

# SUPPLEMENTARY INFORMATION

## Experimental and theoretical investigation on the thermochemistry of 3-methyl-2-benzoxazolinone and 6-nitro-2-benzoxazolinone

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This supplementary information includes:

- data of all the combustion calorimetry experiments of 3-methyl-2-benzoxazolinone and 6-nitro-2-benzoxazolinone (**Tables S1 and S2**);
- the values of standard molar heat capacities in the gaseous phase for the compounds studied (**Tables S3 and S4**);
- optimized geometries of 2-benzoxazolinone derivatives, calculated at the B3LYP/6-31G(d) level of theory (**Figure S1**);
- Gas-phase hypothetical reactions and corresponding values for the enthalpies of reaction and formation, in the gaseous phase, at  $T = 298.15$  K for 3-methyl-2-benzoxazolinone, 6-nitro-2-benzoxazolinone and 2-benzoxazolinone (**Tables S5-S7**);
- G3MP2B3 calculated absolute enthalpies, at  $T = 298.15$  K, and experimental gas-phase values for all the molecules used (**Table S8**);
- Harmonic vibrational frequencies for 2-benzoxazolinone, 3-methyl-2-benzoxazolinone and 6-nitro-2-benzoxazolinone (**Table S9**).

### Acronyms used throughout this supplementary data:

**3MBOA** for 3-methyl-2-benzoxazolinone

**6NBOA** for 6-nitro-2(3*H*)benzoxazolone

### Combustion Calorimetry:

- The calibration experiments were made in an oxygen atmosphere at  $p = 3.04$  MPa, with  $1.00\text{ cm}^3$  of deionized water added to the bomb; the energy equivalent of the calorimeter was determined from the combustion of benzoic acid (NIST SRM 39j) having a massic energy of combustion, under standard bomb conditions, of  $-(26434 \pm 3)\text{ J}\cdot\text{g}^{-1}$ . From six calibration experiments  $\varepsilon_{\text{cal}} = (16002.6 \pm 1.7)\text{ J}\cdot\text{K}^{-1}$ , for an average mass of water added to the calorimeter of  $3119.6\text{ g}$ ; the mentioned uncertainty is the standard deviation of the mean.
- Samples of both compounds were burnt in pellet form, under oxygen at  $p = 3.04$  MPa, with  $1.00\text{ cm}^3$  of deionised water added to the bomb; in the experiments of 6NBOA, a small amount of n-hexadecane (auxiliary of combustion) was used.
- n-Hexadecane (Aldrich, mass fraction  $> 0.999$ ), stored under nitrogen was used as auxiliary combustion. The massic energy of combustion of the sample used, was determined in our laboratory as  $\Delta_c u^\circ = -(47136.7 \pm 2.3)\text{ J}\cdot\text{g}^{-1}$ .
- The cotton thread fuse (empirical formula:  $\text{CH}_{1.686}\text{O}_{0.843}$ ) had a standard massic energy of combustion [S1],  $\Delta_c u^\circ = -16240\text{ J}\cdot\text{g}^{-1}$ ;
- The ignition energy was determined from the change in potential difference on discharge of a  $1400\text{ }\mu\text{F}$  condenser across a platinum wire.
- Pressure coefficient of specific energy  $(\partial u/\partial p)_T = -0.2\text{ J}\cdot\text{g}^{-1}\cdot\text{MPa}^{-1}$  (typical value for organic compounds [S2]).
- The nitric acid formed in the calorimetric experiments was determined using Devarda's alloy method [S3] and the energy correction for the formation of  $0.1\text{ mol}\cdot\text{dm}^{-3}\text{ HNO}_3(\text{aq})$  [S4] from  $\text{N}_2(\text{g})$ ,  $\text{O}_2(\text{g})$  and  $\text{H}_2\text{O}(\text{l})$  was based on  $-59.7\text{ kJ}\cdot\text{mol}^{-1}$ .
- Corrections for carbon formation relied on the standard massic energy of combustion of carbon [S5],  $\Delta_c u^\circ = -32.76\text{ kJ}\cdot\text{g}^{-1}$ .
- The calorimeter temperatures were measured to  $\pm(1\times 10^{-4})\text{ K}$ , at time intervals of  $10\text{ s}$ , with a quartz crystal thermometer (Hewlett-Packard HP 2804 A), interfaced to a PC; the ignition occurs at  $T = (298.150 \pm 0.001)\text{ K}$ .
- Specific density of the studied compounds at  $T = 298.15\text{ K}$ :  
 $\rho = 1.0831\text{ g}\cdot\text{cm}^{-3}$  for 3MBOA [S6] and  $\rho = 1.58\text{ g}\cdot\text{cm}^{-3}$  for 6NBOA [S7].
- The massic heat capacities, at  $T = 298.15\text{ K}$ , were calculated as  $1.245\text{ J}\cdot\text{K}^{-1}\cdot\text{g}^{-1}$  for 3MBOA and as  $1.097\text{ J}\cdot\text{K}^{-1}\cdot\text{g}^{-1}$  for 6NBOA, using Kopp's rule [S8].

**Table S1.** Standard ( $p^\circ = 0.1$  MPa) mass energy of combustion of crystalline **3MBOA**, at  $T = 298.15$  K.

$m(\text{CO}_2, \text{total}) / \text{g}$	1.44346	1.42080	1.77570	1.44647	1.52305	1.50243
$m(\text{cpd}) / \text{g}$	0.60941	0.59983	0.75045	0.61080	0.64339	0.63460
$m(\text{fuse}) / \text{g}$	0.00301	0.00298	0.00257	0.00284	0.00262	0.00270
$T_i / \text{K}$	298.1504	298.1514	298.1592	298.1524	298.1512	298.1507
$T_f / \text{K}$	299.2100	299.1984	299.4260	299.2116	299.2640	299.2570
$\Delta T_{\text{ad}} / \text{K}$	0.98107	0.96581	1.20624	0.98357	1.03534	1.02109
$\varepsilon_i / (\text{J} \cdot \text{K}^{-1})$	15.27	15.26	15.43	15.27	15.31	15.30
$\varepsilon_f / (\text{J} \cdot \text{K}^{-1})$	15.67	15.58	15.97	15.65	15.66	15.68
$-\Delta U(\text{IBP}) / \text{J}$	15713.90	15469.82	19321.53	15754.06	16583.72	16355.35
$\Delta U(\text{HNO}_3) / \text{J}$	27.22	33.73	29.25	28.84	35.58	31.46
$\Delta U(\text{ign}) / \text{J}$	1.15	0.70	0.71	1.02	0.63	0.76
$\Delta U_\Sigma / \text{J}$	12.00	11.76	15.07	12.02	12.69	12.52
$-\Delta U(\text{fuse}) / \text{J}$	48.88	48.40	41.74	46.12	42.55	43.85
$-\Delta_c u^\circ / (\text{J} \cdot \text{g}^{-1})$	25640.85	25633.74	25631.77	25649.99	25634.31	25634.21
$\% \text{ CO}_2 = (100.008 \pm 0.001)^a$						
$-\langle \Delta_c u^\circ \rangle = (25637.48 \pm 6.86) \text{ J} \cdot \text{g}^{-1}^a$						

$m(\text{CO}_2, \text{total})$  is the total mass of  $\text{CO}_2$  recovered in the experiment;  $m(\text{cpd})$  is the mass of compound burnt in each experiment;  $m(\text{fuse})$  is the mass of fuse (cotton) used in each experiment;  $T_i$  is the initial temperature rise;  $T_f$  is the final temperature rise;  $\Delta T_{\text{ad}}$  is the corrected temperature rise;  $\varepsilon_i$  and  $\varepsilon_f$  are the energy equivalents of contents in the initial and final states, respectively;  $\Delta U(\text{IBP})$  is the energy change for the isothermal combustion reaction under actual bomb conditions and includes  $\Delta U(\text{ign})$ ;  $\Delta U(\text{HNO}_3)$  is the energy correction for the nitric acid formation;  $\Delta U(\text{ign})$  is the electrical energy for ignition;  $\Delta U_\Sigma$  is the standard state correction;  $\Delta U(\text{fuse})$  is the energy of combustion of the fuse (cotton);  $\Delta_c u^\circ$  is the standard massic energy of combustion. <sup>a</sup> Mean value and standard deviation of the six experiments.

**Table S2.** Standard ( $p^\circ = 0.1$  MPa) mass energy of combustion of crystalline **6NBOA**, at  $T = 298.15$  K.

$m(\text{CO}_2, \text{total}) / \text{g}$	1.06543	1.31205	1.02819	1.28084	1.26352	1.26658
$m(\text{cpd}) / \text{g}$	0.62026	0.51303	0.52849	0.52977	0.51087	0.52546
$m(\text{fuse}) / \text{g}$	0.00281	0.00265	0.00301	0.00302	0.00291	0.0019
$m(\text{n-hexadec.}) / \text{g}$	—	0.13837	0.03899	0.11927	0.12417	0.11731
$T_i / \text{K}$	298.1506	298.1514	298.1506	298.1509	298.1513	298.1506
$T_f / \text{K}$	298.8918	299.1725	298.9076	299.1394	299.1308	299.125
$\Delta T_{\text{ad}} / \text{K}$	0.64406	0.94067	0.66342	0.90169	0.89586	0.89061
$\varepsilon_i / (\text{J} \cdot \text{K}^{-1})$	15.20	15.39	14.91	15.37	15.36	15.08
$\varepsilon_f / (\text{J} \cdot \text{K}^{-1})$	15.23	15.74	15.00	15.68	15.69	15.38
$-\Delta U(\text{IBP}) / \text{J}$	10315.53	15067.22	10625.74	14443.04	14349.52	14264.63
$\Delta U(\text{HNO}_3) / \text{J}$	27.34	35.58	29.31	34.15	32.48	33.49
$\Delta U(\text{ign}) / \text{J}$	0.91	0.75	0.66	0.48	0.63	1.14
$\Delta U_{\Sigma} / \text{J}$	12.32	11.79	10.88	11.91	11.57	11.78
$\Delta U(\text{carb.}) / \text{J}$	—	—	16.50	9.24	9.90	—
$-\Delta U(\text{n-hexadec.}) / \text{J}$	—	6522.37	1837.78	5621.89	5853.14	5529.38
$-\Delta U(\text{fuse}) / \text{J}$	45.63	43.04	48.88	49.04	47.26	30.86
$-\Delta_c u^\circ / (\text{J} \cdot \text{g}^{-1})$	16493.48	16479.43	16491.11	16488.84	16471.83	16479.13

$$\% \text{ CO}_2 = (100.06 \pm 0.02)^b$$

$$-\langle \Delta_c u^\circ \rangle = (16483.97 \pm 3.45) \text{ J} \cdot \text{g}^{-1}{}^b$$

$m(\text{CO}_2, \text{total})$  is the total mass of  $\text{CO}_2$  recovered in the experiment;  $m(\text{cpd})$  is the mass of compound burnt in each experiment;  $m(\text{fuse})$  is the mass of fuse (cotton) used in each experiment;  $m(\text{n-hexadec.})$  is the mass of n-hexadecane used in each experiment;  $T_i$  and  $T_f$  are the initial and final temperatures rise, respectively;  $\Delta T_{\text{ad}}$  is the corrected temperature rise;  $\varepsilon_i$  and  $\varepsilon_f$  are the energy equivalents of contents in the initial and final states, respectively;  $\Delta U(\text{IBP})$  is the energy change for the isothermal combustion reaction under actual bomb conditions and includes  $\Delta U(\text{ign})$ ;  $\Delta U(\text{HNO}_3)$  is the energy correction for the nitric acid formation;  $\Delta U(\text{ign})$  is the electrical energy for ignition;  $\Delta U_{\Sigma}$  is the standard state correction;  $\Delta U(\text{carb.})$  is the correction energy for carbon soot formation;  $\Delta U(\text{n-hexadec.})$  is the energy of combustion of the n-hexadecane;  $\Delta U(\text{fuse})$  is the energy of combustion of the fuse (cotton);  $\Delta_c u^\circ$  is the standard massic energy of combustion.<sup>a</sup> Mean value and standard deviation of the mean.

**Table S3.** Standard ( $p^\circ = 0.1$  MPa) molar heat capacities in the gaseous phase for **3MBOA** .

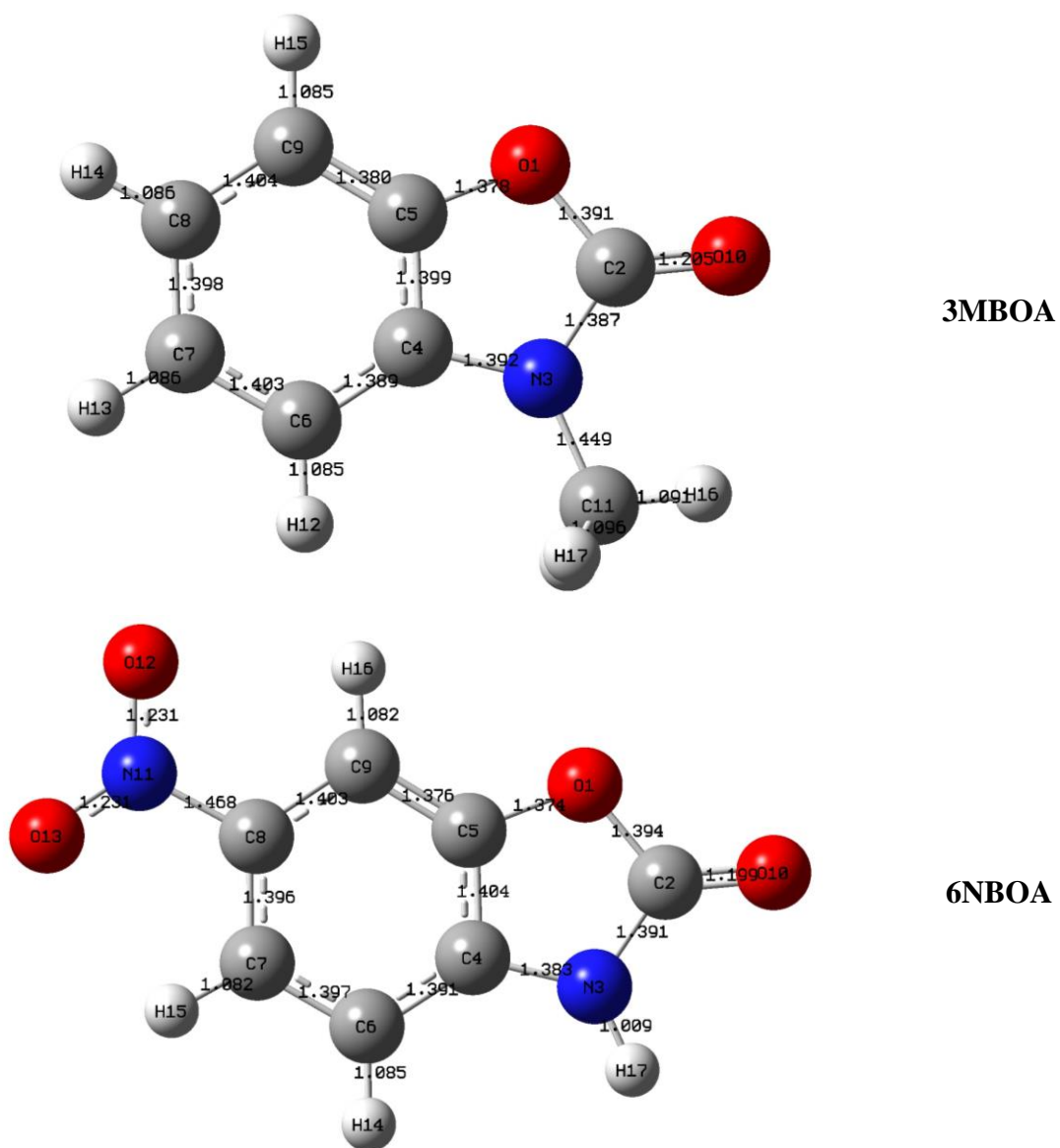
$T / \text{K}$	$C_{p, \text{m}}^\circ (\text{g}) / (\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1})$
150	84.72
200	106.70
250	129.97
298.15	152.58
300	153.44
350	176.09
400	197.25
450	216.59
500	234.06
550	249.73

$$C_{p, \text{m}}^\circ (\text{g}) = -6.769 \times 10^{-7} T^3 + 4.907 \times 10^{-4} T^2 + 3.449 \times 10^{-1} T + 23.94$$

**Table S4.** Standard ( $p^\circ = 0.1$  MPa) molar heat capacities in the gaseous phase for **6NBOA** .

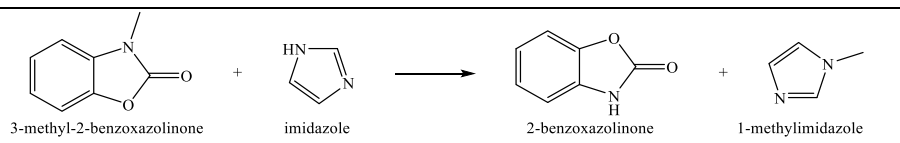
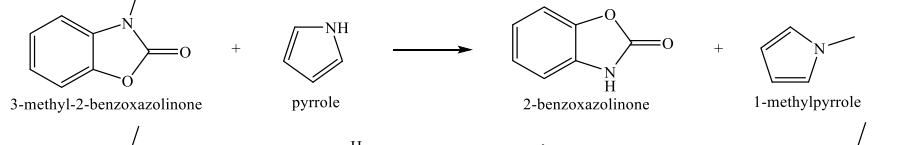
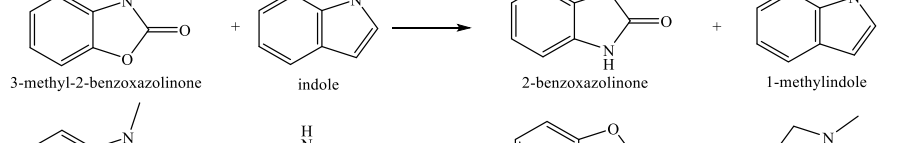
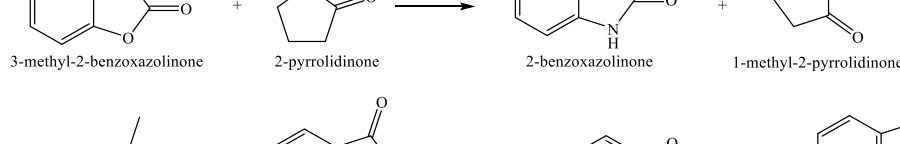
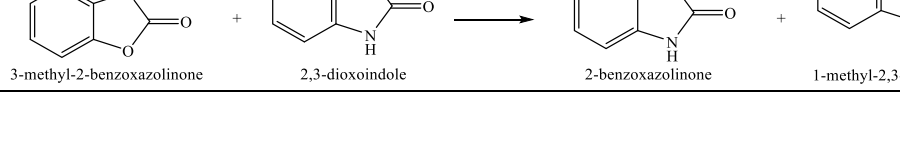
$T / \text{K}$	$C_{p, \text{m}}^\circ (\text{g}) / (\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1})$
300	167.55
350	190.26
400	210.83
450	229.21
500	245.46
550	259.79
600	272.42
650	283.57
700	293.44

$$C_{p, \text{m}}^\circ (\text{g}) = 2.249 \times 10^{-7} T^3 - 7.113 \times 10^{-4} T^2 + 8.484 \times 10^{-1} T - 29.07$$



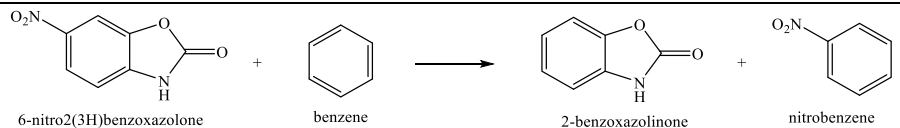
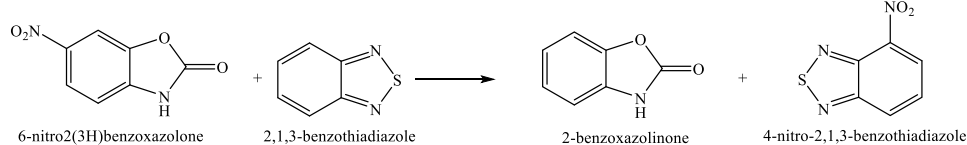
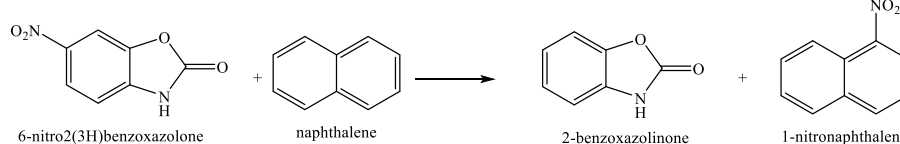
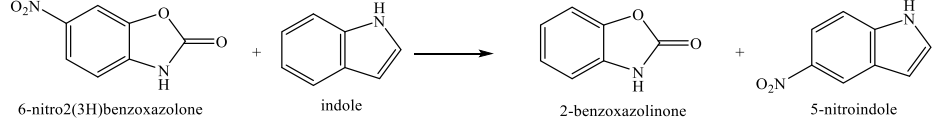
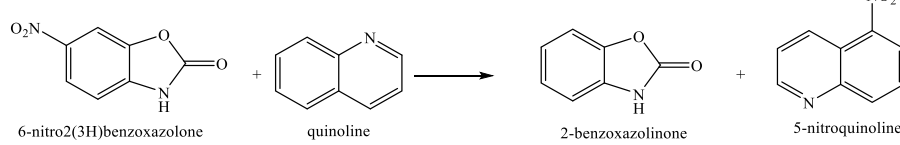
**Figure S1.** Molecular structure of the compounds studied in the gaseous phase, optimized by B3LYP/6-31G(d) level of theory, with the corresponding calculated bond distances ( $10^{-10}$  m).

**Table S5.** Gas-phase hypothetical reactions for **3MBOA** and corresponding values for the enthalpies of reaction  $\Delta_r H_m^\circ$ , and formation,  $\Delta_f H_m^\circ$ , in the gaseous phase, at  $T = 298.15$  K (values in  $\text{kJ}\cdot\text{mol}^{-1}$ ).

Gas-phase hypothetical reactions	Eq.	$\Delta_r H_m^\circ$	$\Delta_f H_m^\circ$
 <p>3-methyl-2-benzoxazolinone + imidazole <math>\longrightarrow</math> 2-benzoxazolinone + 1-methylimidazole</p>	I	10.10	-236.3
 <p>3-methyl-2-benzoxazolinone + pyrrole <math>\longrightarrow</math> 2-benzoxazolinone + 1-methylpyrrole</p>	II	11.46	-235.8
 <p>3-methyl-2-benzoxazolinone + indole <math>\longrightarrow</math> 2-benzoxazolinone + 1-methylindole</p>	III	7.83	-235.3
 <p>3-methyl-2-benzoxazolinone + 2-pyrrolidinone <math>\longrightarrow</math> 2-benzoxazolinone + 1-methyl-2-pyrrolidinone</p>	IV	3.78	-236.2
 <p>3-methyl-2-benzoxazolinone + 2,3-dioxindole <math>\longrightarrow</math> 2-benzoxazolinone + 1-methyl-2,3-dioxindole</p>	V	-0.28	-234.7
		Mean Value	$-235.6 \pm 1.0$ <sup>1</sup>

<sup>1</sup> The assigned uncertainty is an expanded uncertainty of the mean using an appropriate coverage factor,  $k = 2.776$ , to provide a level of confidence of 0.95.

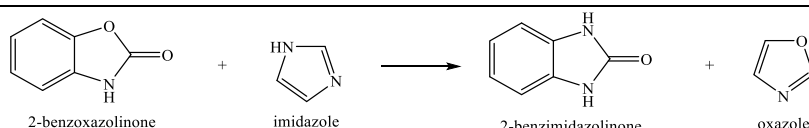
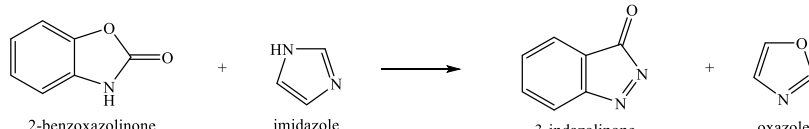
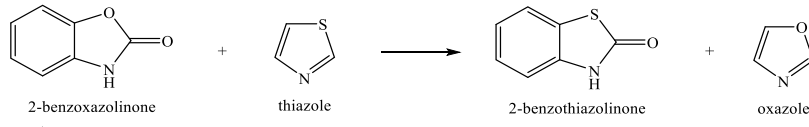
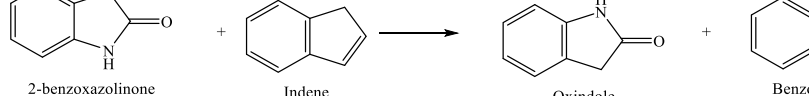
**Table S6.** Gas-phase hypothetical reactions for **6NBOA** and corresponding values for the enthalpies of reaction,  $\Delta_r H_m^\circ$ , and formation,  $\Delta_f H_m^\circ$ , in the gaseous phase, at  $T = 298.15$  K (values in  $\text{kJ}\cdot\text{mol}^{-1}$ ).

Gas-phase hypothetical reactions	Eq.	$\Delta_r H_m^\circ$	$\Delta_f H_m^\circ$
 <p>6-nitro2(3H)benzoxazolone + benzene <math>\rightarrow</math> 2-benzoxazolinone + nitrobenzene</p>	I	-4.42	-229.7
 <p>6-nitro2(3H)benzoxazolone + 2,1,3-benzothiadiazole <math>\rightarrow</math> 2-benzoxazolinone + 4-nitro-2,1,3-benzothiadiazole</p>	II	23.92	-235.7
 <p>6-nitro2(3H)benzoxazolone + naphthalene <math>\rightarrow</math> 2-benzoxazolinone + 1-nitronaphthalene</p>	III	10.43	-234.7
 <p>6-nitro2(3H)benzoxazolone + indole <math>\rightarrow</math> 2-benzoxazolinone + 5-nitroindole</p>	IV	-11.84	-234.6
 <p>6-nitro2(3H)benzoxazolone + quinoline <math>\rightarrow</math> 2-benzoxazolinone + 5-nitroquinoline</p>	V	10.85	-226.9
		Mean Value	$-232.3 \pm 4.7$ <sup>1</sup>

<sup>1</sup> The assigned uncertainty is an expanded uncertainty of the mean using an appropriate coverage factor,  $k = 2.776$ , to provide a level of confidence of 0.95.



**Table S7.** Gas-phase hypothetical reactions for **BOA** and corresponding values for the enthalpies of reaction,  $\Delta_r H_m^\circ$ , and formation,  $\Delta_f H_m^\circ$ , in the gaseous phase, at  $T = 298.15$  K (values in  $\text{kJ}\cdot\text{mol}^{-1}$ ).

Gas-phase hypothetical reactions	Eq.	$\Delta_r H_m^\circ$	$\Delta_f H_m^\circ$
 <p>2-benzoxazolinone + imidazole <math>\longrightarrow</math> 2-benzimidazolinone + oxazole</p>	I	7.33	-219.6
 <p>2-benzoxazolinone + imidazole <math>\longrightarrow</math> 3-indazolinone + oxazole</p>	II	144.40	-222.8
 <p>2-benzoxazolinone + thiazole <math>\longrightarrow</math> 2-benzothiazolinone + oxazole</p>	III	18.20	-219.4
 <p>2-benzoxazolinone + Indene <math>\longrightarrow</math> Oxindole + Benzofuran</p>	IV	7.03	-223.6
		Mean Value	$-221.4 \pm 3.4$ <sup>1</sup>

<sup>1</sup> The assigned uncertainty is an expanded uncertainty of the mean using an appropriate coverage factor,  $k = 3.182$ , to provide a level of confidence of 0.95.

**Table S8.** G3MP2B3 absolute enthalpies (in *Hartrees*\*) and experimental enthalpies of formation (in  $\text{kJ}\cdot\text{mol}^{-1}$ ), in the gaseous phase, at  $T = 298.15\text{ K}$ , for the studied compounds and the auxiliary molecules used in the gas-phase working reactions.

Compounds studied / auxiliary molecules	G3MP2B3 absolute enthalpies	Experimental enthalpies of formation (298.15 K)
3-Methyl-2-benzoxazolinone	-513.535373	$(-239.7 \pm 3.2)^1$
6-Nitro-2-benzoxazolinone	-678.598843	$(-229.9 \pm 3.7)^1$
1 <i>H</i> -imidazole	-225.873394	$(132.9 \pm 0.6)$ [S9]
1-Methylimidazole	-265.103073	$(125.7 \pm 1.1)$ [S10]
2-Benzoxazolinone	-474.301846	$(-219.0 \pm 2.8)$ [S9]
Indole	-363.214962	$(164.3 \pm 1.3)$ [S9]
1-Methylindole	-402.445506	$(155.8 \pm 2.8)$ [S9]
Pyrrole	-209.822531	$(108.4 \pm 0.6)$ [S9]
1-Methylpyrrole	-249.051695	$(103.1 \pm 0.5)$ [S9]
2-Pyrrolidinone	-286.188826	$(-197.4 \pm 3.1)$ [S9]
1-Methyl-1-pyrrolidinone	-325.420913	$(-210.9 \pm 0.6)$ [S9]
2,3-Dioxindole	-512.331688	$(-133.0 \pm 5.6)$ [S9]
1-Methyl-2,3-dioxindole	-551.565323	$(-148.6 \pm 4.4)$ [S9]
Benzene	-231.835164	$(82.6 \pm 0.7)$ [S9]
Nitrobenzene	-436.133844	$(67.5 \pm 0.5)$ [S9]
2,1,3-Benzothiadiazole	-737.775911	$(276.5 \pm 2.5)$ [S11]
4-Nitro-2,1,3-benzothiadiazole	-942.063797	$(283.7 \pm 4.9)$ [S12]
Naphthalene	-385.223727	$(150.3 \pm 1.4)$ [S9]
1-Nitronaphthalene	-589.516753	$(145.0 \pm 1.9)$ [S13]
5-Nitroindole	-567.51647	$(136.9 \pm 2.1)$ [S14]
Quinoline	-401.263696	$(200.5 \pm 0.9)$ [S15]
5-Nitroquinoline	-605.556561	$(203.4 \pm 2.6)$ [S16]
Oxazole	-245.727307	$(-15.5 \pm 0.5)$ [S9]
Thiazole	-568.350825	$[151.5]^2$
3-Indazolinone	-454.392934	$(70.0 \pm 2.2)$ [S9]
Indene	-347.156638	$(163.4 \pm 2.0)$ [S9]
Oxindole	-438.385869	$(-66.8 \pm 3.2)$ [S9]
2-Benzimidazolinone	-454.445141	$(-63.9 \pm 2.9)$ [S9]
2-Benzothiazolinone	-796.918431	$(-34.2 \pm 2.7)$ [S9]

<sup>1</sup> This work. <sup>2</sup> Value estimated at the G3(MP2)//B3LYP level of theory.

\* 1 Hartree =  $2625.5\text{ kJ}\cdot\text{mol}^{-1}$

**Table S9.** Harmonic vibrational frequencies (scaling vibrational frequencies by 1.0029 [S17]) .

2-benzoxazolinone		3-methyl-2- benzoxazolinone		6-nitro-2-benzoxazolinone	
126.0	1279.7	121.9	1120.4	61.8	964
243.3	1295.8	129.4	1153.2	92.5	966.5
318.2	1313.2	138.3	1172.2	164.4	1080
320.7	1368.9	241.8	1193.7	188.6	1132.4
419.8	1446.3	263.5	1255.8	270.5	1165.5
463.3	1530.8	334.8	1302.2	335.6	1271.4
511.5	1532.6	341.6	1347.8	347.3	1286.2
577.1	1681.4	439.1	1402.4	354.6	1306.3
580.6	1682.9	507.7	1436.9	433.1	1363.3
629.4	1918.2	569.5	1478.8	470.1	1395.6
708.5	3206.4	580.7	1522	525.3	1462.2
733.3	3218.7	636.2	1525.4	562.7	1501.6
744.3	3228.0	692.9	1539.4	579.5	1533.4
759.5	3241.5	729.5	1546.9	597.8	1637.7
860.2	3683.8	740.1	1673.3	698.8	1677.9
870.6		754.1	1684.3	717.6	1686.5
903.0		759.6	1895.5	723.8	1930.9
922.9		859.3	3064	744.5	3232.3
940.1		886	3122.1	752.9	3268.3
968.9		921.1	3185.9	838.1	3280.6
1043.4		957.5	3205.7	841.2	3682.8
1112.1		968.9	3219	885.1	
1164.2		1043.2	3228.5	913.2	
1193.4		1070.6	3240.6	935.4	

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