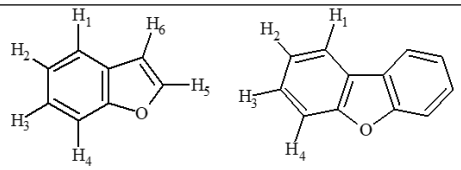
S2. Supplemental figures and tables for theoretical calculations

Table S2. Test of the used method with other OPAHs (benzofuran and dibenzofuran). Calculated barrier heights at 0 K including the ZPE (E_0) and reaction energies ($\Delta_r H°_{298K}$) for the H-abstraction reaction of benzofuran and dibenzofuran (in kcal/mol) at the CCSD(T)-F12/CBS//CAM-B3LYP/6-311++G(d,p) [1] and the CBS-Q/CAM-B3LYP/6-311+G(2d,p) (used in this work) levels of theory. MSD: Mean Square deviation

H-site (group)	E_0	$\Delta_r H°_{298K}$	E_0	$\Delta_r H°_{298K}$	E_0	$\Delta_r H°_{298K}$
	CCSD(T)-F12		CBS		Deviation	
		Benzofuran				
H_1 (g1)	16.16	9.49	16.90	10.03	0.736	0.540
H_2 (g1)	15.83	9.29	16.69	9.99	0.862	0.697
H_3 (g1)	15.77	9.15	16.61	9.77	0.842	0.623
H_4 (g2)	17.34	11.08	18.21	11.79	0.872	0.709
H_5 (g4)	21.14	15.48	22.36	16.65	1.221	1.169
H_6 (g4)	21.09	16.20	21.85	16.90	0.765	0.703
		Dibenzofuran				
H_1 (g1)	16.04	9.54	16.06	10.42	0.021	0.848
H_2 (g1)	15.97	9.50	16.24	11.02	0.270	1.485
H_3 (g1)	15.76	9.13	16.06	10.65	0.304	1.492
H_4 (g2)	17.41	11.24	17.58	12.80	0.169	1.522
		MSD			0.709	1.049



Benzofuran (C_8H_6O) Dibenzofuran ($C_{12}H_8O$)

Positions of H-atoms in the structures of benzofuran and dibenzofuran

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