

Bond Dissociation Energies of Organic Molecules *Blanksby and Ellison***Table 1. Molecular Bond Dissociation Energies for $\text{RH} \rightarrow \text{R} + \text{H}$: Experimental Bond Enthalpies and Radical Heats of Formation at 298 K**

	DH_{298} (kcal mol ⁻¹)	$\Delta_f H_{298}(\text{R})$ (kcal mol ⁻¹)	ref		DH_{298} (kcal mol ⁻¹)	$\Delta_f H_{298}(\text{R})$ (kcal mol ⁻¹)	ref
Inorganics							
H ₂	104.206 ± 0.003	52.103 ± 0.003	4	OH ⁻ → O ⁻ + H	110.21 ± 0.07	-33.23 ± 0.07	34
HF	136.25 ± 0.01	18.83 ± 0.17	6	OH ⁺ → O + H ⁺	115.2 ± 0.1	59.55 ± 0.02	34
HCl	103.15 ± 0.03	29.03 ± 0.04	9	H ₂ S	91.2 ± 0.1	34.2 ± 0.2	6
HBr	87.54 ± 0.05	28.62 ± 0.06	9	SH	84.1 ± 0.2	66.2 ± 0.3	6
HI	71.32 ± 0.06	26.04 ± 0.08	9	H-NO	49.5 ± 0.7	21.8 ± 0.1	4
H-CN	126.3 ± 0.2	105.0 ± 0.7	6	H-ONO (trans)	79.1 ± 0.2	8.2 ± 0.1	4
NH ₃	107.6 ± 0.1	44.5 ± 0.1	6	H-ONO ₂	101.7 ± 0.4	17.6 ± 0.3	35
H ₂ O	118.82 ± 0.07	8.86 ± 0.07	34	SiH ₄	91.7 ± 0.5	47.9 ± 0.6	9
OH	101.76 ± 0.07	59.55 ± 0.02	34	GeH ₄	83 ± 2	53 ± 2	9
Hydrocarbons							
CH ₄	104.99 ± 0.03	35.05 ± 0.07	31	CH ₃ CH-H	110.7 ± 0.6	71.1 ± 0.7	6
CH ₃	110.4 ± 0.2	93.3 ± 0.2	31	HCC-H	133.32 ± 0.07	135.6 ± 0.2	36
CH ₂	101.3 ± 0.3	142.5 ± 0.2	9	C ₆ H ₅ -H	112.9 ± 0.5	80.5 ± 0.5	6
CH	80.9 ± 0.2	171.3 ± 0.1	9	C ₆ H ₅ → <i>o</i> -C ₆ H ₄ + H	78 ± 3	106 ± 3	37
CH ₃ CH ₂ -H	101.1 ± 0.4	29.0 ± 0.4	10	C ₆ H ₅ → <i>m</i> -C ₆ H ₄ + H	94 ± 3	122 ± 3	37
(CH ₃) ₂ CH-H	98.6 ± 0.4	21.5 ± 0.4	10	C ₆ H ₅ → <i>p</i> -C ₆ H ₄ + H	109 ± 3	138 ± 3	37
CH ₃ CH ₂ (CH ₃)CH-H	98.2 ± 0.5	16.1 ± 0.5	10	CH ₃ CHCH ₂ -H	88.8 ± 0.4	41.4 ± 0.4	38
(CH ₃) ₃ C-H	96.5 ± 0.4	12.3 ± 0.4	10	C ₆ H ₅ CH ₂ -H	89.8 ± 0.6	49.7 ± 0.6	38
Alcohols							
H-CH ₂ OH	96.1 ± 0.2	-4.08 ± 0.2	16	CH ₃ CH ₂ O-H	104.7 ± 0.8	-3.6 ± 0.8	6
CH ₃ O-H	104.6 ± 0.7	4.3 ± 0.7	6	(CH ₃) ₂ CHO-H	105.7 ± 0.7	-11.5 ± 0.7	6
CH ₃ S-H	87.4 ± 0.5	29.8 ± 0.4	39,40	(CH ₃) ₃ CO-H	106.3 ± 0.7	-20.5 ± 0.7	6
H-CH ₂ SH	94 ± 2	36 ± 2	39,40	C ₆ H ₅ O-H	90 ± 3	-58 ± 3	41
Peroxides							
HOO-H	87.8 ± 0.5	3.2 ± 0.5	14	CH ₃ CH ₂ OO-H	85 ± 2	-6.8 ± 2.3	42
CH ₃ OO-H	88 ± 1	4.8 ± 1.2	42	(CH ₃) ₃ COO-H	84 ± 2	-25.2 ± 2.3	42
Carbonyls							
H-CHO	88.144 ± 0.008	10.1 ± 0.1	6	H-COOH is ≥	96 ± 1	-46.5 ± 0.7	45
CH ₃ C(O)-H	89.4 ± 0.3	-2.4 ± 0.3	43	CH ₃ COO-H	112 ± 3	-43 ± 3	44
H-CH ₂ CHO	94 ± 2	2.5 ± 2.2	9	C ₆ H ₅ COO-H	111 ± 4	-12 ± 4	44
HCOO-H	112 ± 3	-30 ± 3	44				