller-Plesset order. *J. Chem. Phys.* **1999**, *110*, 4703–4709.
- (10) Curtiss, L. A.; Raghavachari, K.; Redfern, P. C.; Pople, J. A. Assessment of Gaussian-2 and density functional theories for the computation of enthalpies of formation. J. Chem. Phys. **1997**, 106, 1063–1079.

- (11) Curtiss, L. A.; Raghavachari, K.; Redfern, P. C.; Pople, J. A. Assessment of Gaussian-3 and density functional theories for a larger experimental test set. J. Chem. Phys. 2000, 112, 7374–7383.
- (12) Bond, D. Computational methods in organic thermochemistry. 1. Hydrocarbon enthalpies and free energies of formation. J. Org. Chem. 2007, 72, 5555–5566.
- (13) Bond, D. Computational methods in organic thermochemistry. 2. Enthalpies and free energies of formation for functional derivatives of organic hydrocarbons. J. Org. Chem. 2007, 72, 7313–7328.
- (14) Bond, D. Computational methods in organic chemistry. 3. Correction of computed enthalpies for multiple conformations. J. Phys. Chem. A 2008, 112, 1656–1660.
- (15) Nicolaides, A.; Radom, L. An evaluation of the performance of G2, G2(MP2) and G2(MP2, SVP) theories for heats of formation and heats of reaction in the case of "large" hydrocarbons. *Mol. Phys.* **1996**, *88*, 759–765.
- (16) Notario, R.; Castano, O.; Abboud, J. L. M.; Gomperts, R.; Frutos, L. M.; Palmeiro, R. Organic thermochemistry at high ab initio levels. 1. A G2(MP2) and G2 study of cyclic saturated and unsaturated hydrocarbons (including aromatics). J. Org. Chem. **1999**, 64, 9011– 9014.
- (17) Notario, R.; Castano, O.; Gomperts, R.; Frutos, L. M.; Palmeiro, R. Organic thermochemistry at high ab initio levels. 3. A G3 study of cyclic saturated and unsaturated hydrocarbons (including aromatics). *J. Org. Chem.* **2000**, *65*, 4298–4302.
- (18) Redfern, P. C.; Zapol, P.; Curtiss, L. A.; Raghavachari, K. Assessment of Gaussian-3 and density functional theories for enthalpies of formation of C<sub>1</sub>-C<sub>16</sub> alkanes. J. Phys. Chem. A 2000, 104, 5850–5854.
- (19) Haworth, N. L.; Smith, M. H.; Bacskay, G. B.; Mackie, J. C. Heats of formation of hydrofluorocarbons obtained by Gaussian-3 and related quantum chemical computations. *J. Phys. Chem. A* 2000, *104*, 7600– 7611.
- (20) Gomes, J. R. B.; Ribeiro da Silva, M. A. V. Thermochemistry of small organosulfur compounds from ab initio calculations. J. Phys. Chem. A 2004, 108, 11684–11690.
- (21) Blanquart, G.; Pitsch, H. Thermochemical properties of polycyclic aromatic hydrocarbons (PAH) from G3MP2B3 calculations. J. Phys. Chem. A 2007, 111, 6510–6520.
- (22) Taskinen, E.; Taskinen, A. Proximity effects of oxygen atoms on the enthalpies of formation of simple diethers: A computational G3(MP2)// B3 study. J. Phys. Org. Chem. 2008, 21, 449–456.
- (23) Taskinen, E. Enthalpies of formation and isomerization of aromatic hydrocarbons and ethers by G3(MP2)//B3LYP calculations. J. Phys. Org. Chem. 2009, 22, 632–642.
- (24) Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Gaussian-4 theory. J. Chem. Phys. 2007, 126, 84108–84112.
- (25) Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Gaussian-4 theory using reduced order perturbation theory. J. Chem. Phys. 2007, 127, 124105–124108.
- (26) Rayne, S.; Forest, K. Gas phase isomerization enthalpies of organic compounds: A semiempirical, density functional theory, and ab initio post-Hartree-Fock theoretical study. J. Mol. Struct.: THEOCHEM 2010, 948, 102–107.
- (27) Rayne, S.; Forest, K. Computational note on a G4MP2 study into the gas phase enthalpies of formation and isomerization for the  $(CH)_{2n}$  (n = 1-6) isomers. *J. Mol. Struct.: THEOCHEM* **2010**, *948*, 111–112.
- (28) Rayne, S.; Forest, K. Performance of Gaussian-3 and Gaussian-4 level theoretical methods in estimating gas phase enthalpies of formation for representative C<sub>1</sub> and C<sub>2</sub> chlorofluorocarbons and hydrochlorofluorocarbons. J. Mol. Struct.: THEOCHEM 2010, 953, 47–48.
- (29) Rayne, S.; Forest, K. Gas-phase enthalpies of formation, acidities, and strain energies of the [m,n] polyprismanes ( $m \ge 2$ ; n = 3-8;  $m \times n \le 16$ ): A CBS-Q//B3, G4MP2, and G4 theoretical study. *Theor. Chem. Acc.* **2010**; 10.1007/s00214-010-0780-0.
- (30) Dorofeeva, O. V.; Ryzhova, O. N. Enthalpies of formation of β-alanine, sarcosine, and 4-aminobutanoic acid from quantum chemical calculations. J. Chem. Thermodyn. 2010, 42, 1056–1062.
- (31) Mayhall, N. J.; Raghavachari, K.; Redfern, P. C.; Curtiss, L. A. Investigation of Gaussian-4 theory for transition metal thermochemistry. J. Phys. Chem. A 2009, 113, 5170–5175.
- (32) Martin, J. M. L.; de Oliveira, G. Towards standard methods for benchmark quality ab initio thermochemistry - W1 and W2 theory. *J. Chem. Phys.* **1999**, *111*, 1843–1856.
- (33) Parthiban, S.; Martin, J. M. L. Assessment of W1 and W2 theories for the computation of electron affinities, ionization potentials, heats of formation, and proton affinities. *J. Chem. Phys.* 2001, 114, 6014– 6029.
- (34) Barnes, E. C.; Petersson, G. A.; Montgomery, J. A.; Frisch, M. J.; Martin, J. M. L. Unrestricted coupled cluster and Brueckner doubles variations of W1 theory. *J. Chem. Theory Comput.* **2009**, *5*, 2687–2693.
- (35) Afeefy, H. Y.; Liebman, J. F.; Stein, S. E. In NIST Chemistry WebBook, NIST standard reference database number 69; Linstrom, P. J., Mallard,

W. G., Eds.; National Institute of Standards and Technology: Gaithersburg, MD, 2010; http://webbook.nist.gov (accessed July 6, 2010).

- (36) Halgren, T. A. Merck molecular force field. I. Basis, form, scope, parameterization, and performance of MMFF94. J. Comput. Chem. 1996, 17, 490–519.
- (37) Halgren, T. A. Merck molecular force field. III. Molecular geometries and vibrational frequencies for MMFF94. J. Comput. Chem. 1996, 17, 553–586.
- (38) Halgren, T. A. Merck molecular force field. V. Extension of MMFF94 using experimental data, additional computational data, and empirical rules. J. Comput. Chem. 1996, 17, 616–641.
- (39) Halgren, T. A. MMFF VII. Characterization of MMFF94, MMFF94s, and other widely available force fields for conformational energies and for intermolecular-interaction energies and geometries. J. Comput. Chem. 1999, 20, 730–748.
- (40) Halgren, T. A.; Nachbar, R. B. Merck molecular force field. IV. Conformational energies and geometries for MMFF94. J. Comput. Chem. 1996, 17, 587–615.
- (41) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.;

Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J. *Gaussian 09, Revision A.02*; Gaussian, Inc.: Wallingford, CT, 2009.

- (42) Allouche, A. R. Gabedit: A graphical user interface for computational chemistry softwares. J. Comput. Chem. 2010; 10.1002/jcc.21600.
- (43) Saeys, M.; Reyniers, M. F.; Marin, G. B.; Van Speybroeck, V.; Waroquier, M. Ab initio calculations for hydrocarbons: Enthalpy of formation, transition state geometry, and activation energy for radical reactions. J. Phys. Chem. A 2003, 107, 9147–9159.
- (44) van Speybroeck, V.; Gani, R.; Meier, R. J. The calculation of thermodynamic properties of molecules. *Chem. Soc. Rev.* 2010, 39, 1764–1779.
- (45) Cox, J. D.; Wagman, D. D.; Medvedev, V. A. CODATA key values for thermodynamics; Hemisphere: New York, NY, 1984.

Received for review July 24, 2010. Accepted September 25, 2010. This work was made possible by the facilities of the Western Canada Research Grid (WestGrid: http://www.westgrid.ca; project 100185), the Shared Hierarchical Academic Research Computing Network (SHARCNET: http://www.sharcnet.ca; project aqn-965), and Compute/ Calcul Canada.

JE100768S