Supporting information:

Energetics of quinazoline-2,4(1*H*,3*H*)-dione: an experimental and computational study.

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TABLE S1. B3LYP/6-311++G(d,p) optimized bond lengths, bond angles and dihedral angles of quinazoline-2,4(1*H*,3*H*)-dione

Bond length/ nm			Bond angle/ degrees			Dihedral angle/degrees		
	Calc.	Exp.		Calc.	Exp.		Calc.	Exp.
N1—C2	0.1381	0.1348	C10—N1—C2	125.1	124.0	C10—N1—C2—O2	-180.0	-179.3
C2—N3	0.1391	0.1373	N1—C2—N3	113.7	115.6	C10—N1—C2—N3	0.0	0.9
N3—C4	0.1399	0.1389	C2—N3—C4	128.2	127.2	C10—C5—C4—O4	180.0	178.7
C4—C5	0.1478	0.1465	N3—C4—C5	113.9	114.1	C10—C5—C4—N3	0.0	-1.8
C5—C6	0.1399	0.1401	C4—C5—C10	119.7	119.6	C10—C5—C6—C7	0.0	-0.1
C6—C7	0.1386	0.1372	C5—C10—N1	119.2	119.2	C2—N1—C10—C9	180.0	-179.7
C7—C8	0.1400	0.1388	C4—C5—C6	120.4	121.3	C2—N1—C10—C5	0.0	0.0
C8—C9	0.1387	0.1375	C5—C6—C7	120.4	120.2	C2—N3—C4—O4	-180.0	-177.4
C9—C10	0.1401	0.1387	C6—C7—C8	119.5	119.9	C2—N3—C4—C5	0.0	3.1
N1—C10	0.1390	0.1399	C7—C8—C9	121.0	120.9	C4—C5—C6—C7	-180.0	179.8
C5—C10	0.1404	0.1393	C8—C9—C10	119.6	119.3	C4—C5—C10—C9	180.0	-179.9
C2—O2	0.1213	0.1238	C9—C10—C5	119.8	120.5	C4—C5—C10— N1	0.0	0.4
C4—O4	0.1215	0.1221	C10—C5—C6	119.8	119.1	C4—N3—C2—O2	-180.0	177.6
			C9—C10—N1	121.0	120.3	C4—N3—C2—N1	0.0	-2.7
			O2—C2—N1	123.2	123.4	C5—C6—C7—C8	0.0	0.3
			O2—C2—N3	123.1	121.0	C6—C5—C10— N1	180.0	-179.6
			O4—C4—N3	120.7	120.2	C6—C5—C10—C9	0.0	0.1
			O4—C4—C5	125.2	125.4	C6—C5—C4—O4	0.0	-1.3
						C6—C5—C4—N3	-180.0	178.2
						C6—C7—C8—C9	0.0	-0.5
						C7—C8—C9—C10	0.0	0.4
						C8—C9—C10—C5	0.0	-0.3
						C8—C9—C10—N1	-180.0	179.4

TABLE S2. Calculated G3(MP2)//B3LYPabsolute enthalpies, $H_{G3(MP2)//B3LYP}$, and experimental standard molar enthalpies of formation, in the gaseous phase, at T = 298.15 K, for quinazoline-2,4(1*H*,3*H*)-dione, tautomers and auxiliary atoms and molecules used in this study

Compound	$H_{G3(MP2)//B3LYP}$/ a.u.	$\Delta_f H^\circ_m$ (g) exp/ kJ·mol^{-1}
Quinazoline-2,4(1*H*, 3*H*)-dione	-567.667747	–(271.1± 3.3) [a]
Benzene	-231.835172	82.6 ± 0.7 [38]
1,3-Benzoxazine-2,4(3*H*)-dione	-587.519631	–(401.0 ± 3.5) [40]
3,1-Benzoxazine-2,4(1*H*)-dione (isatoic anhydride)	-587.518277	–(406.2 ± 3.4) [40]
1*H*-Benzoimidazol-2(3*H*)-one	-454.445143	–(63.9 ± 2.9) [42]
Carbon (C(^{3}P))	-37.788425	716.67 [39]
Cyclopentane	-196.163575	–(76.4 ± 0.7) [38]
Cyclohexanone	-309.367637	–(226.1 ± 2.1) [38]
2,3-Dihydrophthalazine-1,4-dione (phthalhydrazide)	-567.603696	–(107.4 ± 2.4) [43]
Hydrogen (H(^{2}S))	-0.499780	218.00 [39]
Naphthalene	-385.223696	150.3 ± 1.4 [38]
Nitrogen (N(^{4}S))	-54.524582	472.68 [39]
Isoindoline-1,3-dione (phthalimide)	-512.362458	–(211.1 ± 2.1) [41]
Oxygen (O(^{3}P))	-74.989704	249.18 [39]
Piperidine	-251.439266	–(47.15 ± 0.63) [38]
Pyridine	-247.873416	140.4 ± 0.7 [38]
Quinoline	-401.263671	200.5 ± 0.9 [38]
Uracil	-414.267329	–(302.9 ± 2.3) [38]
Thymine	-453.508739	–(328.7 ± 4.2) [38]
Toluene	-271.074375	50.5 ± 0.5 [38]

[a] Determined in this work.