Table S1 Supplementary data: total BHandHLYP/6-311G** energies (E) and zero point energies (zpe), both in a.u., of reactants and products; also, molecular symmetries and (for radicals) electronic states

	symmetry	E	zpe		symmetry	E	zpe
H_2	$D_{\infty h}$	–1.1695	0.0103	H	$K_h/^2S$	–0.5000	
HO_2	$C_s/\,^2A''$	–150.8716	0.0150	O_2	$D_{\infty h}/^3\Sigma_g$	–150.2888	0.0041
				HO_2NO_2	$C_1/^1A$	–355.9093	0.0315
HCHO	C_{2v}	–114.4688	0.0277	HCO	$C_s/^2A'$	–113.8221	0.0136
H_2O	C_{2v}	–76.4054	0.0222	OH	$D_{\infty h}/\,^2\Pi$	–75.7235	0.0088
CH_3OH	C_s	–115.6869	0.0531	CH_3O	$C_s/\,^2A'$	–115.0232	0.0380
				CH_2OH	$C_1/^2A$	–115.0289	0.0386
H_2S	C_{2v}	–399.3951	0.0156	SH	$D_{\infty h}/\,^2\Pi$	–398.7520	0.0063
HBr	$C_{\infty v}$	–2574.7073	0.0062	Br	$K_h/\,^2P$	–2574.0681	
HI	$C_{\infty v}$	–11.9548	0.0053	I	$K_h/\,^2P$	–11.3432	
NO_2	$C_{2v}/^2A_1$	–205.0119	0.0094	*trans*-HONO	C_s	–205.6422	0.0217
				cis-HONO	C_s	–205.6433	0.0218
				H–NO_2	C_{2v}	–205.6292	0.0234

Note:
For the H atom, the exact value is used for all levels of theory: values for HI and I are from the BHandHLYP/SDD method.