Reactivities of Hydrated Electrons with Organic Compounds in Aqueous-Phase Advanced Reduction Processes

Supporting Information

Contents:

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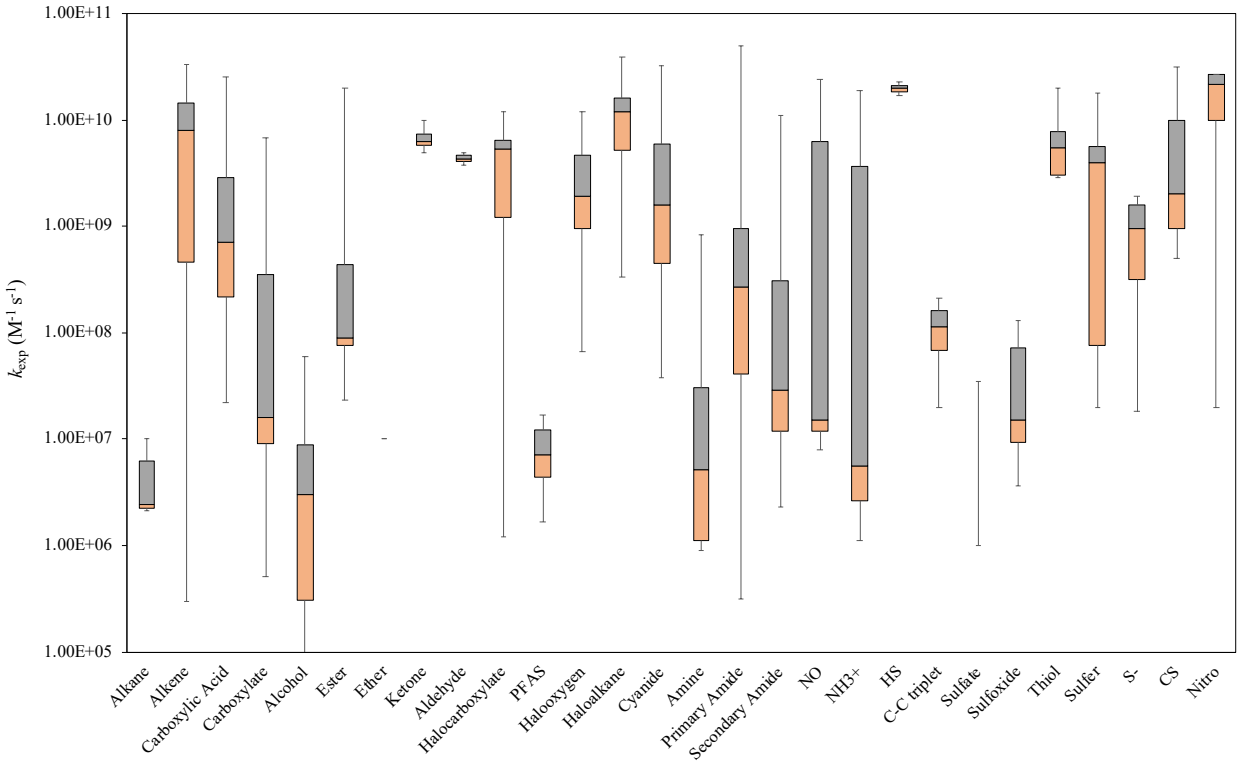


Figure S1: A box and whisker plot of experimentally measured second-order rate constants, k_{exp}, of structurally diverse aliphatic compounds with solvated electrons.

Table S1: Summary of computational method and basis set

Organic compounds	Reaction mechanisms	Optimization and frequency calculation	Single point energy calculation if any
Conventional compounds including fluorinated compounds and selected PFAS for prediction	Associative	M06-2X/cc-pVDZ	M06-2X/Aug-cc-pVTZ
	Concerted and stepwise	M06-2X/Aug-cc-pVTZ	
Iodinated compounds	Concerted	M06-2X/LANL2DZ	
Fluorinated compounds and PFASs	Stepwise	M06-2X/cc-pVDZ	

Table S2: Validation of M06-2X method with various basis sets with experimentally determined one electron reduction potential

		GIBBS FREE ENERGY (HARTREE)				CHANGE IN FREE ENERGY (KCAL/MOL)						
Gaussian Method/Basis Set	*Reaction*	*Radical (g)*	*Anion (g)*	*Radical (aq)*	*Anion (aq)*	*ΔG Solv, Radical (g → aq)*	*ΔG Red (g → g-)*	*ΔG Solv, Anion (g → aq)*	*ΔG Red (aq → aq-)*	*ΔΔG Solv*	**ΔG Reduction (aq) kcal/mol**	**One Electron Reduction Potential (V)**
Experimental (Isse et al 2011) [a]	F* + e- --> F-	--	--	--	--	--	-76.63	--	--	--	--	3.66
	Cl* + e- --> Cl-	--	--	--	--	--	-81.64	--	--	--	--	2.59
	Br* + e- --> Br-	--	--	--	--	--	-75.88	--	--	--	--	2.05
	I* + e- --> I-	--	--	--	--	--	-68.85	--	--	--	--	1.37
M06-2X/cc-pvdz	F* + e- --> F-	-99.710	-99.755	-99.708	-99.903	1.364	-27.811	-92.793	-121.968	-94.156	-121.968	1.01
	Cl* + e- --> Cl-	-460.137	-460.246	-460.137	-460.354	0.143	-68.481	-67.843	-136.467	-67.986	-136.467	1.64
	Br* + e- --> Br-	-2574.148	-2574.254	-2574.149	-2574.341	-0.762	-67.057	-54.098	-120.392	-53.335	-120.392	0.94
M06-2X/LANL2DZ	I* + e- --> I-	-11.323	-11.436	-11.328	-11.538	-3.004	-70.985	-64.119	-132.101	-61.116	-132.101	1.45
M06-2X/aug-cc-pvtz	F* + e- --> F-	-99.747	-99.868	-99.745	-100.007	1.338	-75.585	-87.289	-164.212	-88.627	-164.212	2.84
	Cl* + e- --> Cl-	-460.157	-460.290	-460.157	-460.394	0.188	-83.507	-65.226	-148.920	-65.413	-148.920	2.18
	Br* + e- --> Br-	-2574.215	-2574.341	-2574.217	-2574.426	-0.739	-78.637	-53.306	-131.204	-52.567	-131.204	1.41
M06-2X/LANL2DZ	I* + e- --> I-	-11.323	-11.436	-11.328	-11.538	-3.004	-70.985	-64.119	-132.101	-61.116	-132.101	1.45
B3LYP/cc-pVTZ	F* + e- --> F-	-99.778	-99.864	-99.776	-100.011	1.340	-54.377	-92.110	-147.827	-93.450	-147.827	2.13
	Cl* + e- --> Cl-	-460.190	-460.313	-460.190	-460.420	0.164	-76.692	-67.237	-144.094	-67.401	-144.094	1.97
	Br* + e- --> Br-	-2574.204	-2574.327	-2574.206	-2574.413	-0.747	-77.039	-53.949	-130.242	-53.203	-130.242	1.37
B3LYP/LANL2DZ	I* + e- --> I-	-11.380	-11.489	-11.385	-11.592	-2.994	-68.296	-64.502	-129.803	-61.507	-129.803	1.35
M06-2X/aug-cc-pVDZ	F* + e- --> F-	-99.720	-99.837	-99.718	-99.976	1.314	-73.484	-86.906	-161.703	-88.220	-161.703	2.73
	Cl* + e- --> Cl-	-460.139	-460.272	-460.139	-460.376	0.115	-83.444	-65.060	-148.619	-65.175	-148.619	2.16
	Br* + e- --> Br-	-2574.150	-2574.278	-2574.151	-2574.363	-0.781	-80.259	-53.240	-132.719	-52.460	-132.719	1.47
M06-2X/LANL2DZ	I* + e- --> I-	-11.323	-11.436	-11.328	-11.538	-3.004	-70.985	-64.119	-132.101	-61.116	-132.101	1.45
M06-2X/cc-pVTZ	F* + e- --> F-	-99.745	-99.832	-99.743	-99.979	1.344	-54.784	-92.118	-148.246	-93.462	-148.246	2.15
	Cl* + e- --> Cl-	-460.156	-460.280	-460.156	-460.387	0.166	-77.391	-67.251	-144.808	-67.417	-144.808	2.00
	Br* + e- --> Br-	-2574.215	-2574.335	-2574.216	-2574.421	-0.753	-75.209	-53.956	-128.412	-53.203	-128.412	1.29
M06-2X/LANL2DZ	I* + e- --> I-	-11.323	-11.436	-11.328	-11.538	-3.004	-70.985	-64.119	-132.101	-61.116	-132.101	1.45
M06-2X/Aug-cc-pVTZ//M06-2X/cc-pVDZ	F* + e- --> F-	-99.747	-99.868	-99.745	-100.007	1.338	-75.586	-87.289	-164.213	-88.627	-164.213	2.84
	Cl* + e- --> Cl-	-460.157	-460.290	-460.157	-460.394	0.188	-83.506	-65.223	-148.918	-65.412	-148.918	2.18
	Br* + e- --> Br-	-2574.215	-2574.341	-2574.217	-2574.426	-0.753	-78.656	-53.338	-131.241	-52.585	-131.241	1.41
M06-2X/LANL2DZ//M06-2X/LANL2DZ	I* + e- --> I-	-11.323	-11.436	-11.328	-11.538	-3.005	-70.984	-64.120	-132.100	-61.116	-132.100	1.45
CCSD(T)/cc-pVTZ//M06-2X/cc-pVTZ	F* + e- --> F-	-99.635	-99.713	-99.633	-99.859	1.332	-48.550	-92.123	-142.004	-93.454	-142.004	1.88
	Cl* + e- --> Cl-	-459.687	-459.800	-459.687	-459.907	0.182	-70.699	-67.282	-138.162	-67.463	-138.162	1.71
	Br* + e- --> Br-	-2572.67803	-2572.792	-2572.679	-2572.878	-0.753	-71.690	-53.966	-124.903	-53.213	-124.903	1.14
CCSD(T)/LANL2DZ//M06-2X/LANL2DZ	I* + e- --> I-	-11.185	-11.267	-11.190	-11.369	-3.065	-51.601	-63.985	-112.522	-60.920	-112.522	0.60

Text S1: Critical data evaluation

Experimentally measured second-order rate constants with the solvated electron (k_{exp}) for 268 structurally diverse aliphatic compounds were obtained from the NIST database[1] and compiled with the experimental conditions for the critical data evaluation in Table S2 in the SI. The statistical average of k_{exp} was adopted when multiple experimental values were reported for a given compound. All datapoints were investigated for experimental accuracy. When the pH described in the papers did not provide consistent form of dissociated or non-dissociated species based on the pKa value of the species, we did not include the k_{exp} values in our study because of the uncertainty about the form of species. All k_{exp} values were corrected to an ionic strength of 0 M to ensure uniform experimental conditions[2]. The second-order reaction rate constant for the chemical reaction (k_{chem}) was calculated for each compound to eliminate diffusive effects. For reactions classified as diffusion limited (k_{exp} > diffusion limited rate constant (k_D)), the k_{exp} value was used in place of k_{chem}.

A thorough description of the procedure for correcting second-order rate constants for diffusive effects is found in our previous publication[3]. Experimentally measured second-order rate constants for aqueous compounds (k_{exp}) are made up of both the diffusion-limited rate constant (k_D) and the rate constant for the chemical reaction (k_{chem}), as shown in equation S1.

$$k_{exp} = \frac{k_D k_{chem}}{k_D + k_{chem}} \quad \text{(S1)}$$

To eliminate the contribution of diffusive effects on the second-order rate constant, equation 1 was solved for k_{chem}. To determine k_D for a compound, the liquid phase diffusion coefficient (D_l) of that compound needs to be calculated. The method to calculate D_l varies depending on the charge state of the solute. For neutral compounds, the Hayduk-Laudie correlation[4] as below

$$D_l = \frac{13.26\times10^{-5}}{(\mu_\omega)^{1.14}(V_b)^{0.589}} \quad \text{(S2)}$$

where μ_ω is the viscosity of water and V_b is the molar volume of the solute. For electrolyte compounds, the Nernst-Haskell correlation[5] was used to calculate as below

$$D_l = \frac{RT\left[\left(\frac{1}{n_+}\right)+\left(\frac{1}{n_-}\right)\right]}{F^2\left[\left(\frac{1}{\lambda_+}\right)+\left(\frac{1}{\lambda_-}\right)\right]} \quad \text{(S3)}$$

where R is the universal gas constant, T is the absolute temperature in Kelvins, F is Faraday's constant, n_+ and n_- are the charge numbers of the cation and anion, respectively, and λ_+ and λ_- are the molar conductivities of the cation and anion, respectively. When molar conductivity values could not be found in the literature or databases, we assumed $k_{exp} = k_{chem}$.

The following seven compounds were identified as outliers and were discarded from the investigation: tert-butyl hydroperoxide, glyoxylic acid, o-methylhydroxylamine, methanol, ethanol and pyruvonitrile. The justification for removing each of these compounds from the dataset is described in more detail below.

The experimental pH for tert-butyl hydroperoxide ($(CH_3)_3COOH$, $E_{red,aq}^\circ$ = -1.02 V) was reported as 8.2[6], which is significantly greater than the pKa of 4.75. This disparity would result in dissociation of the OH group and thus an inaccurate k_{exp} would be obtained for this carboxylic acid.

Similarly, the experimental pH range for glyoxylic acid (HOCCOOH, $E_{red,aq}^\circ$ = -1.20 V) was reported as 3 – 4[7], which encompasses the pKa of 3.3. Thus, it cannot be determined whether HOCCOOH was dissociated during the experiment which brings into question the accuracy of the reported k_{exp} value.

O-methylhydroxylamine (CH_3ONH_2, $E_{red,aq}^\circ$ = -5.50 V) is unlike any of the other amine and amide compounds in the dataset due to the presence of a single ether functional group. Due to this unique molecular structure, we were not able to achieve an accurate aqueous-phase optimization of this compound with M06-2X. For this reason and the inability to place this compound within one of the classes in our dataset, it was discarded from the investigation.

The k_{exp} values for both methanol (CH_3OH, $E_{red,aq}^\circ$ = -4.32 V) and ethanol (CH_3CH_2OH, $E_{red,aq}^\circ$ = -4.33 V) appear to be significantly underestimated, with reported values of 1.0 x 10^4 M^{-1} s^{-1} [8] and 1.2 x 10^3 M^{-1} s^{-1} [9], respectively. These reaction rates exceed the lower measurement limit of the pulse radiolysis technique and therefore likely have some degree of uncertainty.

Pyruvonitrile (CH_3COCN, $E_{red,aq}^\circ$ = -1.51 V) is the only compound in our dataset that is a true statistical outlier as it is located over three standard deviations away from the average on the

$E_{red,aq}^{\circ}$ vs k_{chem} plot. It is also the only compound in the cyanide class that contains a carbonyl group. While we did not experience any computational difficulties with this compound, the experimental data may be questionable. Previous publications[10] have classified this datapoint as an outlier and the need for new experimental data for pyruvonitrile is the general consensus in the literature. For this reason, this datapoint was discarded from our investigation.

Table S3. Compilation of k_{exp} values with experimental conditions in the literature

No.	Name	Chemical Formula	Identified Exp. Products	Proposed Mechanism	Arrhenius Parameters	Ionic Strength (M)	Exp. pH[a]	pKa	Adequate Exp. pH?	k_{exp} (M^{-1} s^{-1})	Average k_{exp} (M^{-1} s^{-1})	Ref.
1	Methane	CH_4	--	--	--	--		50.00	--	1.00E+07	1.00E+07	11
2	Propane	$CH_3CH_2CH_3$	--	--	--	--	7.6-8.5	50.00	Y	2.10E+06	2.10E+06	12
3	Butane	C_4H_{10}	various	H abstraction	--	--	7.6-8.5	50.00	Y	2.40E+06	2.40E+06	12
4	Oxalate	$^{-}OOCCOO^{-}$	$C_2O_4^{*3-}$	Reduction of COO^{-}	Log(A) = 9.714; Ea = 15.48 kJ/RT (temp 283-328 K)	0.000	9.15	3.81	Y	1.00E+07	2.32E+07	13
					Log(A) = 9.714; Ea = 15.48 kJ/RT (temp 283-328 K)	0.0021	--		--	1.20E+07		13
					--	--	--		--	4.60E+07		14
					--	--	7.60		Y	3.10E+07		15
					--	--	--		--	1.70E+07		16
5	Formate	$HCOO^{-}$	--	--	--	--	9.15	3.75	Y	8.00E+03	5.04E+05	13
			--	--	--	--	~10		Y	1.00E+06		17
6	Succinate	$^{-}OOC(CH_2)_2COO^{-}$	--	--	--	--	--	5.64	--	7.00E+05	1.59E+07	18
			--	--	--	--	10.00		Y	3.10E+07		19
7	Acetate	CH_3COO^{-}	--	--	--	--	9-11.5	4.75	Y	1.10E+06	1.05E+06	20
			--	--	--	--	~10		Y	1.00E+06		17
8	Hydrogen Oxalate	$HOOCCOO^{-}$	--	--	--	--	--	1.30	--	3.20E+09	3.20E+09	16
9	Malonate	$^{-}OOC\text{-}CH_2\text{-}COO^{-}$	--	--	--	--	7.20	5.69	Y	1.00E+07	1.00E+07	18
10	Malonate(1-)	$HOOC\text{-}CH_2\text{-}COO^{-}$	$OCCH_2COO^{-} + OH^{-}$	Reduction of COO^{-}	--	0.000	--	2.83	--	4.00E+08	5.50E+08	21
					--	--	--		--	7.00E+08		18
					--	0.050	3-4		N	6.10E+08		7
11	Succinate(1-)	$HOOC(CH_2)_2COO^{-}$	--	--	--	--	--	4.21	--	7.00E+07	2.05E+08	18
			--	--	--	--	6.00		Y	3.40E+08		19
12	Lactate	$CH_3CHOHCOO^{-}$	--	--	--	--	9.00	3.86	Y	1.00E+07	1.00E+07	11
13	Glycolate	$HOCH_2COO^{-}$	--	--	--	--	7.00	3.83	Y	8.20E+06	8.20E+06	22
14	Pyruvate	CH_3COCOO^{-}	--	--	--	--	12.70	2.45	Y	6.80E+09	6.80E+09	11
15	CID_4134252	$HOCH_2(CHOH)_4COO^{-}$	--	--	--	--		3.60	--	1.00E+06	1.00E+06	23
16	Malate	$^{-}OOCCH_2CHOHCOO^{-}$	--	--	--	--	11.00	5.03	Y	6.00E+07	6.00E+07	24
17	Oxalic Acid	HOOCCOOH	--	--	--	0.000	1.30	1.3-4.4	Y	2.50E+10	2.50E+10	25

18	Formic Acid	HCOOH	--	--	--	--	5.00	3.75	N	1.40E+08	1.40E+08	[17]
19	Succinic Acid	$HOOC(CH_2)_2COOH$	--	--	--	--	--	4.21	--	3.70E+08	2.28E+08	[18]
			--	--	--	--	3-4		Y	8.60E+07		[7]
20	Propionic Acid	CH_3CH_2COOH	$CH_3CH_2CO_2^- + H^*$	H radical leaving	--	0.050	3-4	4.87	Y	2.20E+07	2.20E+07	[7]
21	Acetic Acid	CH_3COOH	$CH_3CO_2^- + H^*$	H radical leaving	--	--	--	4.75	--	2.20E+08	2.00E+08	[26]
					--	--	5.40		N	1.80E+08		[17]
22	Malonic Acid	HOOC-CH_2-COOH	$OCCH_2CO_2H + OH^-$	OH^- leaving	--	0.000	--	2.83	--	1.60E+09	2.70E+09	[21]
					--	--	--		--	5.00E+09		[18]
					--	0.050	3-4		N	1.50E+09		[7]
23	Lactic Acid	$CH_3CH(OH)COOH$	$CH_3CHOHCO + OH^-$	OH^- leaving	--	--	--	3.86	--	8.00E+08	7.15E+08	[18]
					--	0.050	--		Y	6.30E+08		[7]
24	Malic Acid	$HOOCCH_2CH(OH)COOH$	--	--	--	--	2.40	3.54	Y	3.00E+09	3.00E+09	[27]
25	Glycolic acid	$HOCH_2COOH$	$HOCH_2CO + OH^-$	OH^- leaving	--	0.050	3-4	8.20	Y	4.30E+08	4.30E+08	[7]
26	Methanediol	$CH_2(OH)_2$	$^*CH_2OH + OH^-$	OH^- leaving	--	--	7.00	12.5-13.6	Y	~1.0E7	1.00E+07	[28]
					--	--	7.00		Y	<1.0E7		[17]
27	Tert-Butanol	$(CH_3)_3$-C-OH	--	--	--	--	9-11.5	16-19	Y	4.00E+05	4.00E+05	[20]
28	Butane-1,2,3,4	$HOCH_2[CH(OH)]_2CH_2OH$	--	--	--	--	7.00	13.90	Y	5.00E+06	5.00E+06	[29]
29	Mannitol	$HOCH_2[CH(OH)]_4CH_2OH$	--	--	--	--	7.00	13.60	Y	7.00E+06	8.50E+06	[29]
			--	--	--	--	--		--	1.00E+07		[30]
30	Methyl Acetate	CH_3COOCH_3	$CH_3C(O^-)OCH_3$	--	--	--	7.8-13	~25	Y	8.70E+07	8.70E+07	[31]
31	Methyl Propionate	$C_2H_5COOCH_3$	--	--	--	--	6.81	~25	Y	9.00E+07	9.00E+07	[19]
32	Ethyl Propionate	$C_2H_5COOC_2H_5$	--	--	--	--	--	--	--	7.50E+07	7.50E+07	[32]
33	Dimethyl Oxalate	$CH_3OOCCOOCH_3$	--	--	--	--	--	--	--	2.00E+10	2.00E+10	[21]
34	Tert-butyl Acetate	$(CH_3)_3CCOOCH_3$	--	--	--	--	5.91	~25	Y	2.30E+07	2.30E+07	[19]
35	2-Hydroxyethyl Acetate	$CH_3COOCH_2CH_2OH$	--	--	--	--	--	--	--	2.60E+07	2.60E+07	[33]
36	Di-tert-butyl Peroxide	$(CH_3)_3$-$COOC(CH_3)_3$	--	--	--	--	--	--	--	1.40E+08	1.40E+08	[34]
37	Methylene glycol monoacetate	$HOCH_2COOCH_3$	--	--	--	--	10.60	13.00	Y	4.80E+08	4.80E+08	[19]
38	Methyl methoxyacetate	$CH_3OCH_2COOCH_3$	--	--	--	--	~7	~25	Y	4.40E+08	4.40E+08	[35]
39	Methyl trifluoroacetate	CF_3COOCH_3	--	--	--	--	10.62	--	Y	1.90E+09	1.90E+09	[19]
40	Ethyl glycinate	$NH_2CH_2COOC_2H_5$	--	--	--	--	6.70	--	Y	8.30E+08	8.30E+08	[36]
41	Acetoxymethylamine	$H_2NCH_2COOCH_3$	--	--	--	--	11.20	7.59	Y	3.30E+08	3.10E+08	[37]

			--	--	--	--	10.70		Y	2.90E+08		19
42	Diethyl Ether	$(C_2H_5)_2O$	--	--	--	--	--	--	--	1.00E+07	1.00E+07	11
43	Acetone	CH_3COCH_3	$(CH_3)_2CO^-$	--	Log(A) = 12.517, Ea = 15 kJ/RT (temp 276-320 K)	--	--	--	--	7.70E+09		38
				--	Log(A) = 12.166, Ea = 13 kJ/RT (temp 280-330 K)	--	--	--	--	7.70E+09		39
				--	--	--	--	--	--	6.50E+09		40
				--	Log(A) = 11.832, Ea = 11 kJ/RT (temp 280-340 K)	--	--	--	--	8.00E+09		41
				--	Log(A) = 12.744, Ea = 17 kJ/RT (temp 298-343 K)	--	--	--	--	5.80E+09	6.84E+09	42
				--	--	--	--	--	--	5.60E+09		43
				--	Log(A) = 11.917, Ea =12 kJ/RT (temp 298-340 K)	--	--	--	--	6.60E+09		44
				--	--	--	--	--	--	7.20E+09		44
				--	--	--	--	--	--	6.50E+09		45
				--	--	--	7, 11, 14	19.20	Y	5.9E9, 5.6E9, 5.2E9		46
44	Methyl Ethyl Ketone	$CH_3CH_2COCH_3$	$CH_3CH_2COCH_3^{*-}$	--	Log(A) = 12.580, Ea = 16.4 kJ/RT (temp 274.5-343 K)	--	--	--	--	4.90E+09	4.90E+09	47
45	2,3-Butanedione	$CH_3COCOCH_3$		--	--	--	--	--	--	9.90E+09	9.95E+09	21
				--	--	--	--	--	--	1.00E+10		48
46	Acetoin	$CH_3COCH(OH)CH_3$	--	--	--	--	--	--	--	6.00E+09	6.00E+09	48
47	Acetaldehyde	CH_3CHO		--	--	--	--	13.57	--	4.40E+09	4.90E+09	21
				--	--	--	6.60		Y	5.40E+09		17
48	Propionaldehyde	CH_3CH_2CHO	$CH_3CH_2CHO^-$	--	Log(A) = 12.681; Ea = 18.0 (temp 275-310 K)	--	--	--	--	3.40E+09	3.75E+09	47
				--	--	--	--	--	--	4.10E+09		44
49	Chloroacetate	$ClCH_2COO^-$	$^*CH_2CO_2^- + Cl^-$	Cl^- leaving	--	--			--	1.00E+09		40
					Log(A) = 11.053; Ea = 12 kJ/RT (temp 275-335 K)	--	11.00	2.87	Y	8.90E+08	1.05E+09	49
					Log(A) =11.895; Ea = 16 kJ/RT (temp 293-343 K)	--	7.00		Y	1.10E+09		50

					--	--	~10		Y	1.20E+09		[46]
50	3-Chloropropanoate	$Cl(CH_2)_2COO^-$	--	--	Log(A) = 11.273; Ea = 15 kJ/RT (temp 275-335 K)	--	11.00	2.80	Y	4.40E+08	4.40E+08	[49]
51	Bromoacetate	$BrCH_2COO^-$	--	--	--	--	~10	2.86	Y	6.20E+09	6.20E+09	[46]
52	3-Bromopropanoate	$Br(CH_2)_2COO^-$	--	--	--	--	~10	<4	Y	2.70E+09	2.70E+09	[46]
53	Fluoroacetate	FCH_2COO^-	--	--	--	0.000	~10	2.60	Y	1.20E+06	1.20E+06	[46]
54	2-Bromopropanoate	$CH_3CHBrCOO^-$	--	--	--	--	~10	<4	Y	5.30E+09	5.30E+09	[46]
55	2-Chloropropanoate	$CH_3CHClCOO^-$	--	--	--	--	~10	<4	Y	1.40E+09	1.40E+09	[46]
56	Trichloroacetate	Cl_3CCOO-	--	--	--	--	~10	0.66	Y	8.50E+09	8.50E+09	[46]
57	2-Iodoacetate	ICH_2COO-	--	--	--	--	~10	3.18	Y	1.20E+10	1.20E+10	[46]
58	2-Iodopropanoate	$CH_3CHICOO^-$	--	--	--	--	~10	<4	Y	6.60E+09	6.60E+09	[46]
59	3-Iodanylpropanoate	$I(CH_2)_2COO^-$	--	--	--	--	7.00	<4	Y	5.80E+09	5.80E+09	[51]
60	Chloromethane	CH_3Cl	$^*CH_3 + Cl^-$	Cl^- leaving	--	--	--	--	--	4.70E+08	8.06E+08	[52]
					Log(A) = 11.163; Ea = 14.24 kJ/RT (temp 276-358 K)	--	--	--	--	4.60E+08		[52]
					--	--	--	--	--	1.20E+09		[53]
					--	--	--	--	--	1.10E+09		[54]
					--	--	10.00	--	Y	~8.0E8		[54]
61	Dibromomethane	CH_2Br_2	$Br^- + {}^*CH_2Br$	Br^- leaving	--	--	4.00	--	Y	2.00E+10	2.00E+10	[55]
62	Bromoform	$CHBr_3$	--	--	--	--	7.00	13.70	Y	1.00E+10	1.00E+10	[56]
63	Bromoethane	CH_3CH_2Br	$Br^- + {}^*CH_2CH_3$	Br^- leaving	--	--	7.00	--	Y	8.00E+09	1.07E+10	[56]
					--	--	9-10	--	Y	1.20E+10		[57]
					--	--	7.10	--	Y	1.20E+10		[58]
64	Bromopropane	$CH_3CH_2CH_2Br$	--	--	--	--	7.00	--	Y	1.00E+10	9.25E+09	[56]
			--	--	--	--	6.15	--	Y	8.50E+09		[58]
65	Chloropropane	$CH_3CH_2CH_2Cl$	$^*CH_2CH_2CH_3 + Cl^-$	Cl^- leaving	--	--	7.6-8.5	--	Y	6.20E+08	6.67E+08	[12]
					--	--	9-10	--	Y	6.90E+08		[57]
					--	--	6.30	--	Y	6.90E+08		[58]
66	Chloroethane	CH_3CH_2Cl	$^*CH_2CH_3 + Cl^-$	Cl^- leaving	--	--	--	--		7.00E+08	7.00E+08	[53]
67	1-Bromo-2-chloroethane	CH_2ClCH_2Br	--	--	--	--	7.00	--	Y	8.00E+09	8.00E+09	[56]
68	Halothane	$CF_3CHClBr$	$CF_3CHCl + Br^-$	Br^- leaving	--	--	7.00	--	Y	1.40E+10	1.40E+10	[59]
69	1,1-Dichloroethane	CH_3CHCl_2	$Cl^- + {}^*CH_3CHCl$	Cl^- leaving	--	--	~7	--	Y	9.00E+09	9.00E+09	[60]

70	Diiodomethane	CH_2I_2	$I^- + {}^*CH_2I$	I^- leaving	--	--	4.00	--	Y	3.40E+10	3.40E+10	[55]
					--	--	--	--	--	3.40E+10		[61]
71	Iodoethane	CH_3CH_2I	$I^- + {}^*CH_2CH_3$	I^- leaving	--	--	9-10	--	Y	1.50E+10	1.50E+10	[57]
					--	--	6.04-6.75	--	Y	1.50E+10		[58]
72	Dichloromethane	CH_2Cl_2	$^*CH_2Cl + Cl^-$	Cl^- leaving	--	--	10	--	Y	6.00E+09	6.00E+09	[62]
73	Chloroform	$CHCl_3$	--	--	--	--	7.00	15.50	Y	3.00E+10	3.00E+10	[11]
74	Trichlorofluoromethane	CCl_3F	$^*CFCl_2 + Cl^-$	Cl^- leaving	--	--	~6	--	Y	1.60E+10	1.60E+10	[63]
75	Dichlorodifluoromethane	CF_2Cl_2	$^*CF_2Cl + Cl^-$	Cl^- leaving	--	--	~6	--	Y	1.40E+10	1.40E+10	[63]
76	Chlorotrifluoromethane	$CClF_3$	$^*CF_3 + Cl^-$	Cl^- leaving	--	--	9-10	--	Y	4.40E+09	4.40E+09	[57]
77	Bromotrifluoromethane	CF_3Br	$Br^- + {}^*CF_3$	Br^- leaving	--	--	9-10	--	Y	2.30E+10	2.30E+10	[57]
78	Carbon Tetrachloride	CCl_4	$^*CCl_3 + Cl^-$	Cl^- leaving	--	--	--	--	--	1.30E+10		[44]
					Log(A) = 13.010; Ea = 15 kJ/RT (temp 293-348 K)	--	--	--	--	2.40E+10	1.87E+10	[64]
					--	--	--	--	--	1.90E+10		[65]
79	Chlorodifluoromethane	$CHClF_2$	$^*CHF_2 + Cl^-$	Cl^- leaving	--	--	--	--		2.90E+09	2.90E+09	[66]
80	1,1,2-Trichloroethane	$ClCH_2CHCl_2$	$Cl^- + {}^*CH_2ClCHCl$	Cl^- leaving	--	--	~7	--	Y	8.40E+09	8.40E+09	[60]
81	1,1,1-Trichloroethane	CH_3CCl_3	$Cl^- + {}^*CH_3CCl_2$	Cl^- leaving	--	--	--	--	--	2.50E+10	1.95E+10	[53]
					--	--	~7	--	Y	1.40E+10		[60]
82	Hexachloroethane	CCl_3CCl_3	$Cl^- + {}^*CCl_3CCl_2$	Cl^- leaving	--	--	~7	--	Y	3.90E+10	3.90E+10	[60]
83	2-Chlorobutane	$C_2H_5CH(Cl)CH_3$	--	--	--	--	6.64	--	Y	5.10E+08	5.10E+08	[58]
84	1,2-Dibromoethane	$BrCH_2CH_2Br$	$Br^- + {}^*CH_2CH_2Br$	Br^- leaving	--	--	7.00	--	Y	1.40E+10	1.30E+10	[56]
					--	--	~7	--	Y	1.20E+10		[60]
85	1,2-Dichloroethane	$ClCH_2CH_2Cl$	$Cl^- + {}^*CH_2CH_2Cl$	Cl^- leaving	--	--	--	--	--	6.40E+08	1.77E+09	[67]
					--	--	~7	--	Y	2.90E+09		[60]
86	1,1,2-Trichloro-1,2,2-trifluoroethane	$ClCF_2CCl_2F$	$Cl^- + {}^*CF_2CCl_2F$	Cl^- leaving	--	--	~7	--	Y	1.40E+10	1.40E+10	[60]
87	1-Iodopropane	C_3H_7I	--	I^- leaving	--	--	6.20	--	Y	1.30E+10	1.30E+10	[58]
88	1-Iodobutane	$CH_3(CH_2)_3I$	--	--	--	--	7.60	--	Y	1.20E+10	1.20E+10	[58]
89	1-Bromobutane	$CH_3(CH_2)_3Br$	$Br^- + {}^*CH_2(CH_2)_2CH_3$	Br^- leaving	--	--	7.00	--	Y	9.00E+09	9.67E+09	[56]
					--	--	9-10	--	Y	1.00E+10		[57]
					--	--	6.57	--	Y	1.00E+10		[58]
90	1-Chlorobutane	$CH_3(CH_2)_3Cl$	$Cl^- + {}^*CH_2(CH_2)_2CH_3$	Cl^- leaving	--	--	7.6-8.5	--	Y	4.00E+08	3.37E+08	[12]

					--	--	--	--	--	4.80E+07		26
					--	--	9-10	--	Y	4.50E+08		57
					--	--	7.28	--	Y	4.50E+08		58
91	1-Chloro-2-methylpropane	$(CH_3)_2CHCH_2Cl$	--	--	--	--	5.82	--	Y	5.10E+08	5.10E+08	58
92	1-Bromopentane	$CH_3(CH_2)_4Br$	--	--	--	--	7.00	--	Y	8.00E+09	8.00E+09	56
93	2-Bromo-2-methylpropane	$(CH_3)_3CBr$	--	--	--	--	7.00	--	Y	7.20E+09	7.20E+09	56
94	2-Bromobutane	$CH_3CH_2CH(Br)CH_3$	--	--	--	--	7.00	--	Y	7.20E+09	7.20E+09	56
95	Trifluoroiodomethane	CF_3I	$^{*}CF_3 + I^-$	I^- leaving	--	--	9-10	--	Y	1.30E+10	1.30E+10	57
96	Iodomethane	CH_3I	$^{*}CH_3 + I^-$	I^- leaving	--	--	9-10	--	Y	1.60E+10	1.60E+10	57
					--	--	--	--	--	1.60E+10		68
97	Isoflurane	$CHF_2OCHClCF_3$	CHF_2OCHCF_3	Cl^- leaving	--	--	~7	--	Y	4.70E+09	4.70E+09	60
98	1,1,1-Trifluoroacetone	CF_3COCH_3	--	--	--	--	5.19	--	Y	6.60E+07	6.60E+07	19
99	Fluoroacetone	CH_3COCH_2F	--	--	--	--	6.70	--	Y	1.00E+09	9.40E+08	19
			--	--	--	--	11.00	--	Y	8.80E+08		
100	Methoxyflurane	$CH_3OCF_2CHCl_2$	$Cl^- + {}^{*}CH_3OCF_2CHCl$	--	--	--	~7	--	Y	1.40E+10	1.40E+10	60
101	2-Chloroethanol	$ClCH_2CH_2OH$	various	Cl^- leaving and H-abstraction from OH	--	--	--	--	--	4.20E+08	5.23E+08	69
					--	--	--	--	--	7.00E+08		70
					--	--	6.20	--	Y	6.40E+08		71
					Log(A) = 10.798; Ea =13 kJ/RT (temp 275-335 K)	--	11.00	--	Y	3.30E+08		49
102	2-Bromoethanol	$BrCH_2CH_2OH$	--	--	--	--	~10	--	Y	1.60E+09	1.60E+09	46
103	Chloroacetic acid	$ClCH_2COOH$	$^{*}CH_2CO_2H + Cl^-$	Cl^- leaving	--	--	1.00	--	Y	6.90E+09	6.90E+09	72
104	Chloral hydrate	$CCl_3CH(OH)_2$	--	--	--	--	--	--	--	1.20E+10	1.20E+10	73
105	Enflurane	CHF_2OCF_2CHClF	$Cl^- + CHF_2OCF_2{}^{*}CHF$	Cl^- leaving	--	--	~7	--	Y	2.70E+09	2.70E+09	60
106	Acetonitrile	CH_3CN	--	--	Log(A) = 11.663; Ea = 23 kJ/RT (temp 298-340 K)	--	--	25.00	--	4.40E+07	3.73E+07	44
			--	--	--	--	--		--	3.00E+07		26
			--	--	--	--	12.00		Y	3.80E+07		74
107	Succinonitrile	$NC(CH_2)_2CN$	--	--	--	0.002	3-4	11.00	Y	1.70E+09	1.70E+09	75
108	Trichloroacetonitrile	CCl_3CN	$Cl^- + CCl_2CN$	Cl^- leaving	--	--	~7	15.00	Y	3.20E+10	3.20E+10	60
109	Cyanamide	H_2NCN	H_2NCN^-	--	--	0.002	3-4	10.30	Y	1.50E+09	1.50E+09	75
110	Methylamine	CH_3NH_2	--	--	--	--	11.80	40.00	Y	9.00E+05	9.00E+05	76

111	Butylamine	$CH_3(CH_2)_3NH_2$	--	--	--	--	--	--	--	1.10E+06	1.10E+06	77
112	Propylamine	$CH_3CH_2CH_2NH_2$	--	--	--	--	13.00	10.70	Y	1.10E+06	1.10E+06	77
113	Ethylamine	$CH_3CH_2NH_2$	--	--	--	--	--	--	--	1.00E+06	1.00E+06	77
114	Isobutylamine	$(CH_3)_2CHCH_2NH_2$	--	--	--	--	11.90	10.70	Y	1.10E+07	1.10E+07	76
115	Isoamylamine	$(CH_3)_2CHCH_2CH_2NH_2$	--	--	--	--	11.80	10.70	Y	1.00E+06	1.00E+06	76
116	1,2-Dimethylhydrazine	$CH_3NHNHCH_3$	--	--	--	--	12.40	7.52	Y	6.10E+06	6.10E+06	78
117	Methylhydrazine	CH_3NHNH_2	--	--	--	--	12.00	7.87	Y	6.50E+06	6.50E+06	78
118	Glycinate	$NH_2CH_2COO^-$	--	--	--	--	11.80	2.34	Y	1.70E+06	1.70E+06	37
119	Ethanolamine	$H_2NCH_2CH_2OH$	--	--	--	--	7.80	--	Y	2.00E+07	2.00E+07	79
120	Isopropylamine	$(CH_3)_2CHNH_2$	--	--	--	--	12.30	10.70	Y	1.50E+06	1.50E+06	76
121	Tert-Butylamine	$(CH_3)_3CNH_2$	--	--	--	--	12.30	~10.6	Y	1.10E+06	1.10E+06	76
122	beta-Alaninate	$NH_2(CH_2)_2$-COO^-	--	--	--	--	6.90	2.34	Y	4.20E+06	4.20E+06	80
123	N,N-Diethylhydroxylamine	$(C_2H_5)_2NOH$	--	--	--	--	9.00	--	Y	4.80E+07	4.80E+07	81
124	N-Methyl-N-tritiohydroxylamine	CH_3NHOH	--	--	--	--	9.00	6.20	Y	2.40E+08	2.40E+08	37
125	Amylamine	$CH_3(CH_2)_4NH_2$	--	--	--	--	--	--	--	1.00E+06	1.00E+06	77
126	Trimethylhydrazine	$(CH_3)_2N$-$NHCH_3$	--	--	--	--	10.40	--	Y	1.00E+08	1.00E+08	78
127	1,1-Dimethylhydrazine	$(CH_3)_2NNH_2$	--	--	--	--	12.00	6-7	Y	2.40E+07	2.40E+07	78
128	Propionamide	$CH_3CH_2CONH_2$	--	--	--	--	9.20	17.00	Y	5.40E+07	4.65E+07	82
			--	--	--	--	~6		Y	3.90E+07		83
129	N-Ethylacetamide	$CH_3CONHC_2H_5$	--	--	--	--	6.70	16.62	Y	1.40E+07	1.40E+07	36
130	N-Methylacetamide	$CH_3CONHCH_3$	--	--	--	--	--	--	--	2.30E+06	2.30E+06	84
131	Acetamide	CH_3CONH_2	--	--	--	--	5.20	17.00	Y	4.50E+07	3.83E+07	71
			--	--	--	--	9.20		Y	3.50E+07		82
			--	--	Log(A) = 10.219; Ea = 15 kJ/RT (temp 293-343 K)	--	~5.8		Y	3.50E+07		50
132	Urea	H_2NCONH_2	--	--	--	--	7.00	15.73	Y	3.00E+05	3.10E+05	19
			--	--	Log(A) = 8.002; Ea = 14 kJ/RT (temp 293-343 K)	--	~5.8		Y	3.20E+05		50
133	Glycinamide	$H_2NCH_2CONH_2$	$NH_3 + {}^*CH_2CONH_2$	NH_3 leaving	--	--	11.40	16.37	Y	2.80E+08	2.80E+08	37
134	Formamide	$HCONH_2$	--	--	--	--	--	16.50	--	2.00E+07	2.80E+07	85
			--	--	--	--	6.30		Y	1.80E+07		71

			--	--	--	--	9.20		Y	6.30E+07		82
			--	--	--	--	--		--	<1.0E6		86
			--	--	Log(A) = 9.898, Ea = 13 kJ/RT (temp 293-343K)	--	~5.8		Y	3.80E+07		50
135	3-Chloropropionamide	$ClCH_2CH_2CONH_2$	--	--	--	--	~6	15.92	Y	1.80E+09	1.80E+09	83
136	(S)-2-Hydroxypropanamide	$CH_3CH(OH)CONH_2$	--	--	--	--	7.00	13.34	Y	1.90E+08	1.90E+08	22
137	Aceturate	$CH_3CONHCH_2COO^-$	--	--	--	--	11.50	3.77	Y	2.60E+06	1.13E+07	37
			--	--	--	--	5.95		Y	2.00E+07		87
138	Pivalamide	$(CH_3)_3CCONH_2$	$(CH_3)_3CCONH_2^{*-}$	--	--	--	9.20	--	Y	1.50E+07	1.50E+07	82
139	Malonamide	$H_2NCOCH_2CONH_2$	--	--	--	--	7.00	15-17	Y	1.10E+09	1.10E+09	88
140	2-Hydroxyacetamide	$HOCH_2CONH_2$	--	--	--	--	8.50	15-17	Y	2.90E+08	2.90E+08	22
141	Biuret	$H_2NCONHCONH_2$	$H_2NC(O^-)NHCONH_2$	--	--	--	10.30	15-17	Y	2.50E+08	2.50E+08	88
142	2-Chloropropionamide	$CH_3CH(Cl)CONH_2$	--	--	--	--	~6	~15	Y	5.80E+09	5.80E+09	83
143	Iodoacetamide	ICH_2CONH_2	$I^- + {}^*CH_2CONH_2$	I^- leaving	--	--	--	--	--	5.00E+10	5.00E+10	89
144	Hydroxyurea	$HONHCONH_2$	$[HONHCONH_2]^{*-}$	--	--	--	6.80	10.60	Y	4.80E+08	4.80E+08	90
145	Oxamate	$H_2NCOCOO^-$	--	--	--	--	9.20	2.49	Y	5.70E+09	5.70E+09	88
146	Succinamide	$H_2NCOCH_2CH_2CONH_2$	--	--	--	--	7.10	15-17	Y	2.00E+08	2.00E+08	88
147	Asparaginate	$H_2NCOCH_2CH(NH_2)COO^-$	--	--	--	--	11.70	2-3	Y	2.40E+07	2.40E+07	91
148	N,N-Dimethylformamide	$HCON(CH_3)_2$	--	--	--	--	--		--	4.00E+08		85
			--	--	--	--	9.20	-0.30	Y	4.60E+08	3.04E+08	82
			--	--	--	--	--		--	5.20E+07		86
149	Methyl 2-acetamidoacetate	$CH_3CONHCH_2COOCH_3$	--	--	--	--	8.70	--	--	3.30E+08	3.30E+08	37
150	2-Formamidoacetate	$HCONHCH_2COO^-$	--	--	--	--	10.50	--	--	2.90E+07	2.90E+07	37
151	N-Methylformamide	$HCONHCH_3$	--	--	--	--	9.20	16.54	Y	7.10E+07	4.30E+07	82
			--	--	--	--	--		--	1.50E+07		86
152	N-Tert-Butylacetamide	$CH_3CONHC(CH_3)_3$	--	--	--	--	9.20	16.60	Y	1.20E+07	1.20E+07	82
153	Diacetamide	$(CH_3CO)_2NH$	$(CH_3CO)_2NH^{*-}$	--	--	--	6.50	--	--	1.10E+10	1.10E+10	88
154	N,N-Diethylacetamide	$CH_3CON(C_2H_5)_2$	--	--	--	--	9.20	--	--	8.00E+06	8.00E+06	82
155	N,N-Dimethylacetamide	$CH_3CON(CH_3)_2$	--	--	--	--	--	--	--	9.00E+06	1.50E+07	84
			--	--	--	--	9.20	--	--	2.10E+07		82
156		$(CH_3)_3CCON(CH_3)_2$	$(CH_3)_3CCON(CH_3)_2^{*-}$	--	--	--	9.20	--	--	1.20E+07	1.20E+07	82

157	Methyl Ammonium Hydride	$CH_3NH_3^+$	--	--	--	--	--	--	--	1.90E+06	1.85E+06	[76]
			--	--	--	--	7.60	~10.73	Y	1.80E+06		[91]
158	Ethylammonium	$C_2H_5NH_3^+$	--	--	--	--	--	--	--	2.50E+06	2.50E+06	[77]
159	Trideuterio(propyl)azanium	$CH_3(CH_2)_2NH_3^+$	--	--	--	--	--	--	--	2.80E+06	2.80E+06	[77]
160	Pentylazanium	$CH_3(CH_2)_4NH_3^+$	--	--	--	--	--	--	--	2.70E+06	2.70E+06	[92]
161	2-Methoxy-2-oxoethanaminium	$H_3COOCCH_2NH_3^+$	--	--	--	--	5.30	~10.73	Y	6.80E+09	6.80E+09	[37]
162	Methoxyazanium	$CH_3ONH_3^+$	--	--	--	--	4.50	~10.73	Y	1.90E+10	1.90E+10	[37]
163	Tert-butylammonium	$(CH_3)_3CNH_3^+$	--	--	--	--	7.90	~10.73	Y	1.10E+06	1.10E+06	[76]
164	2-Methylhydrazinium	$CH_3NHNH_3^+$	--	--	--	--	5.50	~10.73	Y	1.40E+09	1.40E+09	[78]
165	1,1-Dimethylhydrazinium	$(CH_3)_2NNH_3^+$	--	--	--	--	5.60	~10.73	Y	5.80E+09	5.80E+09	[78]
166	Tetramethylammonium	$(CH_3)_4N^+$	--	--	--	--	--	--	--	5.60E+06	5.60E+06	[93]
167	Tetraethylammonium	$(C_2H_5)_4N^+$	--	--	--	--	--	--	--	1.20E+07	1.20E+07	[93]
168	Cysteaminium	$HSCH_2CH_2NH_3^+$	$H_2S + H_2NCH_2CH_2$	--	--	--	--	~8.2	--	1.50E+10	2.25E+10	[2]
				--	--	--	5.50		Y	3.00E+10		[94]
169	3-Sulfanylpropylazanium	$HS(CH_2)_3NH_3^+$	--	--	--	--	2.4-4	~8.2	Y	1.70E+10	1.70E+10	[95]
170	Acetylene	HC triplet bond CH	--	--	--	--	--	--	--	2.00E+07	2.00E+07	[96]
171	Propargyl alcohol	HC triplet bond CCH_2OH	--	--	Log(A) = 11.478; Ea =18 kJ/RT (temp 298-370 K)	--	--	--	--	2.10E+08	2.10E+08	[44]
172	Ethanesulfonate	$C_2H_5SO_3^-$	--	Reduction of SO_3^-	--	--	--	--	--	3.50E+07	3.50E+07	[97]
173	Dibutyl sulphoxide	$[CH_3(CH_2)_3SO(CH_2)_3CH_3]$	$[(CH_3CH_2CH_2CH_2)_2SO]^{*-}$	--	--	--	--	--	--	3.60E+06	3.60E+06	[98]
174	Di-tert-butyl sulfoxide	$[(CH_3)_3C]_2SO$	$[(CH_3)_3C]_2SO]^{*-}$	--	--	--	--	--	--	1.50E+07	1.50E+07	[98]
175	Methyl (methylsulfinyl)methyl sulfide	$CH_3SOCH_2SCH_3$	$CH_3SO(-)CH_2SCH_3$	--	--	--	6-11	--	--	1.30E+08	1.30E+08	[99]
176	Methanethiol	CH_3SH	$^*CH_3 + HS^-$	HS^- leaving	--	--	7.00	10.40	Y	7.50E+09	7.50E+09	[100]
177	Thiolactate	$CH_3(CH)SHCOO^-$	$CH_3CHCO_2^- + HS^-$	HS^- leaving	--	--	7.2	3.83	Y	5.00E+09	2.89E+09	[94]
					--	--	12.00		Y	7.70E+08		
178	2-Mercaptopropionic Acid	$CH_3CH(SH)COOH$	$CH_3CHCO_2H + HS^-$	HS^- leaving	--	--	1.6-3	3.83	Y	3.50E+09	3.50E+09	[101]
179	Methyl thioglycolate	$HSCH_2COOCH_3$	$HS^- + ^*CH_2COOCH_3$	HS^- leaving	--	--	5.20	--	--	1.40E+10	7.70E+09	[94]
					--	--	10.00		--	1.40E+09		
180	beta-Mercaptoethanol	$HS(CH_2)_2OH$	--	--	--	--	--	--	--	8.30E+09	1.02E+10	[2]
			--	--	--	--	5.7-9.0		--	1.20E+10		[102]

181	2-Methyl-2-propanethiol	$(CH_3)_3CSH$	$^{*}C(CH_3)_3 + HS^-$	HS^- leaving	--	--	7.00	~10.40	Y	3.00E+09	3.00E+09	100
182	3-Mercaptopropionic acid	$HS(CH_2)_2COOH$	--	--	--	--	1.6-3.0	--	--	5.40E+09	5.40E+09	101
183	Thioglycolate	$HSCH_2COO^-$	$^{*}CH_2CO_2^- + HS^-$	HS^- leaving	--	--	6.50	~4	Y	5.50E+09	3.03E+09	94
					--	--	12.00		Y	5.60E+08		
184		$H_2NC(=NH)NHCH_2CH_2SH$	--	--	--	--	6.74	--	--	2.00E+10	2.00E+10	91
185	Dimethylsulfide	CH_3SCH_3	--	--	--	--	--	--	--	2.00E+07	2.00E+07	103
186	3,3'-Dithiodipropionate	$(SCH_2CH_2COO^-)_2$	$[S(CH_2)_2CO_2]_2^{*-}$	--	--	--	6.40	~3.5	Y	4.40E+09	4.35E+09	104
					--	--	11.00		Y	4.30E+09		
187	2,2'-Disulfanediyldiacetate	$(SCH_2COO^-)_2$	$[S_2(CH_2CO_2^-)_2]^{*-}$	--	--	--	10.80	~3.5	Y	4.30E+09	4.30E+09	104
188	2,2'-Sulfanediyldiacetate	$S(CH_2COO^-)_2$	--	--	--	--	10.80	~3.5	Y	8.30E+07	8.30E+07	94
189	N-Acetylcysteamine	$CH_3CONHCH_2CH_2SH$	$HS^- + {}^{*}CH_2CH_2NHCOCH_3$	HS^- leaving	--	--	7.10	--	--	9.10E+09	9.10E+09	94
190	Cystamine	$S_2(CH_2CH_2NH_2)_2$	$[H_2NCH_2CH_2S]_2^{*-}$	--	--	--	11.10	--	--	1.80E+10	1.80E+10	104
191	L-Cystine anion	$S_2[CH_2CH(NH_2)COO^-]_2$	$[S_2[CH_2CH(NH_2)CO_2^-]_2]^{*-}$	--	--	--	10.50	~3.5	Y	4.20E+09	3.53E+09	105
				--	--	--	--		--	1.50E+09		2
				--	--	--	12.10		Y	5.00E+09		104
				--	--	--	12.00		Y	3.40E+09		11
192	3,3'-Thiodipropanoate	$S(CH_2CH_2COO^-)_2$	--	--	--	--	10.80	~3.5	Y	5.80E+07	5.80E+07	94
193	2-Hydroxyethanethiolate	$HOCH_2CH_2S^-$	--	--	--	--		--	--	1.80E+07	1.80E+07	2
194	2-lambda1-Sulfanylethanamine	$H_2NCH_2CH_2S^-$	$H_2NCH_2CH_2 + HS^- + OH^-$	HS^- leaving, OH^- leaving	--	--	12.50	~7	Y	1.50E+09	9.55E+08	94
			$H_2NCH_2CH_2 + HS^-$	HS^- leaving	--	--			--	4.10E+08		2
195	2-Acetamidoethanethiolate	$CH_3CONHCH_2CH_2S^-$	$^{*}CH_2CH_2NHCOCH_3 + HS^- + OH^-$	HS^- leaving, OH^- leaving	--	--	12.60	~7	Y	1.90E+09	1.90E+09	94
196	Carbon Disulfide	CS_2	CS_2^{*-}	--	--	--		??	--	3.10E+10	3.10E+10	106
					--	--	7.00			3.10E+10		17
197	Thiourea	H_2NCSNH_2	--	--	--	--	6.40	13.87	Y	2.90E+09	2.90E+09	11
198	Thiosemicarbazide	$H_2NNHCSNH_2$	$NH_3 + H_2NNHCS^{*}$	NH_3 leaving	--	--	7.00	~13	Y	1.10E+09	1.10E+09	107
199	N,N'-Diethylthiourea	$CH_3CH_2NHCSNHCH_2CH_3$	$C_2H_5NHC^{*}(S^-)NHC_2H_5$	--	--	--	7.00	~13	Y	5.00E+08	5.00E+08	107
200	Nitromethane	CH_3NO_2	$CH_3NO_2^-$	Reduction of NO_2	--	--	--	10.00	--	2.20E+10	2.15E+10	108
					--	--	7.00		Y	2.10E+10		109

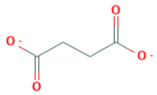
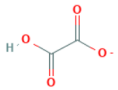
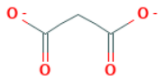
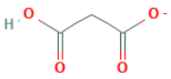
201	1-Nitropropane	$CH_3CH_2CH_2NO_2$	--	--	--	--	0-6	8.98	Y	2.70E+10	2.70E+10	[110]
202	Nitroethane	$CH_3CH_2NO_2$	--	--	--	--	0-6	8.50	Y	2.70E+10	2.70E+10	[110]
203	2-Methyl-2-nitrosopropane	$(CH_3)_3C(NO)$	--	--	--	--	9.20	--	--	6.20E+09	6.20E+09	[111]
204	Trifluoroacetate	CF_3COO^-	--	--	--	--	~10	0.50	Y	1.90E+06	1.65E+06	[112]
			--	--	--	0.000	~10		Y	1.40E+06		[46]
205	Perflurobutanoic Acid	$C_3F_7COO^-$	--	--	--	--	~10	0-3	Y	7.10E+06	7.10E+06	[112]
206	Perflurooctanoic Acid	$C_7F_{15}COO^-$	--	--	--	--	~10	3.80	Y	1.70E+07	1.70E+07	[112]
207	Allylamine	$H_2C=CHCH_2NH_2$	--	--	--	--	11.3	--	--	1.20E+07	1.20E+07	[76]
208	Acrylonitrile	$H_2C=CHCN$	$^*CH(CH_3)CN$	--	--	--	--	--	--	1.30E+10	1.30E+10	[113]
209	Allyl alcohol	$H_2C=CHCH_2OH$	$[CH_2CHCH_2OH]^{*-}$	--	Log(A) = 12.065; Ea = 24 kJ/RT (temp 298-340 K)	--	--	--	--	7.20E+07	3.47E+07	[42]
				--	Log(A) = 9.756; Ea = 14 kJ/RT (temp 298-360 K)	--	--	--	--	2.00E+07		[44]
				--	--	--	--	--	--	1.20E+07		[26]
210	Acrylic acid	$H_2C=CHCOOH$	$[CH_2CHCO_2H]^{*-}$	--	--	--	2.0-3.7	4.2	Y	2.40E+10	2.40E+10	[114]
211	Acrylate	$CH_2=CHCOO^-$	$[CH_2=CHCOO]^{*2-}$	Reduction of COO^-	--	--	9.2	4.2	Y	5.30E+09	5.30E+09	[114]
212	Methyl vinyl ketone	$H_2C=CHCOCH_3$	$CH_3COHCH=CH_2$	--	--	--	5.8	--	--	2.50E+09	2.50E+09	[115]
213	Methyl acrylate	$H_2C=CHCOOCH_3$	$[H_2CCHCO_2CH_3]^{*-}$	--	--	--	11	--	--	9.40E+09	9.40E+09	[116]
214	Senecioic acid amide	$(CH_3)_2C=CHCONH_2$	$[(CH_3)_2CCHCONH_2]^{*-}$	--	--	--	9.2	--	--	5.60E+09	5.60E+09	[117]
215	Vinyl chloride	$CH_2=CHCl$	$CH_2CH^* + Cl^-$	Cl^- leaving	--	--	~6.5	--	--	2.50E+08	2.50E+08	[118]
216	Ethylene	$H_2C=CH_2$	--	--	--	--	--	--	--	3.00E+05	3.00E+05	[26]
217	Ethenesulfonate	$CH_2=CHSO_3^-$	$[CH_2CHSO_3]^{*2-}$	--	--	--	7	--	--	2.30E+09	2.30E+09	[119]
218	Tetrachloroethylene	$Cl_2C=CCl_2$	$CCl_2CCl + Cl^-$	Cl- leaving	--	--	--	--	--	4.20E+10	2.75E+10	[67]
					--	--	~6.5	--	--	1.30E+10		[118]
219	Crotonyl Alcohol	$CH_3CH=CHCH_2OH$	--	--	--	--	--	--	--	5.50E+07	5.50E+07	[26]
220	Crotonic Acid	$CH_3CH=CHCOOH$	$[CH_3CHCHCO_2H]^{*-}$	Reduction of COOH	--	--	2.0-3.7	4.9	Y	1.80E+10	1.80E+10	[114]
221	Dimethyl Fumarate	$CH_3OOCCH=CHCOOCH_3$	Dimethyl fumarate radical anion	--	--	--	9.2	--	--	3.30E+10	3.30E+10	[88]
222	Divinyl Sulfone	$(H_2C=CH)_2SO_2$	--	--	--	--	7	--	--	1.00E+10	1.00E+10	[115]
223	Methacrylic Acid	$H_2C=C(CH_3)COOH$	$[CH_2C(CH_3)CO_2H]^{*-}$	--	--	--	2.0-3.7	4.65	Y	1.90E+10	1.90E+10	[114]
224	Methyl Methacrylate	$H_2C=C(CH_3)COOCH_3$	$[CH_2C(CH_3)CO_2CH_3]^{*-}$	--	--	--	9.2	--	--	1.30E+10	1.30E+10	[117]
225	trans-1,2-Dichloroethylene	ClCH=CHCl	$CHClCH + Cl^-$	Cl^- leaving	--	--	~6.5	--	--	7.50E+09	7.50E+09	[118]

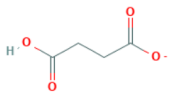
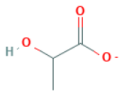
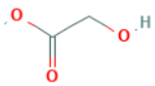
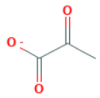
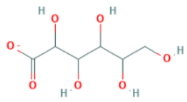
226	Trichloroethylene	$ClCH=CCl_2$	$^{*}CClCHCl + Cl^{-}$	Cl^{-} leaving	--	--	--	--	--	1.90E+10	1.90E+10	118
227	cis-1,2-Dichloroethylene	$H_2C=CCl_2$	$^{*}CClCH_2 + Cl^{-}$	Cl^{-} leaving	--	--	~6.5	--	--	2.30E+10	2.30E+10	118
228	1,3-Butadiene	$H_2C=CHCH=CH_2$	--	--	--	--	7	--	--	8.00E+09	8.00E+09	11
229	Acetaldehyde Oxime	$CH_3CH=NOH$	--	not specified	--	--	10.8	--	--	7.20E+07	7.20E+07	19
230	N,N-Dimethylacrylamide	$CH_2=CHCON(CH_3)_2$	$[CH_2CHCON(CH_3)_2]^{*-}$	--	--	--	9.2	--	--	1.60E+10	1.60E+10	117
231	Methacrylamide	$H_2C=C(CH_3)CONH_2$	$[CH_2C(CH_3)CONH_2]^{*-}$	--	--	--	9.2	--	--	2.40E+10	2.40E+10	117
232	Cyanoguanidine	$NCN=C(NH_2)_2$	$[H_2NC(=NH)NHCN]^{*-}$	--	--	0.002	3-4	--	--	1.20E+10	1.20E+10	120
233	Tetracyanoethylene	$(NC)_2C=C(CN)_2$	--	--	--	--	7	--	--	1.50E+10	1.50E+10	11
234	Methacrylate	$CH_2=C(CH_3)COO^{-}$	$[CH_2C(CH_3)CO_2]^{*2-}$	Reduction of COO^{-}	--	--	9.2	4.65	Y	4.50E+09	4.50E+09	114
235	3-Buten-1-ol	$H_2C=CHCH_2CH_2OH$	--	--	--	--	--	--	--	8.00E+05	2.45E+06	44
			--	--	--	--	--	--	--	4.10E+06		26
236	3-Buten-2-OL	$H_2C=CHCH(OH)CH_3$	--	--	--	--	--	--	--	5.90E+07	5.90E+07	26
237	3-Methylbut-2-enoate	$(CH_3)_2C=CHCO_2^{-}$	--	--	--	--	9.2	5.02	Y	6.40E+08	6.40E+08	121
238	3,3-Dimethylacrylic acid	$(CH_3)_2C=CHCOOH$	$[(CH_3)_2CCHCO_2H]^{*-}$	Reduction of COOH	--	--	2.0-3.7	5.02	Y	1.50E+10	2.45E+06	114
					--	--	3.7		Y	1.00E+10		121
239	Isocrotonate	$CH_3CH=CHCOO^{-}$	$[CH_3CHCHCO_2]^{*2-}$	Reduction of COO^{-}	--	--	9.2	4.9	Y	1.30E+09	1.30E+09	114
240	Hydrogen Fumarate	$HOOCCH=CHCOO^{-}$	--	--	--	0.000	--	--	--	9.00E+09	2.45E+06	21
				--	--	--	--	--	--	1.80E+10		88
241	Monomethyl Fumarate	$CH_3OOCCH=CHCOO^{-}$	--	--	--	--	--	--	--	1.30E+10	1.30E+10	88
242	2-Hydroxyethyl Acrylate	$CH_2=CHCOOCH_2CH_2OH$	$CH_2=CHC(O^{-})OCH_2CH_2OH$	--	--	--	11	--	--	7.50E+09	7.50E+09	122
243	trans-Aconitate(3-)	$^{-}OOCCH=C(COO^{-})CH_2COO^{-}$	--	--	--	--	11	2.8	Y	1.80E+08	1.80E+08	24
244	Acrylamide	$H_2C=CHCONH_2$	$[CH_2CHCONH_2]^{*-}$	--	--	--	--	--	--	1.50E+10	2.30E+10	85
				--	--	--	9.2	--	--	3.10E+10		117
				--	--	--	6.3	--	--	2.00E+10		71
				--	Log(A) = 13.372; Ea = 16 kJ/RT (temp 288-353 K)	--	--	--	--	3.30E+10		123
				--	--	--	7	--	--	2.10E+10		124
				--	--	--	7	--	--	1.80E+10		17
245	Crotonamide	$CH_3CH=CHCONH_2$	$[CH_3CHCHCONH_2]^{*-}$	--	--	--	9.2	--	--	1.30E+10	1.30E+10	117
246	4-(Ethylamino)-4-oxobut-2-enoate	$C_2H_5NHCOCH=CHCOO^{-}$	N-Ethylmaleamic acid, radical anion	--	--	--	7.9	2.85	Y	8.50E+09	8.50E+09	78
247	cis-Dimethyl Fumarate	$CH_3OOCCH=CHCOOCH_3$	--	--	--	--	9.2	--	--	3.20E+10	3.20E+10	88

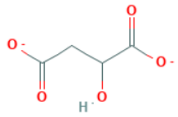
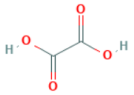
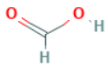
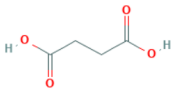
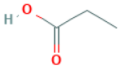
248	4-Penten-2-OL	$H_2C=CHCH_2CH(OH)CH_3$	--	--	--	--	--	--	--	5.00E+05	5.00E+05	44
249	Guanidine	$H_2NC(=NH)NH_2$	--	--	--	--	6.1	--	--	2.50E+08	2.00E+08	91
			--	--	--	--	11.1	--	--	1.90E+08		
			--	--	--	--	11.9	--	--	1.60E+08		
250	Ethyl Acrylate	$H_2C=CHCOOC_2H_5$	--	C-O bond cleavage	--	--	11	--	--	8.70E+09	8.70E+09	116
251	Acetone Oxime	$(CH_3)_2C=NOH$	--	--	--	--	7	--	--	3.50E+08	3.25E+08	71
			--	--		--	7.75	--	--	3.00E+08		19

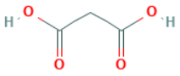
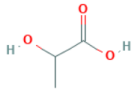
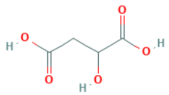
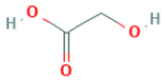
[a]pH shown as reported

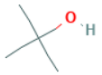
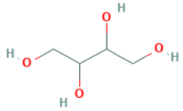
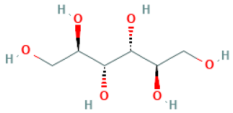
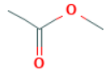
Table S4: E_{red} of all possible attacking sites in each aliphatic compound in the dataset.

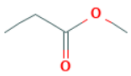
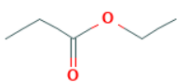
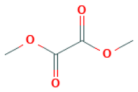
Class	No.	Name	Chemical Formula	2D Chemical Structure	Reduction Mechanism	Association		Concerted		Stepwise		k_{chem} (M^{-1} s^{-1})
						$\Delta G°_{red,aq}$ (k_{cal}/mol)	$E°_{red}$ (V vs SHE)	$\Delta G°_{red,aq}$ (k_{cal}/mol)	$E°_{red}$ (V vs SHE)	$\Delta G°_{red,aq}$ (k_{cal}/mol)	$E°_{red}$ (V vs SHE)	
Alkane	1	Methane	CH_4		$CH_4 + e^- \rightarrow [CH_4]^{*-}$	25.968	-5.41[a]	--	--	--	--	1.00×10^7
	2	Propane	$CH_3CH_2CH_3$		$CH_3CH_2CH_3 + e^- \rightarrow [CH_3CH_2CH_3]^{*-}$	23.745	-5.31[a]	--	--	--	--	2.10×10^6
	3	Butane	C_4H_{10}		$C_4H_{10} + e^- \rightarrow [C_4H_{10}]^{*-}$	22.767	-5.27[a]	--	--	--	--	2.40×10^6
Carboxylate	4	Oxalate	$^-OOCCOO^-$		$^-O_2C_2O_2^- + e^- \rightarrow {}^-OOC{*}COO^{2-}$	-29.943	-2.98[b]	--	--	--	--	2.28×10^7
	5	Formate	$HCOO^-$		$HCOO^- + e^- \rightarrow H{*}CO(-)O^-$	-9.935	-3.85[b]	--	--	--	--	5.04×10^5
	6	Succinate	$^-OOC(CH_2)_2COO^-$		$^-O_2C(CH_2)_2CO_2^- + e^- \rightarrow {}^-OOC(CH_2)_2{*}COO^{2-}$	-8.725	-3.90[b]	--	--	--	--	1.59×10^7
					$^-O_2C(CH_2)_2CO_2^- + e^- \rightarrow [OOC(CH_2)CHCOO]^{3-} + H{*}$	--	--	28.987	-5.54[a]	--	--	
	7	Acetate	CH_3COO^-		$CH_3COO^- + e^- \rightarrow CH_3{*}CO(-)O^-$	-8.070	-3.93[b]	--	--	--	--	1.05×10^6
	8	Hydrogen Oxalate	$HOOCCOO^-$		$HOOCCOO^- + e^- \rightarrow HOOC{*}CO(-)O^-$	-52.207	-2.02[b]	--	--	--	--	3.65×10^9
					$HOOCCOO^- + e^- \rightarrow OC{*}COO^- + OH^-$	--	--	1.670	-4.35[a]	--	--	
	9	Malonate	$^-OOC\text{-}CH_2\text{-}COO^-$		$^-OOCCH_2COO^- + e^- \rightarrow \text{-}OOCCH_2{*}CO(-)O^-$	-9.073	-3.89[b]	--	--	--	--	1.00×10^7
					$^-OOCCH_2COO^- + e^- \rightarrow {}^-OOCCHCO(-)O^- + H{*}$	--	--	13.960	-4.89[a]	--	--	
	10	Malonate(1-)	$HOOC\text{-}CH_2\text{-}COO^-$		$HOOCCH_2COO^- + e^- \rightarrow HOOCCH_2{*}CO(-)O^-$	-35.927	-2.72[b]	--	--	--	--	5.06×10^8

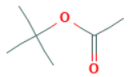
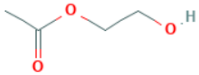
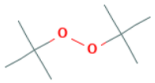
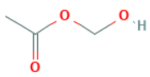
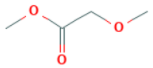
				$HOOCCH_2COO^- + e^- \rightarrow OC^*CH_2COO^- + OH^-$	--	--	5.142	-4.50 [a]	--	--	
11	Succinate(1-)	$HOOC(CH_2)_2COO^-$		$HOOC(CH_2)_2COO^- + e^- \rightarrow HOOC(CH_2)_2{}^*CO(-)O^-$	-32.735	-2.86 [b]	--	--	--	--	2.05×10^8
				$HOOC(CH_2)_2COO^- + e\text{-} \rightarrow OC^*(CH_2)_2COO^- + OH^-$	--	--	7.757	-4.62 [a]	--	--	
12	Lactate	$CH_3CHOHCOO^-$		$CH_3CHOHCOO^- + e^- \rightarrow CH_3CHOH^*CO(-)O^-$	-5.700	-4.03 [b]	--	--	--	--	1.00×10^7
				$CH_3CHOHCOO^- + e^- \rightarrow CH_3CH^*COO^- + OH^-$	--	--	-12.063	-3.76 [a]	--	--	
13	Glycolate	$HOCH_2COO^-$		$HOCH_2COO^- + e^- \rightarrow HOCH_2{}^*CO(-)O^-$	-6.606	-3.99 [b]	--	--	--	--	8.20×10^6
				$HOCH_2COO^- + e^- \rightarrow [OCH_2COO]^{2-} + H^*$	--	--	6.926	-4.58 [a]	--	--	
				$HOCH_2COO^- + e^- \rightarrow [HOCHCOO]^{2-} + H^*$	--	--	28.841	-5.53 [a]	--	--	
				$HOCH_2COO^- + e^- \rightarrow {}^*CH_2COO^- + OH\text{-}$	--	--	-10.115	-3.84 [a]	--	--	
14	Pyruvate	CH_3COCOO^-		$CH_3COCOO^- + e^- \rightarrow [CH_3COCOO]^{*2-}$	-50.939	-2.07 [b]	--	--	--	--	6.80×10^9
				$CH_3COCOO^- + e^- \rightarrow [CH_2COCOO]^{2-} + H^*$	--	--	-3.486	-4.13 [a]	--	--	
15	CID_4134252	$HOCH_2(CHOH)_4COO^-$		$HOCH_2(CHOH)_4COO^- + e^- \rightarrow [HOCH_2(CHOH)_4COO^-]^{*-}$	-13.587	-3.69 [b]	--	--	--	--	1.00×10^6
				$HOCH_2(CHOH)_4COO^- + e^- \rightarrow {}^*CH_2(CHOH)_4COO^- + OH^-$	--	--	-9.684	-3.86 [a]	--	--	
				$HOCH_2(CHOH)_4COO^- + e^- \rightarrow HOCH_2{}^*CH(CHOH)_3COO^- + OH^-$	--	--	-7.585	-3.95 [a]	--	--	
				$HOCH_2(CHOH)_4COO^- + e^- \rightarrow HOCH_2CHOH^*CH(CHOH)_2COO^- + OH^-$	--	--	-8.980	-3.89 [a]	--	--	

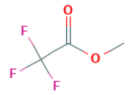
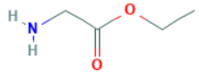
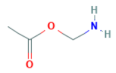
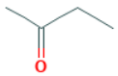
					$HOCH_2(CHOH)_4COO^- + e^- \rightarrow HOCH_2CHOHCHOH^*CHCHOHCOO^- + OH^-$	--	--	-13.703	-3.69 [a]	--	--	
					$HOCH_2(CHOH)_4COO^- + e^- \rightarrow HOCH_2(CHOH)_3{}^*CHCOO^- + OH^-$	--	--	-13.307	-3.70 [a]	--	--	
	16	Malate	$^-OOCCH_2CHOHCOO^-$		$^-OOCCH_2CHOHCOO^- + e^- \rightarrow [^-OOCCH_2CHOHCOO^-]^{*-}$	-11.815	-3.77 [b]	--	--	--	--	
					$^-OOCCH_2CHOHCOO^- + e^- \rightarrow [^-OOCCH_2CHOCOO^-]^- + H^*$	--	--	8.850	-4.66 [a]	--	--	
					$^-OOCCH_2CHOHCOO^- + e^- \rightarrow [^-OOCCH_2COHCOO^-]^- + H^*$	--	--	32.830	-5.70 [a]	--	--	6.01×10^{7}
					$^-OOCCH_2CHOHCOO^- + e^- \rightarrow [^-OOCCHCHOHCOO^-]^- + H^*$	--	--	24.844	-5.36 [a]	--	--	
					$^-OOCCH_2CHOHCOO^- + e^- \rightarrow {}^-OOCCH_2CH^*COO^- + OH^-$	--	--	-11.626	-3.78 [a]	--	--	
Carboxylic Acid	17	Oxalic Acid	HOOCCOOH		$HO_2C_2O_2H + e^- \rightarrow HOOC^*CO(-)OH$	-62.942	-1.55 [b]	--	--	--	--	2.50×10^{10}
					$HO_2C_2O_2H + e^- \rightarrow HOOC^*CO + OH^-$	--	--	10.378	-4.73 [a]	--	--	
	18	Formic Acid	HCOOH		$HCOOH + e^- \rightarrow H^*CO(-)OH$	-39.005	-2.59 [b]	--	--	--	--	1.41×10^{8}
					$HCOOH + e^- \rightarrow H^*CO + OH^-$	--	--	6.357	-4.56 [a]	--	--	
	19	Succinic Acid	$HOOC(CH_2)_2COOH$		$HO_2C(CH_2)_2CO_2H + e^- \rightarrow HOOC(CH_2)_2{}^*CO(-)OH$	-35.299	-2.75 [b]	--	--	--	--	
					$HO_2C(CH_2)_2CO_2H + e^- \rightarrow [HOOC(CH_2)CHCOOH]^- + H^*$	--	--	-2.834	-4.16 [a]	--	--	2.30×10^{8}
					$HO_2C(CH_2)_2CO_2H + e^- \rightarrow HOOC(CH_2)_2{}^*CO + OH^-$	--	--	7.496	-4.60 [a]	--	--	
	20	Propionic Acid	CH_3CH_2COOH		$CH_3CH_2COOH + e^- \rightarrow CH_3CH_2{}^*CO(-)OH$	-35.025	-2.76 [b]	--	--	--	--	2.20×10^{7}

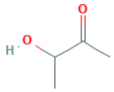
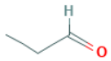
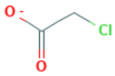
				$CH_3CH_2COOH + e^- \rightarrow [CH_3CHCOOH]^- + H^*$	--	--	1.168	-4.33 [a]	--	--	
				$CH_3CH_2COOH + e^- \rightarrow [CH_2CH_2COOH]^- + H^*$	--	--	33.426	-5.73 [a]	--	--	
				$CH_3CH_2COOH + e^- \rightarrow CH_3CH_2{}^*CO + OH^-$	--	--	6.418	-4.56 [a]	--	--	
21	Acetic Acid	CH_3COOH		$CH_3COOH + e^- \rightarrow CH_3{}^*CO(-)OH$	-32.160	-2.89[b]	--	--	--	--	2.02×10^8
				$CH_3COOH + e^- \rightarrow CH_3{}^*CO + OH^-$	--	--	6.511	-4.56 [a]	--	--	
22	Malonic Acid	$HOOC\text{-}CH_2\text{-}COOH$		$HOOCCH_2COOH + e^- \rightarrow HOOCCH_2{}^*CO(-)OH$	-40.827	-2.51[b]	--	--	--	--	3.03×10^9
				$HOOCCH_2COOH + e^- \rightarrow HOOCCH_2{}^*CO + OH^-$	--	--	9.316	-4.68 [a]	--	--	
23	Lactic Acid	$CH_3CH(OH)COOH$		$CH_3CH(OH)COOH + e^- \rightarrow CH_3CH(OH)^*CO(-)OH$	-38.233	-2.62[b]	--	--	--	--	7.36×10^8
				$CH_3CH(OH)COOH + e^- \rightarrow CH_3CH(OH)^*CO + OH^-$	--	--	7.089	-4.59 [a]	--	--	
				$CH_3CH(OH)COOH + e^- \rightarrow CH_3CH^*COOH + OH^-$	--	--	-18.547	-3.48 [a]	--	--	
24	Malic Acid	$HOOCCH_2CH(OH)COOH$		$HOOCCH_2CH(OH)COOH + e^- \rightarrow HO(-)OC^*CH_2CH(OH)COOH$	-41.244	-2.49[b]	--	--	--	--	3.41×10^9
				$HOOCCH_2CH(OH)COOH + e^- \rightarrow OC^*CH_2CH(OH)COOH + OH^-$	--	--	7.383	-4.60 [a]	--	--	
				$HOOCCH_2CH(OH)COOH + e^- \rightarrow HOOCCH_2CH^*COOH + OH^-$	--	--	6.874	-4.58 [a]	--	--	
25	Glycolic acid	$HOCH_2COOH$		$HOCH_2COOH + e^- \rightarrow HOCH_2{}^*CO(-)OH$	-40.415	-2.53[b]	--	--	--	--	4.38×10^8
				$HOCH_2COOH + e^- \rightarrow [HOCHCOOH]^- + H^*$	--	--	0.331	-4.29 [a]	--	--	

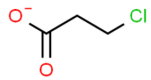
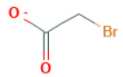
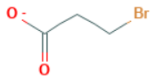
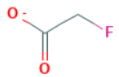
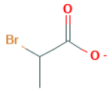
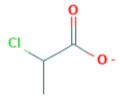
					$HOCH_2COOH + e^- \rightarrow [OCH_2COOH]^- + H^*$	--	--	-4.933	-4.07 [a]	--	--	
					$HOCH_2COOH + e^- \rightarrow HOCH_2{}^*CO + OH^-$	--	--	6.645	-4.57 [a]	--	--	
					$HOCH_2COOH + e^- \rightarrow {}^*CH_2COOH + OH^-$	--	--	-15.503	-3.61 [a]	--	--	
	26	Methanediol	$CH_2(OH)_2$		$CH_2(OH)_2 + e^- \rightarrow [CH_2(OH)_2]^{*-}$	-13.523	-3.69[b]	--	--	--	--	1.00×10^7
					$CH_2(OH)_2 + e^- \rightarrow {}^*CH_2OH + OH^-$	--	--	-6.929	-3.98 [a]	--	--	
	27	Tert-Butanol	$(CH_3)_3$-C-OH		$(CH_3)_3$-C-OH + $e^- \rightarrow [(CH_3)_3$-C-OH$]^{*-}$	-6.326	-4.01[b]	--	--	--	--	4.00×10^5
					$(CH_3)_3$-C-OH + $e^- \rightarrow (CH_3)_3$-*C + OH^-	--	--	-10.962	-3.80 [a]	--	--	
Alcohol	28	Butane-1,2,3,4	$HOCH_2[CH(OH)]_2CH_2OH$		$HOCH_2[CH(OH)]_2CH_2OH + e^- \rightarrow [HOCH_2[CH(OH)]_2CH_2OH]^{*-}$	-11.497	-3.78[b]	--	--	--	--	5.00×10^6
					$HOCH_2[CH(OH)]_2CH_2OH + e^- \rightarrow HOCH_2[CH(OH)]_2{}^*CH_2 + OH^-$	--	--	-8.412	-3.92 [a]	--	--	
					$HOCH_2[CH(OH)]_2CH_2OH + e^- \rightarrow HOCH_2CH(OH)^*CHCH_2OH + OH^-$	--	--	-7.991	-3.93 [a]	--	--	
	29	Mannitol	$HOCH_2[CH(OH)]_4CH_2OH$		$HOCH_2[CH(OH)]_4CH_2OH + e^- \rightarrow [HOCH_2[CH(OH)]_4CH_2OH]^{*-}$	-16.741	-3.55[b]	--	--	--	--	8.50×10^6
					$HOCH_2[CH(OH)]_4CH_2OH + e^- \rightarrow HOCH_2[CH(OH)]_4{}^*CH_2 + OH^-$	--	--	-9.942	-3.85 [a]	--	--	
					$HOCH_2[CH(OH)]_4CH_2OH + e^- \rightarrow [HOCH_2[CH(OH)]_3{}^*CHCH_2OH + OH^-$	--	--	-9.885	-3.85 [a]	--	--	
					$HOCH_2[CH(OH)]_4CH_2OH + e^- \rightarrow HOCH_2[CH(OH)]_2{}^*CHCHOHCH_2OH + OH^-$	--	--	-10.336	-3.83 [a]	--	--	
Ester	30	Methyl Acetate	CH_3COOCH_3		$CH_3COOCH_3 + e^- \rightarrow CH_3{}^*CO(-)OCH_3$	-33.562	-2.82[b]	--	--	--	--	8.73×10^7

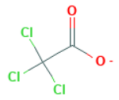
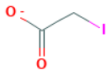
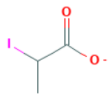
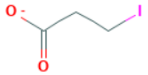
				$CH_3COOCH_3 + e^- \rightarrow [CH_3COOCH_2]^- + H^*$	--	--	0.326	-4.29 [a]	--	--	
				$CH_3COOCH_3 + e^- \rightarrow CH_3{}^*CO + {}^-OCH_3$	--	--	-2.110	-4.19 [a]	--	--	
				$CH_3COOCH_3 + e^- \rightarrow CH_3COO^- + {}^*CH_3$	--	--	-49.229	-2.15 [a]	--	--	
31	Methyl Propionate	$C_2H_5COOCH_3$		$C_2H_5COOCH_3 + e^- \rightarrow C_2H_5{}^*CO(-)OCH_3$	-33.244	-2.84 [b]	--	--	--	--	9.03×10^{7}
				$C_2H_5COOCH_3 + e^- \rightarrow [C_2H_5COOCH_2]^- + H^*$	--	--	0.704	-4.31 [a]	--	--	
				$C_2H_5COOCH_3 + e^- \rightarrow [CH_3CHCOOCH_3]^- + H^*$	--	--	33.583	-5.74 [a]	--	--	
				$C_2H_5COOCH_3 + e^- \rightarrow [CH_2CH_2COOCH_3]^- + H^*$	--	--	28.489	-5.52 [a]	--	--	
				$C_2H_5COOCH_3 + e^- \rightarrow C_2H_5{}^*CO + {}^-OCH_3$	--	--	-2.429	-4.17 [a]	--	--	
				$C_2H_5COOCH_3 + e^- \rightarrow C_2H_5{}^*COO^- + {}^*CH_3$	--	--	-49.257	-2.14 [a]	--	--	
32	Ethyl Propionate	$C_2H_5COOC_2H_5$		$C_2H_5COOC_2H_5 + e^- \rightarrow C_2H_5{}^*CO(-)OC_2H_5$	-33.220	-2.84 [b]	--	--	--	--	7.52×10^{7}
				$C_2H_5COOC_2H_5 + e^- \rightarrow [CH_3CHCOOC_2H_5]^- + H^*$	--	--	0.606	-4.31 [a]	--	--	
				$C_2H_5COOC_2H_5 + e^- \rightarrow [CH_2CH_2COOC_2H_5]^- + H^*$	--	--	33.721	-5.74 [a]	--	--	
				$C_2H_5COOC_2H_5 + e^- \rightarrow C_2H_5COO^- + {}^*C_2H_5$	--	--	-49.535	-2.13 [a]	--	--	
33	Dimethyl Oxalate	$CH_3OOCCOOCH_3$		$CH_3OOCCOOCH_3 + e^- \rightarrow CH_3OOC{}^*CO(-)OCH_3$	-59.029	-1.72 [b]	--	--	--	--	1.04×10^{11}
				$CH_3OOCCOOCH_3 + e^- \rightarrow CH_3OOCCOO^- + {}^*CH_3$	--	--	-59.324	-1.71 [a]	--	--	

34	Tert-butyl Acetate	$(CH_3)_3CCOOCH_3$		$(CH_3)_3CCOOCH_3 + e^- \rightarrow (CH_3)_3C^*CO(-)OCH_3$	-30.196	-2.97[b]	--	--	--	--	2.30×10^7
				$(CH_3)_3CCOOCH_3 + e^- \rightarrow CCOO(-)CH_3 + *(CH_3)_3$	--	--	-53.704	-1.95[a]	--	--	
35	2-Hydroxyethyl Acetate	$CH_3COOCH_2CH_2OH$		$CH_3COOCH_2CH_2OH + e^- \rightarrow CH_3^*CO(-)OCH_2CH_2OH$	-33.275	-2.84[b]	--	--	--	--	2.60×10^7
				$CH_3COOCH_2CH_2OH + e^- \rightarrow CH_3COO^- + *CH_2CH_2OH$	--	--	-51.150	-2.06[a]	--	--	
36	Di-tert-butyl Peroxide	$(CH_3)_3\text{-}COOC(CH_3)_3$		$(CH_3)_3COOC(CH_3)_3 + e^- \rightarrow (CH_3)_3^*CO(-)OC(CH_3)_3$	-134.702	1.56[a]	--	--	--	--	1.41×10^8
				$(CH_3)_3COOC(CH_3)_3 + e^- \rightarrow (CH_3)_3CO^* + {}^-OC(CH_3)_3$	--	--	44.927	-6.23[a]	--	--	
37	Methylene glycol monoacetate	$HOCH_2COOCH_3$		$HOCH_2COOCH_3 + e^- \rightarrow HOCH_2^*CO(-)OCH_3$	-37.368	-2.66[b]	--	--	--	--	4.90×10^8
				$HOCH_2COOCH_3 + e^- \rightarrow [HOCH_2COOCH_2]^- + H^*$	--	--	-3.063	-4.15[a]	--	--	
				$HOCH_2COOCH_3 + e^- \rightarrow [HOCHCOOCH_3]^- + H^*$	--	--	26.806	-5.44[a]	--	--	
				$HOCH_2COOCH_3 + e^- \rightarrow [OCH_2COOCH_3]^- + H^*$	--	--	-18.410	-3.48[a]	--	--	
				$HOCH_2COOCH_3 + e^- \rightarrow {}^*COO(-)CH_3 + HOCH_2$	--	--	-47.078	-2.24[a]	--	--	
38	Methyl methoxyacetate	$CH_3OCH_2COOCH_3$		$CH_3OCH_2COOCH_3 + e^- \rightarrow CH_3OCH_2^*CO(-)OCH_3$	-38.037	-2.63[b]	--	--	--	--	4.48×10^8
				$CH_3OCH_2COOCH_3 + e^- \rightarrow [CH_3OCH_2COOCH_2]^- + H^*$	--	--	26.108	-5.41[a]	--	--	
				$CH_3OCH_2COOCH_3 + e^- \rightarrow [CH_3OCHCOOCH_3]^- + H^*$	--	--	0.321	-4.29[a]	--	--	
				$CH_3OCH_2COOCH_3 + e^- \rightarrow [CH_2OCH_2COOCH_3]^- + H^*$	--	--	31.663	-5.65[a]	--	--	

					$CH_3OCH_2COOCH_3 + e^- \rightarrow CH_3OCH_2COO^- + {}^*CH_3$	--	--	-51.620	-2.04 [a]	--	--	
					$CH_3OCH_2COOCH_3 + e^- \rightarrow {}^*CH_3 + {}^-OCH_2COOCH_3$	--	--	-27.406	-3.09 [a]	--	--	
	39	Methyl trifluoroacetate	CF_3COOCH_3		$CF_3COOCH_3 + e^- \rightarrow CF_3{}^*CO(-)OCH_3$	-55.217	-1.89[b]	--	--	--	--	2.06×10^9
					$CF_3COOCH_3 + e^- \rightarrow CF_2COOCH_3 + F^-$	--	--	10.892	-4.75 [a]	28.138	-5.50[c]	
	40	Ethyl glycinate	$NH_2CH_2COOC_2H_5$		$NH_2CH_2COOC_2H_5 + e^- \rightarrow NH_2CH_2{}^*CO(-)OC_2H_5$	-34.863	-2.77[b]	--	--	--	--	8.58×10^8
	41	Acetoxymethylamine	$H_2NCH_2COOCH_3$		$H_2NCH_2COOCH_3 + e^- \rightarrow H_2NCH_2{}^*CO(-)OCH_3$	-32.451	-2.87[b]	--	--	--	--	3.14×10^8
Ether	42	Diethyl Ether	$(C_2H_5)_2O$		$CH_3CH_2OCH_2CH_3 + e^- \rightarrow [CH_3CH_2OCH_2CH_3]^{*-}$	23.466	-5.30[a]	--	--	--	--	1.00×10^7
					$CH_3CH_2OCH_2CH_3 + e^- \rightarrow CH_3{}^*CH_2 + (-)OCH_2CH_3$	--	--	-38.953	-2.59 [a]	--	--	
					$CH_3CH_2OCH_2CH_3 + e^- \rightarrow [CH_2CH_2OCH_2CH_3]^- + H^*$	--	--	30.857	-5.62 [a]	--	--	
					$CH_3CH_2OCH_2CH_3 + e^- \rightarrow [CH_3CHOCH_2CH_3]^- + H^*$	--	--	37.511	-5.91 [a]	--	--	
Ketone	43	Acetone	CH_3COCH_3		$CH_3COCH_3 + e^- \rightarrow CH_3{}^*CO(-)CH_3$	-38.955	-2.59[b]	--	--	--	--	8.90×10^9
					$CH_3COCH_3 + e^- \rightarrow [CH_2COCH_3]^- + H^*$	--	--	-4.570	-4.08 [a]	--	--	
	44	Methyl Ethyl Ketone	$CH_3CH_2COCH_3$		$CH_3CH_2COCH_3 + e^- \rightarrow CH_3CH_2{}^*CO(-)CH_3$	-38.719	-2.60[b]	--	--	--	--	6.11×10^9
					$CH_3CH_2COCH_3 + e^- \rightarrow [CH_3CH_2COCH_2]^- + H^*$	--	--	-3.653	-4.12 [a]	--	--	
					$CH_3CH_2COCH_3 + e^- \rightarrow [CH_3CHCOCH_3]^- + H^*$	--	--	33.035	-5.71 [a]	--	--	

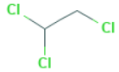
					$CH_3CH_2COCH_3 + e^- \rightarrow [CH_2CH_2COCH_3]^- + H^*$	--	--	-3.304	-4.14 [a]	--	--	
	45	2,3-Butanedione	$CH_3COCOCH_3$		$CH_3COCOCH_3 + e^- \rightarrow CH_3{*}CO(-)COCH_3$	-69.049	-1.29[b]	--	--	--	--	1.67×10^{10}
	46	Acetoin	$CH_3COCH(OH)CH_3$		$CH_3COCH(OH)CH_3 + e^- \rightarrow CH_3{*}CO(-)CH(OH)CH_3$	-43.759	-2.38[b]	--	--	--	--	
					$CH_3COCH(OH)CH_3 + e^- \rightarrow [CH_3COCH(OH)CH_2]^- + H^*$	--	--	11.615	-4.78 [a]	--	--	
					$CH_3COCH(OH)CH_3 + e^- \rightarrow [CH_3COCH(O)CH_3]^- + H^*$	--	--	-1.714	-4.21 [a]	--	--	7.95×10^{9}
					$CH_3COCH(OH)CH_3 + e^- \rightarrow [CH_3COC(OH)CH_3]^- + H^*$	--	--	-2.584	-4.17 [a]	--	--	
					$CH_3COCH(OH)CH_3 + e^- \rightarrow [CH_2COCH(OH)CH_3]^- + H^*$	--	--	-8.967	-3.89 [a]	--	--	
Aldehyde	47	Acetaldehyde	CH_3CHO		$CH_3CHO + e^- \rightarrow CH_3{*}CHO(-)$	-44.971	-2.33[b]	--	--	--	--	6.11×10^{9}
					$CH_3CHO + e^- \rightarrow [CH_2CHO]^- + H^*$	--	--	-7.263	-3.97 [a]	--	--	
	48	Propionaldehyde	CH_3CH_2CHO		$CH_3CH_2CHO + e^- \rightarrow CH_3CH_2{*}CHO(-)$	-44.416	-2.35[b]	--	--	--	--	
					$CH_3CH_2CHO + e^- \rightarrow [CH_3CHCHO]^- + H^*$	--	--	-5.969	-4.02 [a]	--	--	4.43×10^{9}
					$CH_3CH_2CHO + e^- \rightarrow [CH_2CH_2CHO]^- + H^*$	--	--	30.949	-5.62 [a]	--	--	
Halocarboxylate	49	Chloroacetate	$ClCH_2COO^-$		$ClCH_2COO^- + e^- \rightarrow ClCH_2{*}CO(-)O^-$	-12.632	-3.73 [c]	--	--	--	--	
					$ClCH_2COO^- + e^- \rightarrow {*}CH_2COO^- + Cl^-$	--	--	-50.627	-2.08 [c]	10.403	-4.73 [c]	1.09×10^{9}
					$ClCH_2COO^- + e^- \rightarrow [ClCHCOO]^{2-} + H^*$	--	--	5.808	-4.53 [c]	--	--	

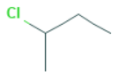
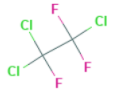
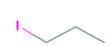
50	3-Chloropropanoate	$Cl(CH_2)_2COO^-$		$Cl(CH_2)_2COO^- + e^- \rightarrow Cl(CH_2)_2{*}CO(-)O^-$	-12.823	-3.72 [c]	--	--	--	--	
				$Cl(CH_2)_2COO^- + e^- \rightarrow {*}(CH_2)_2COO^- + Cl^-$	--	--	-46.439	-2.27 [c]	12.921	-4.84 [c]	4.40×10^8
				$Cl(CH_2)_2COO^- + e^- \rightarrow [ClCH_2CHCOO]^{2-} + H{*}$	--	--	20.851	-5.18 [c]	--	--	
51	Bromoacetate	$BrCH_2COO^-$		$BrCH_2COO^- + e^- \rightarrow BrCH_2{*}CO(-)O^-$	-67.468	-1.35 [c]	--	--	--	--	
				$BrCH_2COO^- + e^- \rightarrow {*}CH_2COO^- + Br^-$	--	--	-19.940	-3.42 [c]	11.540	-4.78 [c]	8.03×10^9
				$BrCH_2COO^- + e^- \rightarrow [BrCHCOO]^{2-} + H{*}$	--	--	7.739	-4.62 [c]	--	--	
52	3-Bromopropanoate	$Br(CH_2)_2COO^-$		$Br(CH_2)_2COO^- + e^- \rightarrow Br(CH_2)_2{*}CO(-)O^-$	-62.640	-1.56 [c]	--	--	--	--	
				$Br(CH_2)_2COO^- + e^- \rightarrow {*}(CH_2)_2COO^- + Br^-$	--	--	-14.680	-3.64 [c]	15.242	-4.94 [c]	2.70×10^9
53	Fluoroacetate	FCH_2COO^-		$FCH_2COO^- + e^- \rightarrow FCH_2{*}CO(-)O^-$	-15.028	-3.63 [c]	--	--	--	--	
				$FCH_2COO^- + e^- \rightarrow {*}CH_2COO^- + F^-$	--	--	4.487	-4.47 [c]	66.820	-7.18 [c]	1.20×10^6
				$FCH_2COO^- + e^- \rightarrow [FCHCOO]^{2-} + H{*}$	--	--	11.537	-4.78 [c]	--	--	
54	2-Bromopropanoate	$CH_3CHBrCOO^-$		$CH_3CHBrCOO^- + e^- \rightarrow CH_3CHBr{*}CO(-)O^-$	-71.420	-1.18 [c]	--	--	--	--	
				$CH_3CHBrCOO^- + e^- \rightarrow CH_3{*}CHCOO^- + Br^-$	--	--	-22.907	-3.29 [c]	6.181	-4.55 [c]	5.30×10^9
55	2-Chloropropanoate	$CH_3CHClCOO^-$		$CH_3CHClCOO^- + e^- \rightarrow CH_3CHCl{*}CO(-)O^-$	-73.686	-1.09 [c]	--	--	--	--	
				$CH_3CHClCOO^- + e^- \rightarrow CH_3{*}CHCOO^- + Cl^-$	--	--	-54.101	-1.93 [c]	5.260	-4.51 [c]	1.40×10^9

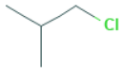
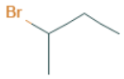
	56	Trichloroacetate	Cl_3CCOO^-		$Cl_3CCOO^- + e^- \rightarrow Cl_3C^*CO(-)O^-$	-84.532	-0.61 [c]	--	--	--	--	1.22×10^{10}
					$Cl_3CCOO^- + e^- \rightarrow Cl_2{}^*CCOO^- + Cl^-$	--	--	-65.405	-1.44 [c]	1.905	-4.36 [c]	
	57	2-Iodoacetate	ICH_2COO^-		$ICH_2COO^- + e^- \rightarrow ICH_2{}^*CO(-)O^-$	-76.428	-0.97[d]	--	--	--	--	1.20×10^{10}
					$ICH_2COO^- + e^- \rightarrow {}^*CH_2COO^- + I^-$	--	--	-78.042	-0.90 [d]	5.889	-4.54 [d]	
	58	2-Iodopropanoate	$CH_3CHICOO^-$		$CH_3CHICOO^- + e^- \rightarrow CH_3CHI^*CO(-)O^-$	-81.881	-0.73 [d]	--	--	--	--	6.60×10^{9}
					$CH_3CHICOO^- + e^- \rightarrow CH_3CH^*COO^- + I^-$	--	--	-83.383	-0.66 [d]	-1.077	-4.23 [d]	
	59	3-Iodanylpropanoate	$ICH_2CH_2COO^-$		$ICH_2CH_2COO^- + e^- \rightarrow ICH_2CH_2{}^*CO(-)O^-$	-74.691	-1.04 [d]	--	--	--	--	5.80×10^{9}
					$ICH_2CH_2COO^- + e^- \rightarrow {}^*CH_2CH_2COO^- + I^-$	--	--	-76.123	-0.98 [d]	6.459	-4.56 [d]	
Haloalkane	60	Chloromethane	CH_3Cl		$CH_3Cl + e^- \rightarrow [CH_3Cl]^{*-}$	-65.941	-1.42 [c]	--	--	--	--	8.33×10^{8}
					$CH_3Cl + e^- \rightarrow {}^*CH_3 + Cl^-$	--	--	-69.845	-1.25 [c]	-66.194	-1.41 [c]	
	61	Dibromomethane	CH_2Br_2		$CH_2Br_2 + e^- \rightarrow [CH_2Br_2]^{*-}$	-68.953	-1.29 [c]	--	--	--	--	1.10×10^{11}
					$CH_2Br_2 + e^- \rightarrow {}^*CH_2Br + Br^-$	--	--	-73.001	-1.11 [c]	-74.164	-1.06 [c]	
	62	Bromoform	$CHBr_3$		$CHBr_3 + e^- \rightarrow [CHBr_3]^{*-}$	-76.889	-0.95 [c]	--	--	--	--	1.67×10^{10}
					$CHBr_3 + e^- \rightarrow {}^*CHBr_2 + Br^-$	--	--	-80.061	-0.81 [c]	-83.885	-0.64 [c]	
	63	Bromoethane	CH_3CH_2Br		$CH_3CH_2Br + e^- \rightarrow [CH_3CH_2Br]^{*-}$	-64.174	-1.50 [c]	--	--	--	--	1.89×10^{10}

				$CH_3CH_2Br + e^- \rightarrow {}^*CH_3CH_2 + Br^-$	--	--	-67.927	-1.33 [c]	-66.744	-1.39 [c]	
64	Bromopropane	$CH_3CH_2CH_2Br$		$CH_3CH_2CH_2Br + e^- \rightarrow [CH_3CH_2CH_2Br]^{*-}$	-63.130	-1.54 [c]	--	--	--	--	1.47×10^{10}
				$CH_3CH_2CH_2Br + e^- \rightarrow {}^*CH_3CH_2CH_2 + Br^-$	--	--	-67.546	-1.35 [c]	-68.672	-1.30 [c]	
65	Chloropropane	$CH_3CH_2CH_2Cl$		$CH_3CH_2CH_2Cl + e^- \rightarrow [CH_3CH_2CH_2Cl]^{*-}$	-65.761	-1.43 [c]	--	--	--	--	6.85×10^{8}
				$CH_3CH_2CH_2Cl + e^- \rightarrow {}^*CH_3CH_2CH_2 + Cl^-$	--	--	-70.862	-1.21 [c]	-70.353	-1.23 [c]	
66	Chloroethane	CH_3CH_2Cl		$CH_3CH_2Cl + e^- \rightarrow [CH_3CH_2Cl]^{*-}$	-13.127	-3.71 [c]	--	--	--	--	7.21×10^{8}
				$CH_3CH_2Cl + e^- \rightarrow {}^*CH_3CH_2 + Cl^-$	--	--	-71.030	-1.20 [c]	-68.735	-1.30 [c]	
67	1-Bromo-2-chloroethane	CH_2ClCH_2Br		$CH_2ClCH_2Br + e^- \rightarrow [CH_2Cl{}^*CH_2Br]^{*-}$	-67.334	-1.36 [c]	--	--	--	--	
				$CH_2ClCH_2Br + e^- \rightarrow CH_2Cl{}^*CH_2 + Br^-$	--	--	-70.607	-1.22 [c]	-72.145	-1.15 [c]	1.18×10^{10}
				$CH_2ClCH_2Br + e^- \rightarrow {}^*CH_2CH_2Br + Cl^-$	--	--	-63.714	-1.52 [c]	-76.683	-0.96 [c]	
68	Halothane	$CF_3CHClBr$		$CF_3CHClBr + e^- \rightarrow [CF_3{}^*CHClBr]^{*-}$	-75.421	-1.01 [c]	--	--	--	--	
				$CF_3CHClBr + e^- \rightarrow CF_3{}^*CHCl + Br^-$	--	--	-79.440	-0.84 [c]	-82.086	-0.72 [c]	3.22×10^{10}
				$CF_3CHClBr + e^- \rightarrow CF_3{}^*CHBr + Cl^-$	--	--	-69.655	-1.26 [c]	-84.961	-0.60 [c]	
69	1,1-Dichloroethane	CH_3CHCl_2		$CH_3CHCl_2 + e^- \rightarrow [CH_3CHCl_2]^{*-}$	-72.516	-1.14 [c]	--	--	--	--	1.42×10^{10}
				$CH_3CHCl_2 + e^- \rightarrow CH_3{}^*CHCl + Cl^-$	--	--	-77.004	-0.94 [c]	-76.499	-0.96 [c]	

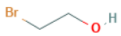
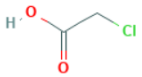
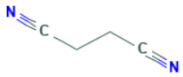
70	Diiodomethane	CH_2I_2		$CH_2I_2 + e^- \rightarrow [CH_2I_2]^{*-}$	-80.495	-0.79 [d]	--	--	--	--	3.40×10^{10}
				$CH_2I_2 + e^- \rightarrow {}^*CH_2I + I^-$	--	--	-80.133	-0.81 [d]	-93.538	-0.22 [d]	
71	Iodoethane	CH_3CH_2I		$CH_3CH_2I + e^- \rightarrow [CH_3CH_2I]^{*-}$	-75.941	-0.99 [d]	--	--	--	--	3.85×10^{10}
				$CH_3CH_2I + e^- \rightarrow CH_3{}^*CH_2 + I^-$	--	--	-75.941	-0.99 [d]	-87.734	-0.48 [d]	
72	Dichloromethane	CH_2Cl_2		$CH_2Cl_2 + e^- \rightarrow [CH_2Cl_2]^{*-}$	-71.833	-1.17 [c]	--	--	--	--	7.95×10^{9}
				$CH_2Cl_2 + e^- \rightarrow {}^*CH_2Cl + Cl^-$	--	--	-75.690	-1.00 [c]	-74.257	-1.06 [c]	
73	Chloroform	$CHCl_3$		$CHCl_3 + e^- \rightarrow [CHCl_3]^{*-}$	-79.543	-0.83 [c]	--	--	--	--	3.00×10^{10}
				$CHCl_3 + e^- \rightarrow {}^*CHCl_2 + Cl^-$	--	--	-81.972	-0.73 [c]	-82.310	-0.71 [c]	
74	Trichlorofluoromethane	CCl_3F		$CCl_3F + e^- \rightarrow [CCl_3F]^{*-}$	-79.113	-0.85 [c]	--	--	--	--	4.60×10^{10}
				$CCl_3F + e^- \rightarrow {}^*CCl_2F + Cl^-$	--	--	-82.747	-0.69 [c]	-77.563	-0.92 [c]	
				$CCl_3F + e^- \rightarrow {}^*CCl_3 + F^-$	--	--	-25.048	-3.19 [c]	-37.457	-2.66 [c]	
75	Dichlorodifluoromethane	CF_2Cl_2		$CF_2Cl_2 + e^- \rightarrow [CF_2Cl_2]^{*-}$	-74.271	-1.06 [c]	--	--	--	--	3.28×10^{10}
				$CF_2Cl_2 + e^- \rightarrow {}^*CF_2Cl + Cl^-$	--	--	-77.164	-0.93 [c]	-62.436	-1.57 [c]	
				$CF_2Cl_2 + e^- \rightarrow {}^*CFCl_2 + F^-$	--	--	-15.382	-3.61 [c]	-20.224	-3.40 [c]	
76	Chlorotrifluoromethane	$CClF_3$		$CClF_3 + e^- \rightarrow [CClF_3]^{*-}$	-70.255	-1.23 [c]	--	--	--	--	5.36×10^{9}

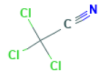
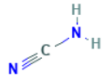
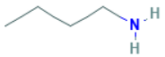
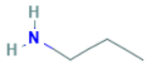
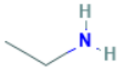
				$CClF_3 + e^- \rightarrow *CF_3 + Cl^-$	--	--	-71.187	-1.19 [c]	-69.497	-1.27 [c]	
				$CClF_3 + e^- \rightarrow *CClF_2 + F^-$	--	--	-6.059	-4.02 [c]	-3.135	-4.14 [c]	
77	Bromotrifluoromethane	CF_3Br		$CF_3Br + e^- \rightarrow [CF_3Br]^{*-}$	-70.849	-1.21 [c]	--	--	--	--	3.93×10^{11}
				$CF_3Br + e^- \rightarrow *CF_3 + Br^-$	--	--	-70.324	-1.23 [c]	-70.396	-1.23 [c]	
				$CF_3Br + e^- \rightarrow *CF_2Br + F^-$	--	--	-7.619	-3.95 [c]	-6.574	-3.99 [c]	
78	Carbon Tetrachloride	CCl_4		$CCl_4 + e^- \rightarrow [CCl_4]^{*-}$	-86.869	-0.51 [c]	--	--	--	--	7.61×10^{10}
				$CCl_4 + e^- \rightarrow *CCl_3 + Cl^-$	--	--	-91.148	-0.33 [c]	-89.364	-0.41 [c]	
79	Chlorodifluoromethane	$CHClF_2$		$CHClF_2 + e^- \rightarrow [CHClF_2]^{*-}$	-66.256	-1.41 [c]	--	--	--	--	3.29×10^{9}
				$CHClF_2 + e^- \rightarrow *CHF_2 + Cl^-$	--	--	-70.221	-1.24 [c]	-63.028	-1.55 [c]	
				$CHClF_2 + e^- \rightarrow *CHClF + F^-$	--	--	-10.444	-3.83 [c]	-18.607	-3.47 [c]	
80	1,1,2-Trichloroethane	$ClCH_2CHCl_2$		$ClCH_2CHCl_2 + e^- \rightarrow [ClCH_2CHCl_2]^{*-}$	-76.948	-0.94 [c]	--	--	--	--	1.27×10^{10}
				$ClCH_2CHCl_2 + e^- \rightarrow *CH_2CHCl_2 + Cl^-$	--	--	-75.169	-1.02 [c]	-82.211	-0.72 [c]	
				$ClCH_2CHCl_2 + e^- \rightarrow ClCH_2*CHCl + Cl^-$	--	--	-63.785	-1.51 [c]	--	--	
81	1,1,1-Trichloroethane	CH_3CCl_3		$CH_3CCl_3 + e^- \rightarrow [CH_3CCl_3]^{*-}$	-79.429	-0.84 [c]	--	--	--	--	9.24×10^{10}
				$CH_3CCl_3 + e^- \rightarrow CH_3*CCl_2 + Cl^-$	--	--	-84.087	-0.63 [c]	-84.836	-0.60 [c]	

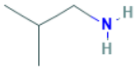
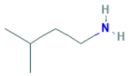
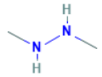
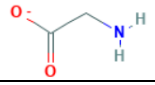
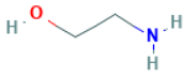
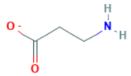
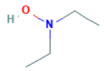
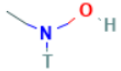
82	Hexachloroethane	CCl_3CCl_3		$CCl_3CCl_3 + e^- \rightarrow [CCl_3CCl_3]^{*-}$	-85.483	-0.57 [c]	--	--	--	--	3.90×10^{10}
				$CCl_3CCl_3 + e^- \rightarrow CCl_3{*}CCl_2 + Cl^-$	--	--	-89.801	-0.39 [c]	-94.942	-0.16 [c]	
83	2-Chlorobutane	$C_2H_5CH(Cl)CH_3$		$C_2H_5CH(Cl)CH_3 + e^- \rightarrow [C_2H_5CH(Cl)CH_3]^{*-}$	-67.500	-1.35 [c]	--	--	--	--	5.21×10^{8}
				$C_2H_5CH(Cl)CH_3 + e^- \rightarrow C_2H_5{*}CHCH_3 + Cl^-$	--	--	-71.791	-1.17 [c]	-72.500	-1.14 [c]	
84	1,2-Dibromoethane	$BrCH_2CH_2Br$		$BrCH_2CH_2Br + e^- \rightarrow [BrCH_2CH_2Br]^{*-}$	-67.072	-1.37 [c]	--	--	--	--	2.74×10^{10}
				$BrCH_2CH_2Br + e^- \rightarrow BrCH_2{*}CH_2 + Br^-$	--	--	-72.813	-1.12 [c]	-74.200	-1.06 [c]	
85	1,2-Dichloroethane	$ClCH_2CH_2Cl$		$ClCH_2CH_2Cl + e^- \rightarrow [ClCH_2CH_2Cl]^{*-}$	-69.404	-1.27 [c]	--	--	--	--	1.91×10^{9}
				$ClCH_2CH_2Cl + e^- \rightarrow ClCH_2{*}CH_2 + Cl^-$	--	--	-74.111	-1.07 [c]	-73.303	-1.10 [c]	
86	1,1,2-Trichloro-1,2,2-trifluoroethane	$ClCF_2CCl_2F$		$ClCF_2CCl_2F + e^- \rightarrow [ClCF_2CCl_2F]^{*-}$	-77.672	-0.91 [c]	--	--	--	--	3.17×10^{10}
				$ClCF_2CCl_2F + e^- \rightarrow ClCF_2{*}CClF + Cl^-$	--	--	-80.517	-0.79 [c]	-84.396	-0.62 [c]	
				$ClCF_2CCl_2F + e^- \rightarrow {*}CF_2CCl_2F + Cl^-$	--	--	-74.448	-1.05 [c]	--	--	
				$ClCF_2CCl_2F + e^- \rightarrow ClCF_2{*}CCl_2 + F^-$	--	--	-26.570	-3.13 [c]	--	--	
				$ClCF_2CCl_2F + e^- \rightarrow Cl{*}CFCCl_2F + F^-$	--	--	-15.564	-3.61 [c]	--	--	
87	1-Iodopropane	C_3H_7I		$C_3H_7I + e^- \rightarrow [C_3H_7I]^{*-}$	-75.555	-1.00 [d]	--	--	--	--	2.73×10^{10}
				$C_3H_7I + e^- \rightarrow {*}C_3H_7 + I^-$	--	--	-75.555	-1.00 [d]	-89.251	-0.41 [d]	

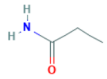
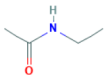
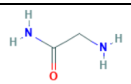
88	1-Iodobutane	$CH_3(CH_2)_3I$		$CH_3(CH_2)_3I + e^- \rightarrow [CH_3(CH_2)_3I]^{*-}$	-75.508	-1.01 [d]	--	--	--	--	2.29×10^{10}
				$CH_3(CH_2)_3I + e^- \rightarrow CH_3{*}(CH_2)_3 + I^-$	--	--	-75.500	-1.01 [d]	-91.800	-0.30 [d]	
89	1-Bromobutane	$CH_3(CH_2)_3Br$		$CH_3(CH_2)_3Br + e^- \rightarrow [CH_3(CH_2)_3Br]^{*-}$	-54.063	-1.94 [c]	--	--	--	--	1.59×10^{10}
				$CH_3(CH_2)_3Br + e^- \rightarrow CH_3{*}(CH_2)_3 + Br^-$	--	--	-67.540	-1.35 [c]	-70.843	-1.21 [c]	
90	1-Chlorobutane	$CH_3(CH_2)_3Cl$		$CH_3(CH_2)_3Cl + e^- \rightarrow [CH_3(CH_2)_3Cl]^{*-}$	-12.529	-3.74 [c]	--	--	--	--	3.42×10^{8}
				$CH_3(CH_2)_3Cl + e^- \rightarrow CH_3{*}(CH_2)_3 + Cl^-$	--	--	-70.825	-1.21 [c]	-73.047	-1.11 [c]	
91	1-Chloro-2-methylpropane	$(CH_3)_2CHCH_2Cl$		$(CH_3)_2CHCH_2Cl + e^- \rightarrow [(CH_3)_2CHCH_2Cl]^{*-}$	-66.405	-1.40 [c]	--	--	--	--	5.21×10^{8}
				$(CH_3)_2CHCH_2Cl + e^- \rightarrow (CH_3)_2CH{*}CH_2 + Cl^-$	--	--	-70.620	-1.22 [c]	-71.911	-1.16 [c]	
92	1-Bromopentane	$CH_3(CH_2)_4Br$		$CH_3(CH_2)_4Br + e^- \rightarrow [CH_3(CH_2)_4Br]^{*-}$	-54.106	-1.93 [c]	--	--	--	--	1.17×10^{10}
				$CH_3(CH_2)_4Br + e^- \rightarrow CH_3{*}(CH_2)_4 + Br^-$	--	--	-67.451	-1.36 [c]	-72.978	-1.12 [c]	
93	2-Bromo-2-methylpropane	$(CH_3)_3CBr$		$(CH_3)_3CBr + e^- \rightarrow [(CH_3)_3CBr]^{*-}$	-67.447	-1.36 [c]	--	--	--	--	1.02×10^{10}
				$(CH_3)_3CBr + e. \rightarrow (CH_3)_3{*}C + Br^-$	--	--	-70.359	-1.23 [c]	-72.263	-1.15 [c]	
94	2-Bromobutane	$CH_3CH_2CH(Br)CH_3$		$CH_3CH_2CH(Br)CH_3 + e^- \rightarrow [CH_3CH_2CH(Br)CH_3]^{*-}$	-65.083	-1.46 [c]	--	--	--	--	1.01×10^{10}
				$CH_3CH_2CH(Br)CH_3 + e^- \rightarrow CH_3CH_2{*}CHCH_3 + Br^-$	--	--	-69.183	-1.28 [c]	-71.233	-1.19 [c]	
95	Trifluoroiodomethane	CF_3I		$CF_3I + e^- \rightarrow [CF_3I]^{*-}$	-79.974	-0.81 [d]	--	--	--	--	2.77×10^{10}

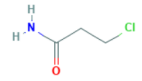
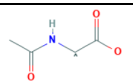
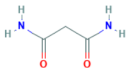
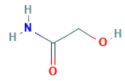
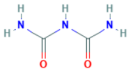
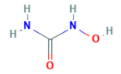
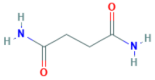
				$CF_3I + e^- \rightarrow {}^*CF_3 + I^-$	--	--	-77.058	-0.94 [d]	-91.195	-0.33 [d]	
	96	Iodomethane	CH_3I	$CH_3I + e^- \rightarrow [CH_3]^{*-}$	-72.925	-1.12 [d]	--	--	--	--	4.64×10^{10}
				$CH_3I + e^- \rightarrow {}^*CH_3 + I^-$	--	--	-73.395	-1.10 [d]	-83.781	-0.65 [d]	
Halooxygen	97	Isoflurane	$CHF_2OCHClCF_3$	$CHF_2OCHClCF_3 + e^- \rightarrow [CHF_2OCHClCF_3]^{*-}$	-75.427	-1.01 [c]	--	--	--	--	5.80×10^{9}
				$CHF_2OCHClCF_3 + e^- \rightarrow CHF_2O{}^*CHCF_3 + Cl^-$	--	--	-53.746	-1.95 [c]	0.870	-4.32 [c]	
				$CHF_2OCHClCF_3 + e^- \rightarrow CHF_2OCHCl{}^*CF_2 + F^-$	--	--	18.124	-5.07 [c]	31.949	-5.67 [c]	
	98	1,1,1-Trifluoroacetone	CF_3COCH_3	$CF_3COCH_3 + e^- \rightarrow CF_3{}^*CO(-)CH_3$	-50.673	-2.08 [c]	--	--	--	--	6.62×10^{7}
				$CF_3COCH_3 + e^- \rightarrow {}^*CF_2COCH_3 + F^-$	--	--	6.470	-4.56 [c]	-50.673	-5.36 [c]	
	99	Fluoroacetone	CH_3COCH_2F	$CH_3COCH_2F + e^- \rightarrow CH_3{}^*CO(-)CH_2F$	-37.268	-2.66 [c]	--	--	--	--	9.77×10^{8}
				$CH_3COCH_2F + e^- \rightarrow CH_3CO{}^*CH_2 + F^-$	--	--	-0.651	-4.25 [c]	-37.268	-5.12 [c]	
	100	Methoxyflurane	$CH_3OCF_2CHCl_2$	$CH_3OCF_2CHCl_2 + e^- \rightarrow [CH_3OCF_2CHCl_2]^{*-}$	48.587	-6.39 [c]	--	--	--	--	3.16×10^{10}
				$CH_3OCF_2CHCl_2 + e^- \rightarrow CH_3OCF_2{}^*CHCl + Cl^-$	--	--	-67.898	-1.34 [c]	1.306	-4.34 [c]	
				$CH_3OCF_2CHCl_2 + e^- \rightarrow CH_3O{}^*CFCHCl_2 + F^-$	--	--	-8.857	-3.90 [c]	29.840	-5.57 [c]	
	101	2-Chloroethanol	$ClCH_2CH_2OH$	$ClCH_2CH_2OH + e^- \rightarrow [ClCH_2CH_2OH]^{*-}$	-70.321	-1.23 [c]	--	--	--	--	5.34×10^{8}
				$ClCH_2CH_2OH + e^- \rightarrow {}^*CH_2CH_2OH + Cl^-$	--	--	-58.474	-1.74 [c]	15.251	-4.94 [c]	

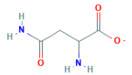
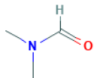
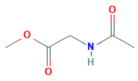
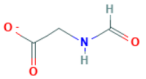
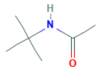
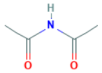
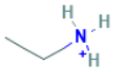
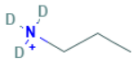
				$ClCH_2CH_2OH + e^- \rightarrow [ClCH_2CH_2O]^- + H^*$	--	--	-1.422	-4.22 [c]	--	--	
	102	2-Bromoethanol	$BrCH_2CH_2OH$		$BrCH_2CH_2OH + e^- \rightarrow [BrCH_2CH_2OH]^{*-}$	-69.500	-1.27 [c]	--	--	--	--	1.71×10^9
					$BrCH_2CH_2OH + e^- \rightarrow {}^*CH_2CH_2OH + Br^-$	--	--	-14.719	-3.64 [c]	18.641	-5.09 [c]	
	103	Chloroacetic acid	$ClCH_2COOH$		$ClCH_2COOH + e^- \rightarrow ClCH_2{}^*CO(-)OH$	-42.366	-2.44 [c]	--	--	--	--	9.60×10^9
					$ClCH_2COOH + e^- \rightarrow {}^*CH_2COOH + Cl^-$	--	--	-54.820	-1.90 [c]	5.395	-4.51 [c]	
	104	Chloral hydrate	$CCl_3CH(OH)_2$		$CCl_3CH(OH)_2 + e^- \rightarrow [CCl_3CH(OH)_2]^{*-}$	-84.704	-0.61 [c]	--	--	--	--	2.31×10^{10}
					$CCl_3CH(OH)_2 + e^- \rightarrow {}^*CCl_2CH(OH)_2 + Cl^-$	--	--	-58.870	-1.73 [c]	-0.786	-4.25 [c]	
	105	Enflurane	CHF_2OCF_2CHClF		$CHF_2OCF_2CHClF + e^- \rightarrow [CHF_2OCF_2CHClF]^{*-}$	-70.858	-1.21 [c]	--	--	--	--	3.03×10^9
					$CHF_2OCF_2CHClF + e^- \rightarrow CHF_2OCF_2{}^*CHCl + F^-$	--	--	2.174	-4.37 [c]	--	--	
					$CHF_2OCF_2CHClF + e^- \rightarrow CHF_2OCF_2{}^*CHF + Cl^-$	--	--	-50.059	-2.11 [c]	4.142	-4.46 [c]	
					$CHF_2OCF_2CHClF + e^- \rightarrow {}^*CHFOCF_2CHClF + F^-$	--	--	18.080	-5.06 [c]	16.319	-4.99 [c]	
Cyanide	106	Acetonitrile	CH_3CN		$CH_3CN + e^- \rightarrow [CH_3CN]^{*-}$	-14.829	-3.64 [a]	--	--	--	--	3.74×10^7
					$CH_3CN + e^- \rightarrow {}^*CH_3 + CN^-$	--	--	-21.899	-3.33 [a]	119.687	-9.47 [c]	
	107	Succinonitrile	$NC(CH_2)_2CN$		$NC(CH_2)_2CN + e^- \rightarrow [NC(CH_2)_2CN]^{*-}$	-21.837	-3.33 [a]	--	--	--	--	1.83×10^9
					$NC(CH_2)_2CN + e^- \rightarrow NCCH_2{}^*CH_2 + CN^-$	--	--	-28.089	-3.06 [a]	108.910	-9.00 [c]	

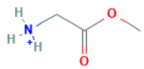
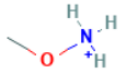
	108	Trichloroacetonitrile	CCl_3CN		$CCl_3CN + e^- \rightarrow *CCl_2CN + Cl^-$	--	--	-98.667	0.00 [c]	35.993	-5.84 [c]	3.20×10^{10}
	109	Cyanamide	H_2NCN		$H_2NCN + e^- \rightarrow [H_2NCN]^{*-}$	-21.233	-3.36 [a]	--	--	--	--	1.60×10^{9}
					$H_2NCN + e^- \rightarrow H_2N^* + CN^-$	--	--	-26.831	-3.12 [a]	113.625	-9.21 [c]	
Amine	110	Methylamine	CH_3NH_2		$CH_3NH_2 + e^- \rightarrow [CH_3NH_2]^{*-}$	19.277	-5.12 [a]	--	--	--	--	9.00×10^{5}
	111	Butylamine	$CH_3(CH_2)_3NH_2$		$CH_3(CH_2)_3NH_2 + e^- \rightarrow [CH_3(CH_2)_3NH_2]^{*-}$	17.068	-5.02 [a]	--	--	--	--	1.10×10^{6}
					$CH_3(CH_2)_3NH_2 + e^- \rightarrow [CH_3CH_2CH_2CHNH_2]^- + H^*$	--	--	43.125	-6.15 [a]	--	--	
					$CH_3(CH_2)_3NH_2 + e^- \rightarrow [CH_3CH_2CHCH_2NH_2]^- + H^*$	--	--	39.521	-5.99 [a]	--	--	
					$CH_3(CH_2)_3NH_2 + e^- \rightarrow [CH_3CHCH_2CH_2NH_2]^- + H^*$	--	--	40.696	-6.04 [a]	--	--	
					$CH_3(CH_2)_3NH_2 + e^- \rightarrow [CH_2CH_2CH_2CH_2NH_2]^- + H^*$	--	--	38.869	-5.97 [a]	--	--	
	112	Propylamine	$CH_3CH_2CH_2NH_2$		$CH_3CH_2CH_2NH_2 + e^- \rightarrow [CH_3CH_2CH_2NH_2]^{*-}$	19.795	-5.14 [a]	--	--	--	--	1.10×10^{6}
					$CH_3CH_2CH_2NH_2 + e^- \rightarrow [CH_3CH_2CHNH_2]^- + H^*$	--	--	43.023	-6.15 [a]	--	--	
					$CH_3CH_2CH_2NH_2 + e^- \rightarrow [CH_3CHCH_2NH_2]^- + H^*$	--	--	40.090	-6.02 [a]	--	--	
					$CH_3CH_2CH_2NH_2 + e^- \rightarrow [CH_2CH_2CH_2NH_2]^- + H^*$	--	--	38.631	-5.95 [a]	--	--	
	113	Ethylamine	$CH_3CH_2NH_2$		$CH_3CH_2NH_2 + e^- \rightarrow [CH_3CH_2NH_2]^{*-}$	20.420	-5.17 [a]	--	--	--	--	1.00×10^{6}
					$CH_3CH_2NH_2 + e^- \rightarrow [CH_3CHNH_2]^- + H^*$	--	--	43.284	-6.16 [a]	--	--	

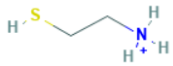
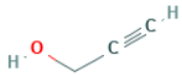
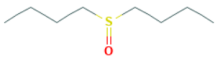
				$CH_3CH_2NH_2 + e^- \rightarrow [CH_2CH_2NH_2]^- + H^*$	--	--	35.972	-5.84 [a]	--	--	
114	Isobutylamine	$(CH_3)_2CHCH_2NH_2$		$(CH_3)_2CHCH_2NH_2 + e^- \rightarrow [(CH_3)_2CHCH_2NH_2]^{*-}$	18.633	-5.09 [a]	--	--	--	--	1.10×10^7
115	Isoamylamine	$(CH_3)_2CHCH_2CH_2NH_2$		$(CH_3)_2CHCH_2CH_2NH_2 + e^- \rightarrow [(CH_3)_2CHCH_2CH_2NH_2]^{*-}$	20.072	-5.15 [a]	--	--	--	--	1.00×10^6
116	1,2-Dimethylhydrazine	$CH_3NHNHCH_3$		$CH_3NHNHCH_3 + e^- \rightarrow [CH_3NHNHCH_3]^{*-}$	27.980	-5.49 [a]	--	--	--	--	6.10×10^6
117	Methylhydrazine	CH_3NHNH_2		$CH_3NHNH_2 + e^- \rightarrow [CH_3NHNH_2]^{*-}$	12.204	-4.81 [a]	--	--	--	--	6.50×10^6
118	Glycinate	$NH_2CH_2COO^-$		$NH_2CH_2COO^- + e^- \rightarrow [NH_2CH_2COO]^{*2-}$	-9.945	-3.85 [b]	--	--	--	--	1.70×10^6
119	Ethanolamine	$H_2NCH_2CH_2OH$		$H_2NCH_2CH_2OH + e^- \rightarrow [H_2NCH_2CH_2OH]^{*-}$	-0.269	-4.27 [a]	--	--	--	--	2.00×10^7
				$H_2NCH_2CH_2OH + e^- \rightarrow [H_2NCH_2CH_2O]^- + H^*$	--	--	-1.157	-4.23 [a]	--	--	
120	Isopropylamine	$(CH_3)_2CHNH_2$		$(CH_3)_2CHNH_2 + e^- \rightarrow [(CH_3)_2CHNH_2]^{*-}$	18.203	-5.07 [a]	--	--	--	--	1.50×10^6
121	Tert-Butylamine	$(CH_3)_3CNH_2$		$(CH_3)_3CNH_2 + e^- \rightarrow [(CH_3)_3CNH_2]^{*-}$	18.200	-5.07 [a]	--	--	--	--	1.10×10^6
122	beta-Alaninate	$NH_2(CH_2)_2\text{-}COO^-$		$NH_2(CH_2)_2COO^- + e^- \rightarrow NH_2(CH_2)_2{}^*CO(-)O^-$	-9.804	-3.85 [b]	--	--	--	--	4.20×10^6
123	N,N-Diethylhydroxylamine	$(C_2H_5)_2NOH$		$(C_2H_5)_2NOH + e^- \rightarrow [(C_2H_5)_2NOH]^{*-}$	-2.508	-4.17 [a]	--	--	--	--	4.81×10^7
124	N-Methyl-N-tritiohydroxylamine	CH_3NHOH		$CH_3NHOH + e^- \rightarrow [CH_3NHOH]^{*-}$	-15.916	-3.59 [a]	--	--	--	--	2.42×10^8
125	Amylamine	$CH_3(CH_2)_4NH_2$		$CH_3(CH_2)_4NH_2 + e^- \rightarrow [CH_3(CH_2)_4NH_2]^{*-}$	21.111	-5.20 [a]	--	--	--	--	1.00×10^6
126	Trimethylhydrazine	$(CH_3)_2N\text{-}NHCH_3$		$(CH_3)_2N\text{-}NHCH_3 + e^- \rightarrow [(CH_3)_2N\text{-}NHCH_3]^{*-}$	-16.761	-3.55 [a]	--	--	--	--	1.00×10^8

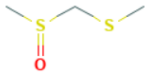
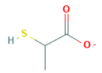
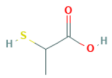
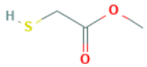
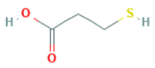
	127	1,1-Dimethylhydrazine	$(CH_3)_2NNH_2$		$(CH_3)_2NNH_2 + e^- \rightarrow [(CH_3)_2NNH_2]^{*-}$	18.277	-5.07[a]	--	--	--	--	2.40×10^7
Amide	128	Propionamide	$CH_3CH_2CONH_2$		$CH_3CH_2CONH_2 + e^- \rightarrow [CH_3CH_2CONH_2]^{*-}$	-23.714	-3.25[b]	--	--	--	--	4.66×10^7
					$CH_3CH_2CONH_2 + e^- \rightarrow [CH_3CHCONH_2]^- + H^*$	--	--	9.667	-4.70[a]	--	--	
	129	N-Ethylacetamide	$CH_3CONHC_2H_5$		$CH_3CONHC_2H_5 + e^- \rightarrow [CH_3CONHC_2H_5]^{*-}$	-23.750	-3.25[b]	--	--	--	--	1.40×10^7
					$CH_3CONHC_2H_5 + e\text{-} \rightarrow [CH_3CONHC_2H_4]^- + H^*$	--	--	33.619	-5.74[a]	--	--	
					$CH_3CONHC_2H_5 + e^- \rightarrow [CH_3CONHC_2H_4]^- + H^*$	--	--	31.040	-5.63[a]	--	--	
					$CH_3CONHC_2H_5 + e^- \rightarrow [CH_2CONHC_2H_5]^- + H^*$	--	--	7.925	-4.62[a]	--	--	
	130	N-Methylacetamide	$CH_3CONHCH_3$		$CH_3CONHCH_3 + e^- \rightarrow [CH_3CONHCH_3]^{*-}$	-21.793	-3.34[b]	--	--	--	--	2.30×10^6
					$CH_3CONHCH_3 + e^- \rightarrow [CH_2CONHCH_3]^- + H^*$	--	--	31.293	-5.64[a]	--	--	
					$CH_3CONHCH_3 + e^- \rightarrow [CH_3CONHCH_2]^- + H^*$	--	--	8.714	-4.66[a]	--	--	
	131	Acetamide	CH_3CONH_2		$CH_3CONH_2 + e^- \rightarrow [CH_3CONH_2]^{*-}$	-25.725	-3.16[b]	--	--	--	--	3.84×10^7
					$CH_3CONH_2 + e^- \rightarrow [CH_2CONH_2]^- + H^*$	--	--	5.776	-4.53[a]	--	--	
	132	Urea	H_2NCONH_2		$H_2NCONH_2 + e^- \rightarrow [H_2NCONH_2]^{*-}$	-17.397	-3.53[b]	--	--	--	--	3.10×10^5
	133	Glycinamide	$H_2NCH_2CONH_2$		$H_2NCH_2CONH_2 + e^- \rightarrow [H_2NCH_2CONH_2]^{*-}$	-27.344	-3.09[b]	--	--	--	--	2.83×10^8
	134	Formamide	$HCONH_2$		$HCONH_2 + e^- \rightarrow [HCONH_2]^{*-}$	-28.171	-3.06[b]	--	--	--	--	2.80×10^7

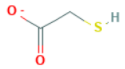
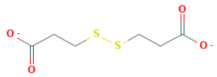
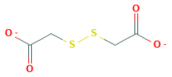
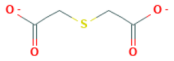
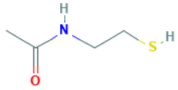
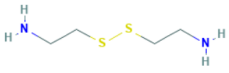
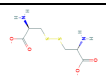
135	3-Chloropropionamide	$ClCH_2CH_2CONH_2$		$ClCH_2CH_2CONH_2 + e^- \rightarrow [ClCH_2CH_2CONH_2]^{*-}$	-61.908	-1.60 [a]	--	--	--	--	1.94×10^{9}
				$ClCH_2CH_2CONH_2 + e^- \rightarrow {}^*CH_2CH_2CONH_2 + Cl^-$	--	--	-60.223	-1.67 [a]	10.524	-4.74 [c]	
136	(S)-2-Hydroxypropanamide	$CH_3CH(OH)CONH_2$		$CH_3CH(OH)CONH_2 + e^- \rightarrow [CH_3CH(OH)CONH_2]^{*-}$	-29.161	-3.02 [b]	--	--	--	--	1.91×10^{8}
				$CH_3CH(OH)CONH_2 + e^- \rightarrow [CH_3CH(O)CONH_2]^- + H^*$	--	--	-11.924	-3.76[a]	--	--	
137	Aceturate	$CH_3CONHCH_2COO^-$		$CH_3CONHCH_2COO^- + e^- \rightarrow [CH_3CONHCH_2COO]^{*2-}$	-25.837	-3.16 [b]	--	--	--	--	1.13×10^{7}
138	Pivalamide	$(CH_3)_3CCONH_2$		$(CH_3)_3CCONH_2 + e^- \rightarrow (CH_3)_3C{}^*CO(-)NH_2$	-27.032	-3.11 [b]	--	--	--	--	1.50×10^{7}
139	Malonamide	$H_2NCOCH_2CONH_2$		$H_2NCOCH_2CONH_2 + e^- \rightarrow H_2N{}^*CO(-)CH_2CONH_2$	-30.467	-2.96 [b]	--	--	--	--	1.15×10^{9}
140	2-Hydroxyacetamide	$HOCH_2CONH_2$		$HOCH_2CONH_2 + e^- \rightarrow HOCH_2{}^*CO(-)NH_2$	-29.101	-3.02 [b]	--	--	--	--	2.93×10^{8}
141	Biuret	$H_2NCONHCONH_2$		$H_2NCONHCONH_2 + e^- \rightarrow H_2N{}^*CO(-)NHCONH_2$	-26.984	-3.11 [b]	--	--	--	--	2.53×10^{8}
142	2-Chloropropionamide	$CH_3CH(Cl)CONH_2$		$CH_3CH(Cl)CONH_2 + e^- \rightarrow CH_3{}^*CHCONH_2 + Cl^-$	--	--	-70.689	-1.22 [a]	0.907	-4.32 [c]	7.58×10^{9}
143	Iodoacetamide	ICH_2CONH_2		$ICH_2CONH_2 + e^- \rightarrow {}^*CH_2CONH_2 + I^-$	-81.461	-0.75 [d]	--	--	--	--	5.00×10^{10}
				$ICH_2CONH_2 + e^- \rightarrow ICH_2{}^*CO(-)NH_2$	--	--	-35.569	-2.74 [d]	-2.753	-4.16[d]	
144	Hydroxyurea	$HONHCONH_2$		$HONHCONH_2 + e^- \rightarrow HONH{}^*CO(-)NH_2$	-27.450	-3.09 [b]	--	--	--	--	4.90×10^{8}
145	Oxamate	$H_2NCOCOO^-$		$H_2NCOCOO^- + e^- \rightarrow H_2N{}^*CO(-)COO^-$	-44.349	-2.36 [b]	--	--	--	--	5.70×10^{9}
146	Succinamide	$H_2NCOCH_2CH_2CONH_2$		$H_2NCOCH_2CH_2CONH_2 + e^- \rightarrow H_2N{}^*CO(-)CH_2CH_2CONH_2$	-26.232	-3.14 [b]	--	--	--	--	2.02×10^{8}

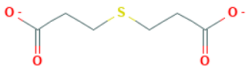
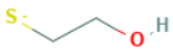
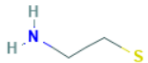
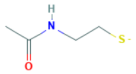
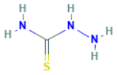
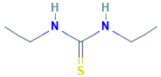
	147	Asparaginate	$H_2NCOCH_2CH(NH_2)COO^-$		$H_2NCOCH_2CH(NH_2)COO^- + e^- \rightarrow H_2N{*}CO(-)CH_2CH(NH_2)COO^-$	-26.514	-3.13 [b]	--	--	--	--	2.40×10^{7}
	148	N,N-Dimethylformamide	$HCON(CH_3)_2$		$HCON(CH_3)_2 + e^- \rightarrow H{*}CO(-)N(CH_3)_2$	-30.349	-2.96 [b]	--	--	--	--	3.08×10^{8}
	149	Methyl 2-acetamidoacetate	$CH_3CONHCH_2COOCH_3$		$CH_3CONHCH_2COOCH_3 + e^- \rightarrow CH_3{*}CO(-)NHCH_2COOCH_3$	-38.384	-2.62 [b]	--	--	--	--	3.34×10^{8}
	150	2-Formamidoacetate	$HCONHCH_2COO^-$		$HCONHCH_2COO^- + e^- \rightarrow H{*}CO(-)NHCH_2COO^-$	-25.927	-3.16 [b]	--	--	--	--	2.90×10^{7}
	151	N-Methylformamide	$HCONHCH_3$		$HCONHCH_3 + e^- \rightarrow H{*}CO(-)NHCH_3$	-25.681	-3.17 [b]	--	--	--	--	4.31×10^{7}
	152	N-Tert-Butylacetamide	$CH_3CONHC(CH_3)_3$		$CH_3CONHC(CH_3)_3 + e^- \rightarrow CH_3{*}CO(-)NHC(CH_3)_3$	-21.692	-3.34 [b]	--	--	--	--	1.20×10^{7}
	153	Diacetamide	$(CH_3CO)_2NH$		$(CH_3CO)_2NH + e^- \rightarrow (CH_3CO)NH(CH_3{*}CO(-))$	-43.290	-2.40 [b]	--	--	--	--	1.98×10^{10}
	154	N,N-Diethylacetamide	$CH_3CON(C_2H_5)_2$		$CH_3CON(C_2H_5)_2 + e^- \rightarrow CH_3{*}CO(-)N(C_2H_5)_2$	-23.892	-3.24 [b]	--	--	--	--	8.00×10^{6}
	155	N,N-Dimethylacetamide	$CH_3CON(CH_3)_2$		$CH_3CON(CH_3)_2 + e^- \rightarrow CH_3{*}CO(-)N(CH_3)_2$	-27.415	-3.09 [b]	--	--	--	--	1.50×10^{7}
	156		$(CH_3)_3CCON(CH_3)_2$		$(CH_3)_3CCON(CH_3)_2 + e^- \rightarrow [(CH_3)_3CCON(CH_3)_2]^{*-}$	-29.955	-2.98 [b]	--	--	--	--	1.20×10^{7}
Ammonia	157	Methyl Ammonium Hydride	$CH_3NH_3^+$		$CH_3NH_3^+ + e^- \rightarrow [CH_3NH_3]{*}$	-7.523	-3.95 [a]	--	--	--	--	1.85×10^{6}
					$CH_3NH_3^+ + e^- \rightarrow {*}CH_3 + NH_3$	--	--	-50.076	-2.11 [a]	--	--	
	158	Ethylammonium	$C_2H_5NH_3^+$		$C_2H_5NH_3^+ + e^- \rightarrow [C_2H_5NH_3]{*}$	-25.234	-3.19 [a]	--	--	--	--	2.50×10^{6}
					$C_2H_5NH_3^+ + e^- \rightarrow {*}C_2H_5 + NH_3$	--	--	-51.524	-2.05 [a]	--	--	
	159	Trideuterio(propyl)azanium	$CH_3(CH_2)_2NH_3^+$		$CH_3(CH_2)_2NH_3^+ + e^- \rightarrow [CH_3(CH_2)_2NH_3]{*}$	-25.506	-3.17 [a]	--	--	--	--	2.80×10^{6}

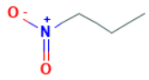
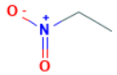
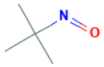
				$CH_3(CH_2)_2NH_3^+ + e^- \rightarrow {}^*CH_3(CH_2)_2 + NH_3$	--	--	-50.987	-2.07 [a]	--	--	
160	Pentylazanium	$CH_3(CH_2)_4NH_3^+$		$CH_3(CH_2)_4NH_3^+ + e^- \rightarrow [CH_3(CH_2)_4NH_3]$	-25.230	-3.19 [a]	--	--	--	--	2.70×10^6
				$CH_3(CH_2)_4NH_3^+ + e^- \rightarrow {}^*CH_3(CH_2)_4 + NH_3$	--	--	-51.570	-2.04 [a]	--	--	
161	2-Methoxy-2-oxoethanaminium	$H_3COOCCH_2NH_3^+$		$H_3COOCCH_2NH_3^+ + e^- \rightarrow [H_3COOCCH_2NH_3]^*$	-55.615	-1.87 [a]	--	--	--	--	6.80×10^9
				$H_3COOCCH_2NH_3^+ + e^- \rightarrow H_3COOC^*CH_2 + NH_3$	--	--	-59.487	-1.70 [a]	--	--	
				$H_3COOCCH_2NH_3^+ + e^- \rightarrow H_3C^* + OOCCH_2NH_3$	--	--	-61.013	-1.63 [a]	--	--	
				$H_3COOCCH_2NH_3^+ + e^- \rightarrow H_3CO^- + OC^*CH_2NH_3$	--	--	-0.132	-4.27 [a]	--	--	
162	Methoxyazanium	$CH_3ONH_3^+$		$CH_3ONH_3^+ + e^- \rightarrow [CH_3ONH_3]^*$	-37.582	-2.65 [a]	--	--	--	--	1.90×10^{10}
				$CH_3ONH_3^+ + e^- \rightarrow [CH_3O]^* + NH_3$	--	--	-96.506	-0.10 [a]	--	--	
				$CH_3ONH_3^+ + e^- \rightarrow {}^*CH_3 + ONH_3$	--	--	-49.198	-2.15 [a]	--	--	
163	Tert-butylammonium	$(CH_3)_3CNH_3^+$		$(CH_3)_3CNH_3^+ + e^- \rightarrow [(CH_3)_3CNH_3]$	-24.443	-3.22 [a]	--	--	--	--	1.10×10^6
				$(CH_3)_3CNH_3^+ + e^- \rightarrow (CH_3)_3{}^*C + NH_3$	--	--	-53.400	-1.96 [a]	--	--	
164	2-Methylhydrazinium	$CH_3NHNH_3^+$		$CH_3NHNH_3^+ + e^- \rightarrow [CH_3NHNH_3]^*$	-27.873	-3.07 [a]	--	--	--	--	1.40×10^9
				$CH_3NHNH_3^+ + e^- \rightarrow CH_3{}^*NH + NH_3$	--	--	-80.617	-0.78 [a]	--	--	
165	1,1-Dimethylhydrazinium	$(CH_3)_2NNH_3^+$		$(CH_3)_2NNH_3^+ + e^- \rightarrow [(CH_3)_2NNH_3]^*$	-29.065	-3.02 [a]	--	--	--	--	5.80×10^9

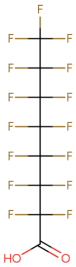
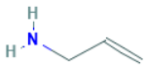
					$(CH_3)_2NNH_3^+ + e^- \rightarrow (CH_3)_2{}^*N + NH_3$	--	--	-85.826	-0.56 [a]	--	--	
	166	Tetramethylammonium	$(CH_3)_4N^+$		$(CH_3)_4N^+ + e^- \rightarrow [(CH_3)_4N]^*$	9.144	-4.68 [a]	--	--	--	--	5.60×10^6
					$(CH_3)_4N^+ + e^- \rightarrow [(CH_3)_3N + {}^*CH_3$	--	--	-49.224	-2.15 [a]	--	--	
	167	Tetraethylammonium	$(C_2H_5)_4N^+$		$(C_2H_5)_4N^+ + e^- \rightarrow [(C_2H_5)_4N^+]^{*-}$	24.703	-5.35 [a]	--	--	--	--	1.20×10^7
					$(C_2H_5)_4N^+ + e^- \rightarrow (C_2H_5)_3N + {}^*C_2H_5$	--	--	-52.937	-1.98 [a]	--	--	
Hydrogen Sulfide	168	Cysteaminium	$HSCH_2CH_2NH_3^+$		$HSCH_2CH_2NH_3^+ + e^- \rightarrow {}^*CH_2CH_2NH_3^+ + HS^-$	--	--	-51.154	-2.06 [c]	35.675	-5.83 [c]	2.25×10^{10}
					$HSCH_2CH_2NH_3^+ + e^- \rightarrow HSCH_2{}^*CH_2 + NH_3$	--	--	-53.409	-1.96 [a]	--	--	
	169	3-Sulfanylpropylazanium	$HS(CH_2)_3NH_3^+$		$HS(CH_2)_3NH_3^+ + e^- \rightarrow {}^*(CH_2)_3NH_3^+ + HS^-$	--	--	-52.077	-2.02 [c]	33.887	-5.75 [c]	1.70×10^{10}
					$HS(CH_2)_3NH_3^+ + e^- \rightarrow HS(CH_2)_3{}^* + NH_3$	--	--	-53.531	-1.96 [a]	--	--	
Alkyne	170	Acetylene	HC triplet bond CH		$HC\equiv CH + e^- \rightarrow [HC\equiv CH]^{*-}$	-21.817	-3.33 [a]	--	--	--	--	2.00×10^7
	171	Propargyl alcohol	HC triplet bond CCH_2OH		$HC\equiv CCH_2OH + e^- \rightarrow [HC\equiv CCH_2OH]^{*-}$	-24.162	-3.23 [a]	--	--	--	--	2.12×10^8
Sulfate	172	Ethanesulfonate	$C_2H_5SO_3^-$		$C_2H_5SO_3^- + e^- \rightarrow [C_2H_5SO_3]^{*2-}$	7.650	-4.61 [a]	--	--	--	--	
					$C_2H_5SO_3^- + e^- \rightarrow [CH_2CH_2SO_3]^{2-} + H^*$	--	--	31.977	-5.67 [a]	--	--	3.50×10^7
					$C_2H_5SO_3^- + e^- \rightarrow [CH_3CHSO_3]^{2-} + H^*$	--	--	23.473	-5.30 [a]	--	--	
Sulfoxide	173	Dibutyl sulphoxide	$[CH_3(CH_2)_3SO(CH_2)_3CH_3]$		$[CH_3(CH_2)_3SO(CH_2)_3CH_3] + e^- \rightarrow [[CH_3(CH_2)_3SO(CH_2)_3CH_3]]^{*-}$	-33.031	-2.85 [a]	--	--	--	--	3.60×10^6

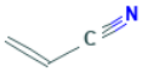
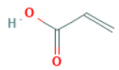
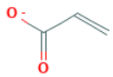
				$[CH_3(CH_2)_3SO(CH_2)_3CH_3] + e^- \rightarrow CH_3(CH_2)_3S(-)O + *(CH_2)_3CH_3$	--	--	-35.991	-2.72 [a]	22.095	-5.24 [c]	
	174	Di-tert-butyl sulfoxide	$[(CH_3)_3C]_2SO$		$[(CH_3)_3C]_2SO + e^- \rightarrow [[(CH_3)_3C]_2SO]^{*-}$	-42.905	-2.42 [a]	--	--	--	--	1.50×10^{7}
					$[(CH_3)_3C]_2SO + e^- \rightarrow (CH_3)_3CS(-)O + (CH_3)_3C^*$	--	--	-47.194	-2.23 [a]	-63.617	-1.52 [c]	
	175	Methyl (methylsulfinyl)methyl sulfide	$CH_3SOCH_2SCH_3$		$CH_3SOCH_2SCH_3 + e^- \rightarrow [CH_3SOCH_2SCH_3]^{*-}$	-30.720	-2.95 [a]	--	--	--	--	1.31×10^{8}
					$CH_3SOCH_2SCH_3 + e^- \rightarrow CH_3S(-)O + *CH_2SCH_3$	--	--	-41.576	-2.48 [a]	22.053	-5.24 [c]	
Thiol	176	Methanethiol	CH_3SH		$CH_3SH + e^- \rightarrow *CH_3 + SH^-$	--	--	-47.753	-2.21 [c]	42.899	-6.14 [c]	1.08×10^{10}
	177	Thiolactate	$CH_3(CH)SHCOO^-$		$CH_3(CH)SHCOO^- + e^- \rightarrow CH_3(CH)SH*CO(-)O^-$	-17.629	-3.52 [a]	--	--	--	--	2.89×10^{9}
					$CH_3(CH)SHCOO^- + e^- \rightarrow *CH_3(CH)COO^- + SH^-$	--	--	-58.463	-1.75 [c]	27.383	-5.47 [c]	
	178	2-Mercaptopropionic Acid	$CH_3(CH)SHCOOH$		$CH_3CH(SH)COOH + e^- \rightarrow *CH_3CHCOOH + SH^-$	--	--	-62.497	-1.57 [c]	22.838	-5.27 [c]	4.08×10^{9}
	179	Methyl thioglycolate	CH_3COOCH_2SH		$HSCH_2COOCH_3 + e^- \rightarrow *CH_2COOCH_3 + HS^-$	--	--	-56.076	-1.85 [c]	26.953	-5.45 [c]	1.12×10^{10}
	180	beta-Mercaptoethanol	$HS(CH_2)_2OH$		$HS(CH_2)_2OH + e^- \rightarrow [HS(CH_2)_2OH]^{*-}$	-23.177	-3.28 [a]	--	--	--	--	1.73×10^{10}
					$HS(CH_2)_2OH + e^- \rightarrow HSCH_2*CH_2 + OH^-$	--	--	-11.456	-3.78 [a]			
					$HS(CH_2)_2OH + e^- \rightarrow *(CH_2)_2OH + HS^-$	--	--	-49.878	-2.12 [c]	38.682	-5.96 [c]	
	181	2-Methyl-2-propanethiol	$(CH_3)_3CSH$		$(CH_3)_3CSH + e^- \rightarrow (CH_3)_3*C + HS^-$	--	--	-54.275	-1.93 [c]	32.693	-5.70 [c]	3.41×10^{9}
	182	3-Mercaptopropionic acid	$HS(CH_2)_2COOH$		$HS(CH_2)_2COOH + e^- \rightarrow *(CH_2)_2COOH + HS^-$	--	--	-50.098	-2.11 [c]	34.898	-5.79 [c]	6.91×10^{9}

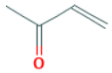
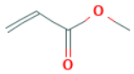
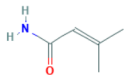
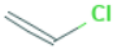
	183	Thioglycolate	$HSCH_2COO^-$		$HSCH_2COO^- + e^- \rightarrow {}^*CH_2COO^- + HS^-$	--	--	-54.298	-1.93 [c]	33.123	-5.72 [c]	3.03×10^{9}
	184		$H_2NC(=NH)NHCH_2CH_2SH$		$H_2NC(=NH)NHCH_2CH_2SH + e^- \rightarrow [H_2NC(=NH)NHCH_2CH_2SH]^{*-}$	0.881	-4.32 [a]	--	--	--	--	1.02×10^{11}
					$H_2NC(=NH)NHCH_2CH_2SH + e^- \rightarrow H_2NC(=NH)NHCH_2{}^*CH_2 + HS^-$	--	--	-51.249	-2.06 [c]	31.333	-5.64 [c]	
Sulfide/Disulfide	185	Dimethylsulfide	CH_3SCH_3		$CH_3SCH_3 + e^- \rightarrow [CH_3SCH_3]^{*-}$	5.808	-4.53 [a]	--	--	--	--	2.00×10^{7}
					$CH_3SCH_3 + e^- \rightarrow [CH_2SCH_3]^- + H^*$	--	--	24.723	-5.35[a]	--	--	
					$CH_3SCH_3 + e^- \rightarrow CH_3S^- + {}^*CH_3$	--	--	-38.239	-2.62[c]	52.271	-6.55 [c]	
	186	3,3'-Dithiodipropionate	$(SCH_2CH_2COO^-)_2$		$(SCH_2CH_2COO^-)_2 + e^- \rightarrow (SCH_2CH_2{}^*CO(-)O^-)(SCH_2CH_2COO^-)$	-49.957	-2.11[a]	--	--	--	--	4.35×10^{9}
					$(SCH_2CH_2COO^-)_2 + e^- \rightarrow [(SCHCH_2COO^-)(SCH_2CH_2COO^-)]^- + H^*$	--	--	--	--	20.221	-5.16 [c]	
	187	2,2'-Disulfanediyldiacetate	$(SCH_2COO^-)_2$		$(SCH_2COO^-)_2 + e^- \rightarrow {}^*SCH_2COO^- + [SCH_2COO^-]^-$	--	--	--	--	25.319	-5.38 [c]	4.30×10^{9}
	188	2,2'-Sulfanediyldiacetate	$S(CH_2COO^-)_2$		$S(CH_2COO^-)_2 + e^- \rightarrow S(-)CH_2COO- + {}^*CH_2COO^-$	--	--	-91.208	-0.33 [a]	34.861	-5.79 [c]	8.30×10^{7}
	189	N-Acetylcysteamine	$CH_3CONHCH_2CH_2SH$		$CH_3CONHCH_2CH_2SH + e^- \rightarrow [CH_3CONHCH_2CH_2SH]^{*-}$	-23.670	-3.25 [a]	--	--	--	--	1.43×10^{10}
					$CH_3CONHCH_2CH_2SH + e^- \rightarrow CH_3CONHCH_2{}^*CH_2 + SH^-$	--	--	-37.013	-2.68 [a]	29.283	-5.55 [c]	
	190	Cystamine	$S_2(CH_2CH_2NH_2)_2$		$S_2(CH_2CH_2NH_2)_2 + e^- \rightarrow [S_2(CH_2CH_2NH_2)_2]^{*-}$	-53.594	-1.96[c]	--	--	--	--	5.85×10^{10}
					$S_2(CH_2CH_2NH_2)_2 + e^- \rightarrow {}^*SCH_2CH_2NH_2 + [SCH2CH2NH_2]^-$	--	--	--	--	24.232	-5.33 [c]	
	191	L-Cystine anion	$S_2[CH_2CH(NH_2)COO^-]_2$		$S_2[CH_2CH(NH_2)COO^-]_2 + e^- \rightarrow {}^*SCH_2CH(NH_2)COO^- + [SCH_2CH(NH_2)COO^-]^-$	--	--	--	--	15.237	-4.94 [c]	3.53×10^{9}

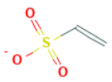
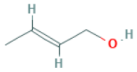
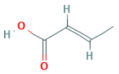
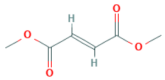
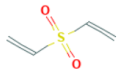
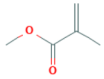
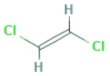
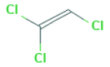
	192	3,3'-Thiodipropanoate	$S(CH_2CH_2COO^-)_2$		$(CH_2CH_2COO^-)_2 + e^- \rightarrow S(-)CH_2CH_2COO^- + {}^*CH_2CH_2COO^-$	--	--	-96.927	-0.08 [a]	33.508	-5.73 [c]	5.80×10^{7}
S-	193	2-Hydroxyethanethiolate	$HOCH_2CH_2S^-$		$HOCH_2CH_2S^- + e^- \rightarrow [HOCH_2CH_2S^-]^{*-}$	3.129	-4.42 [a]	--	--	--	--	
					$HOCH_2CH_2S^- + e^- \rightarrow HOCH_2{}^*CH_2 + S_2^-$	--	--	-15.197	-3.62[c]	71.881	-7.40 [c]	1.80×10^{7}
					$HOCH_2CH_2S^- + e^- \rightarrow (-)OCH_2CH_2S^- + H^*$	--	--	4.802	-4.49 [a]	--	--	
	194	2-lambda1-Sulfanylethanamine	$H_2NCH_2CH_2S^-$		$H_2NCH_2CH_2S^- + e^- \rightarrow [H_2NCH_2CH_2S^-]^{*-}$	20.995	-5.19 [a]	--	--	--	--	
					$H_2NCH_2CH_2S^- + e^- \rightarrow H_2NCH_2{}^*CH_2 + S_2^-$	--	--	-16.842	-3.55[c]	69.605	-7.30 [c]	
					$H_2NCH_2CH_2S^- + e^- \rightarrow H(-)NCH_2CH_2S^- + H^*$	--	--	31.804	-5.66 [a]	--	--	9.55×10^{8}
					$H_2NCH_2CH_2S^- + e^- \rightarrow H_2NCH_2CHS^- + H^*$	--	--	53.644	-6.61 [a]	--	--	
					$H_2NCH_2CH_2S^- + e^- \rightarrow H_2NCHCH_2S^- + H^*$	--	--	51.827	-6.53 [a]	--	--	
	195	2-Acetamidoethanethiolate	$CH_3CONHCH_2CH_2S^-$		$CH_3CONHCH_2CH_2S^- + e^- \rightarrow [CH_3CONHCH_2CH_2S^-]^{*-}$	-9.487	-3.87 [a]	--	--	--	--	
					$CH_3CONHCH_2CH_2S^- + e^- \rightarrow CH_3CONHCH_2{}^*CH_2 + S_2^-$	--	--	-16.106	-3.58[c]	62.816	-7.00 [c]	1.90×10^{9}
CS	196	Carbon Disulfide	CS_2		$CS_2 + e^- \rightarrow [CS_2]^{*-}$	-57.796	-1.77 [a]	--	--	--	--	3.10×10^{10}
	197	Thiourea	H_2NCSNH_2		$H_2NCSNH_2 + e^- \rightarrow [H_2NCSNH_2]^{*-}$	-18.118	-3.49 [a]	--	--	--	--	3.29×10^{9}
	198	Thiosemicarbazide	$H_2NNHCSNH_2$		$H_2NNHCSNH_2 + e^- \rightarrow [H_2NNHCSNH_2]^{*-}$	-19.102	-3.45 [a]	--	--	--	--	1.15×10^{9}
	199	N,N'-Diethylthiourea	$CH_3CH_2NHCSNHCH_2CH_3$		$CH_3CH_2NHCSNHCH_2CH_3 + e^- \rightarrow [CH_3CH_2NHCSNHCH_2CH_3]^{*-}$	-19.126	-3.45 [a]	--	--	--	--	5.10×10^{8}

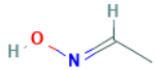
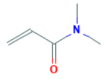
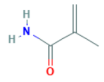
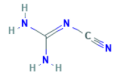
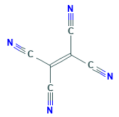
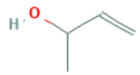
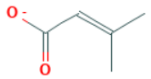
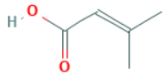
Nitro	200	Nitromethane	CH_3NO_2		$CH_3NO_2 + e^- \rightarrow [CH_3NO_2]^{*-}$	-61.020	-1.63 [a]	--	--	--	--	1.80×10^{11}
					$CH_3NO_2 + e^- \rightarrow [CH_2NO_2]^- + H^*$	--	--	-15.324	-3.62 [a]	--	--	
					$CH_3NO_2 + e^- \rightarrow {}^*CH_3 + NO_2^-$	--	--	-46.434	-2.27 [a]	51.633	-6.52 [c]	
	201	1-Nitropropane	$CH_3CH_2CH_2NO_2$		$CH_3CH_2CH_2NO_2 + e^- \rightarrow [CH_3CH_2CH_2NO_2]^{*-}$	-60.847	-1.64 [a]	--	--	--	--	2.70×10^{10}
					$CH_3CH_2CH_2NO_2 + e^- \rightarrow [CH_3CH_2CHNO_2]^- + H^*$	--	--	-16.349	-3.57 [a]	--	--	
					$CH_3CH_2CH_2NO_2 + e^- \rightarrow [CH_3CHCH_2NO_2]^- + H^*$	--	--	33.614	-5.74 [a]	--	--	
					$CH_3CH_2CH_2NO_2 + e^- \rightarrow [CH_3CH_2{}^*CH_2 + NO_2^-$	--	--	-46.496	-2.26 [a]	48.013	-6.36 [c]	
	202	Nitroethane	$CH_3CH_2NO_2$		$CH_3CH_2NO_2 + e^- \rightarrow [CH_3CH_2NO_2]^{*-}$	-60.174	-1.67[a]	--	--	--	--	2.70×10^{10}
					$CH_3CH_2NO_2 + e^- \rightarrow [CH_3CHNO_2]^- + H^*$	--	--	-16.097	-3.58 [a]	--	--	
					$CH_3CH_2NO_2 + e^- \rightarrow CH_3{}^*CH_2 + NO_2^-$	--	--	-46.401	-2.27 [a]	49.591	-6.43 [c]	
	203	2-Methyl-2-nitrosopropane	$(CH_3)_3C(NO)$		$(CH_3)_3C(NO) + e^- \rightarrow [(CH_3)_3C(NO)]^{*-}$	-63.457	-1.53 [a]	--	--	--	--	8.26×10^{9}
					$(CH_3)_3C(NO) + e^- \rightarrow (CH_3)_3{}^*C + NO^-$	--	--	4.387	-4.47 [a]	20.961	-5.19[c]	
PFAS	204	Trifluoroacetate	CF_3COO^-		$CF_3COO^- + e^- \rightarrow CF_3{}^*CO(-)O^-$	--	--	--	--	--	--	1.65×10^{6}
					$CF_3COO^- + e^- \rightarrow {}^*CF_2COO^- + F^-$	--	--	-8.995	-3.89[a]	88.105	-8.10 [a]	
	205	Perflurobutanoic Acid	$C_3F_7COO^-$		$C_3F_7COO^- + e^- \rightarrow C_3F_7{}^*CO(-)O^-$	-36.211	-2.71[b]	--	--	--	--	7.10×10^{6}

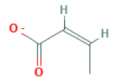
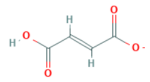
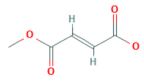
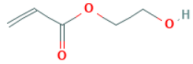
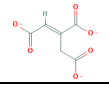
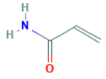
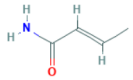
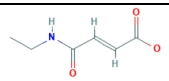
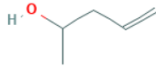
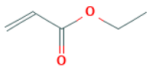
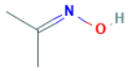
					$C_3F_7COO^- + e^- \rightarrow CF_3CF_2CFCOO^- + F^-$	--	--	-19.143	-3.45[a]	59.505	-6.86[a]	
					$C_3F_7COO^- + e^- \rightarrow CF_3{}^*CFCF_2COO^- + F^-$	--	--	-13.608	-3.69[a]	65.733	-7.13[a]	
					$C_3F_7COO^- + e^- \rightarrow {}^*CF_2CF_2CF_2COO^- + F^-$	--	--	-5.305	-4.05[a]	73.344	-7.46[a]	
					$C_7F_{15}COO^- + e^- \rightarrow C_7F_{15}{}^*CO(-)O^-$	-32.059	-2.89[b]	--	--	--	--	
					$C_7F_{15}COO^- + e^- \rightarrow CF_3CF_2CF_2CF_2CF_2CF_2{}^*CFCOO^- + F^-$	--	--	-18.451	-3.48[c]	42.899	-6.14[c]	
					$C_7F_{15}COO^- + e^- \rightarrow CF_3CF_2CF_2CF_2CF_2{}^*CFCF_2COO^- + F^-$	--	--	-15.222	-3.62[c]	46.128	-6.28[c]	
					$C_7F_{15}COO^- + e^- \rightarrow CF_3CF_2CF_2CF_2{}^*CFCF_2CF_2COO^- + F^-$	--	--	-16.145	-3.58[c]	45.436	-6.25[c]	
	206	Perfluorooctanoic Acid	$C_7F_{15}COO^-$		$C_7F_{15}COO^- + e^- \rightarrow CF_3CF_2CF_2{}^*CFCF_2CF_2CF_2COO^- + F^-$	--	--	-16.606	-3.56[c]	45.206	-6.24[c]	1.70×10^7
					$C_7F_{15}COO^- + e^- \rightarrow CF_3CF_2{}^*CFCF_2CF_2CF_2CF_2COO^- + F^-$	--	--	-16.837	-3.55[c]	46.589	-6.30[c]	
					$C_7F_{15}COO^- + e^- \rightarrow CF_3{}^*CFCF_2CF_2CF_2CF_2CF_2COO^- + F^-$	--	--	-15.684	-3.60[c]	46.589	-6.30[c]	
					$C_7F_{15}COO^- + e^- \rightarrow {}^*CF_2CF_2CF_2CF_2CF_2CF_2CF_2COO^- + F^-$	--	--	-6.227	-4.01[c]	54.892	-6.66[c]	
					$H_2C{=}CHCH_2NH_2 + e^- \rightarrow [H_2C{=}CHCH_2NH_2]^{*-}$	-23.127	-3.28[b]	--	--	--	--	
Alkene	207	Allylamine	$H_2C{=}CHCH_2NH_2$		$H_2C{=}CHCH_2NH_2 + e^- \rightarrow [H_2C{=}CHCHNH_2]^- + H^*$	--	--	19.091	-5.11[a]	--	--	1.20×10^7
					$H_2C{=}CHCH_2NH_2 + e^- \rightarrow [H_2C{=}CCH_2NH_2]^- + H^*$	--	--	26.763	-5.44[a]	--	--	
					$H_2C{=}CHCH_2NH_2 + e^- \rightarrow [HC{=}CHCH_2NH_2]^- + H^*$	--	--	26.076	-5.41[a]	--	--	

				$H_2C{=}CHCN + e^- \rightarrow [H_2C{=}CHCN]^{*-}$	-53.943	-1.94[b]	--	--	--	--	
208	Acrylonitrile	$H_2C{=}CHCN$		$H_2C{=}CHCN + e^- \rightarrow [H_2C{=}CCN]^- + H^*$	--	--	3.716	-4.44[a]	--	--	2.78×10^{10}
				$H_2C{=}CHCN + e^- \rightarrow [HC{=}CHCN]^- + H^*$	--	--	14.285	-4.90[a]	--	--	
				$H_2C{=}CHCH_2OH + e^- \rightarrow [H_2C{=}CHCH_2OH]^{*-}$	-27.368	-3.09[b]	--	--	--	--	
				$H_2C{=}CHCH_2OH + e^- \rightarrow [H_2C{=}CHCH_2O]^- + H^*$	--	--	0.364	-4.30[a]	--	--	
209	Allyl alcohol	$H_2C{=}CHCH_2OH$		$H_2C{=}CHCH_2OH + e^- \rightarrow [H_2C{=}CHCHOH]^- + H^*$	--	--	17.836	-5.05[a]	--	--	3.47×10^{7}
				$H_2C{=}CHCH_2OH + e^- \rightarrow [H_2C{=}CCH_2OH]^- + H^*$	--	--	23.083	-5.28[a]	--	--	
				$H_2C{=}CHCH_2OH + e^- \rightarrow [HC{=}CHCH_2OH]^- + H^*$	--	--	19.174	-5.11[a]	--	--	
				$H_2C{=}CHCOOH + e^- \rightarrow H_2C{=}CH^*CO(-)OH$	-59.268	-1.71[b]	--	--	--	--	
				$H_2C{=}CHCOOH + e^- \rightarrow H_2C{=}CH^*CO + OH^-$	--	--	7.683	-4.61[a]	--	--	
210	Acrylic acid	$H_2C{=}CHCOOH$		$H_2C{=}CHCOOH + e^- \rightarrow [H_2C{=}CCOOH]^- + H^*$	--	--	11.370	-4.77[a]	--	--	1.03×10^{12}
				$H_2C{=}CHCOOH + e^- \rightarrow [HC{=}CHCOOH]^- + H^*$	--	--	17.443	-5.04[a]	--	--	
				$CH_2{=}CHCOO^- + e^- \rightarrow CH_2{=}CH^*CO(-)O^-$	-40.739	-2.51[b]	--	--	--	--	
211	Acrylate	$CH_2{=}CHCOO^-$		$CH_2{=}CHCOO^- + e^- \rightarrow [CH_2{=}CCOO]^{2-} + H^*$	--	--	28.234	-5.50[a]	--	--	5.30×10^{9}
				$CH_2{=}CHCOO^- + e^- \rightarrow [CH{=}CHCOO]^{2-} + H^*$	--	--	27.304	-5.46[a]	--	--	

212	Methyl vinyl ketone	$H_2C=CHCOCH_3$		$H_2C=CHCOCH_3 + e^- \rightarrow H_2C=CH^*CO(-)CH_3$	-63.318	-1.53[b]	--	--	--	--	2.78×10^9
				$H_2C=CHCOCH_3 + e^- \rightarrow [H_2C=CHCOCH_2]^- + H^*$	--	--	-8.414	-3.92[a]	--	--	
				$H_2C=CHCOCH_3 + e^- \rightarrow [H_2C=CCOCH_3]^- + H^*$	--	--	8.306	-4.64[a]	--	--	
				$H_2C=CHCOCH_3 + e^- \rightarrow [HC=CHCOCH_3]^- + H^*$	--	--	18.815	-5.10[a]	--	--	
213	Methyl acrylate	$H_2C=CHCOOCH_3$		$H_2C=CHCOOCH_3 + e^- \rightarrow H_2C=CH^*CO(-)OCH_3$	-57.171	-1.80[b]	--	--	--	--	1.52×10^{10}
				$H_2C=CHCOOCH_3 + e^- \rightarrow [H_2C=CHCOOCH_2]^- + H^*$	--	--	26.012	-5.41[a]	--	--	
				$H_2C=CHCOOCH_3 + e^- \rightarrow [H_2C=CCOOCH_3]^- + H^*$	--	--	11.779	-4.79[a]	--	--	
				$H_2C=CHCOOCH_3 + e^- \rightarrow [HC=CHCOOCH_3]^- + H^*$	--	--	17.747	-5.05[a]	--	--	
214	Senecioic acid amide	$(CH_3)_2C=CHCONH_2$		$(CH_3)_2C=CHCONH_2 + e^- \rightarrow [(CH_3)_2C=CHCONH_2]^{*-}$	-44.000	-2.37[b]	--	--	--	--	7.23×10^9
				$(CH_3)_2C=CHCONH_2 + e^- \rightarrow [(CH_3)_2C=CCONH_2]^- + H^*$	--	--	17.846	-5.05[a]	--	--	
				$(CH_3)_2C=CHCONH_2 + e^- \rightarrow [CH_3CH_2C=CHCONH_2]^- + H^*$	--	--	-1.305	-4.22[a]	--	--	
215	Vinyl chloride	$CH_2=CHCl$		$CH_2=CHCl + e^- \rightarrow [CH_2=CHCl]^{*-}$	-58.079	-1.76[c]	--	--	--	--	2.53×10^8
				$CH_2=CHCl + e^- \rightarrow {}^*CH_2=CH + Cl^-$	--	--	-62.086	-1.59[c]	27.100	-5.45[c]	
216	Ethylene	$H_2C=CH_2$		$H_2C=CH_2 + e^- \rightarrow [H_2C=CH_2]^{*-}$	-24.747	-3.21[b]	--	--	--	--	3.00×10^5
				$H_2C=CH_2 + e^- \rightarrow [H_2C=CH]^- + H^*$	--	--	27.495	-5.47[a]	--	--	

				$CH_2=CHSO_3^- + e^- \rightarrow [CH_2=CHSO_3]^{*2-}$	-37.671	-2.65[b]	--	--	--	--	
217	Ethenesulfonate	$CH_2=CHSO_3^-$		$CH_2=CHSO_3^- + e^- \rightarrow [CH_2=CSO_3]^{2-} + H^*$	--	--	13.000	-4.84[a]	--	--	2.30×10^{9}
				$CH_2=CHSO_3^- + e^- \rightarrow [CH=CHSO_3]^{2-} + H^*$	--	--	19.342	-5.12[a]	--	--	
				$Cl_2C=CCl_2 + e^- \rightarrow [Cl_2C=CCl_2]^{*-}$	-67.930	-1.33[c]	--	--	--	--	
218	Tetrachloroethylene	$Cl_2C=CCl_2$		$Cl_2C=CCl_2 + e^- \rightarrow {}^*Cl_2C=CCl + Cl^-$	--	--	-70.102	-1.24[c]	15.166	-4.94[c]	2.67×10^{10}
219	Crotonyl Alcohol	$CH_3CH=CHCH_2OH$		$CH_3CH=CHCH_2OH + e^- \rightarrow [CH_3CH=CHCH_2OH]^{*-}$	-24.308	-3.23[b]	--	--	--	--	5.51×10^{7}
220	Crotonic Acid	$CH_3CH=CHCOOH$		$CH_3CH=CHCOOH + e^- \rightarrow CH_3CH=CH{}^*CO(-)OH$	-54.359	-1.92[b]	--	--	--	--	6.62×10^{10}
221	Dimethyl Fumarate	$CH_3OOCCH=CHCOOCH_3$		$CH_3OOCCH=CHCOOCH_3 + e^- \rightarrow CH_3OOCCH=CH{}^*CO(-)OCH_3$	-76.951	-0.94[b]	--	--	--	--	3.30×10^{10}
222	Divinyl Sulfone	$(H_2C=CH)_2SO_2$		$(H_2C=CH)_2SO_2 + e^- \rightarrow [(H_2C=CH)_2SO_2]^{*-}$	-55.621	-1.87[b]	--	--	--	--	1.66×10^{10}
223	Methacrylic Acid	$H_2C=C(CH_3)COOH$		$H_2C=C(CH_3)COOH + e^- \rightarrow H_2C=C(CH_3){}^*CO(-)OH$	-56.591	-1.83[b]	--	--	--	--	8.26×10^{10}
224	Methyl Methacrylate	$H_2C=C(CH_3)COOCH_3$		$H_2C=C(CH_3)COOCH_3 + e^- \rightarrow H_2C=C(CH_3){}^*CO(-)OCH_3$	-54.409	-1.92[b]	--	--	--	--	2.72×10^{10}
				$ClCH=CHCl + e^- \rightarrow [ClCH=CHCl]^{*-}$	-60.299	-1.67[c]	--	--	--	--	
225	trans-1,2-Dichloroethylene	$ClCH=CHCl$		$ClCH=CHCl + e^- \rightarrow {}^*CH=CHCl + Cl^-$	--	--	-64.409	-1.49[c]	22.702	-5.26[c]	1.08×10^{10}
				$ClCH=CCl_2 + e^- \rightarrow [ClCH=CCl_2]^{*-}$	-60.732	-1.65[c]	--	--	--	--	
226	Trichloroethylene	$ClCH=CCl_2$		$ClCH=CCl_2 + e^- \rightarrow {}^*CH=CCl_2 + Cl^-$	--	--	-64.187	-1.50[c]	21.118	-5.20[c]	8.28×10^{10}

				$ClCH=CCl_2 + e^- \rightarrow ClCH=C^*Cl + Cl^-$	--	--	-66.977	-1.38[c]	18.451	-5.08[c]	
227	cis-1,2-Dichloroethylene	$H_2C=CCl_2$		$H_2C=CCl_2 + e^- \rightarrow [H_2C=CCl_2]^{*-}$	-64.626	-1.48[c]	--	--	--	--	3.86×10^{11}
				$H_2C=CCl_2 + e^- \rightarrow H_2C=C^*Cl + Cl^-$	--	--	-67.503	-1.35[c]	19.855	-5.14[c]	
228	1,3-Butadiene	$H_2C=CHCH=CH_2$		$H_2C=CHCH=CH_2 + e^- \rightarrow [H_2C=CHCH=CH_2]^{*-}$	-42.651	-2.43[b]	--	--	--	--	1.19×10^{10}
229	Acetaldehyde Oxime	$CH_3CH=NOH$		$CH_3CH=NOH + e^- \rightarrow [CH_3CH=NOH]^{*-}$	-30.634	-2.95[b]	--	--	--	--	7.22×10^{7}
230	N,N-Dimethylacrylamide	$CH_2=CHCON(CH_3)_2$		$CH_2=CHCON(CH_3)_2 + e^- \rightarrow CH_2=CH^*CO(-)N(CH_3)_2$	-51.043	-2.07[b]	--	--	--	--	4.51×10^{10}
231	Methacrylamide	$H_2C=C(CH_3)CONH_2$		$H_2C=C(CH_3)CONH_2 + e^- \rightarrow H_2C=C(CH_3)^*CO(-)NH_2$	-49.796	-2.12[b]	--	--	--	--	7.10×10^{11}
232	Cyanoguanidine	$NCN=C(NH_2)_2$		$NCN=C(NH_2)_2 + e^- \rightarrow [NCN=C(NH_2)_2]^{*-}$	-31.890	-2.90[b]	--	--	--	--	1.96×10^{10}
233	Tetracyanoethylene	$(NC)_2C=C(CN)_2$		$(NC)_2C=C(CN)_2 + e^- \rightarrow [(NC)_2C=C(CN)_2]^{*-}$	-107.391	0.38[a]	--	--	--	--	3.74×10^{10}
				$(NC)_2C=C(CN)_2 + e^- \rightarrow (NC)_2C=C^*CN + CN^-$	--	--	--	--	36.901	-5.88[c]	
234	Methacrylate	$CH_2=C(CH_3)COO^-$		$CH_2=C(CH_3)COO^- + e^- \rightarrow CH_2=C(CH_3)^*CO(-)O^-$	-49.796	-2.12[b]	--	--	--	--	4.50×10^{9}
235	3-Buten-1-ol	$H_2C=CHCH_2CH_2OH$		$H_2C=CHCH_2CH_2OH + e^- \rightarrow [H_2C=CHCH_2CH_2OH]^{*-}$	-22.989	-3.28[b]	--	--	--	--	2.45×10^{6}
236	3-Buten-2-OL	$H_2C=CHCH(OH)CH_3$		$H_2C=CHCH(OH)CH_3 + e^- \rightarrow [H_2C=CHCH(OH)CH_3]^{*-}$	-26.409	-3.13[b]	--	--	--	--	5.91×10^{7}
237	3-Methylbut-2-enoate	$(CH_3)_2C=CHCO_2^-$		$(CH_3)_2C=CHCO_2^- + e^- \rightarrow (CH_3)_2C=CH^*CO(-)O^-$	-31.707	-2.91[b]	--	--	--	--	6.40×10^{8}
238	3,3-Dimethylacrylic acid	$(CH_3)_2C=CHCOOH$		$(CH_3)_2C=CHCOOH + e^- \rightarrow (CH_3)_2C=CH^*CO(-)OH$	-50.403	-2.09[b]	--	--	--	--	2.53×10^{10}

239	Isocrotonate	$CH_3CH=CHCOO^-$		$CH_3CH=CHCOO^- + e^- \rightarrow CH_3CH=CH^*CO(-)O^-$	-35.702	-2.73[b]	--	--	--	--	1.30×10^{9}
240	Hydrogen Fumarate	$HOOCCH=CHCOO^-$		$HOOCCH=CHCOO^- + e^- \rightarrow HO(-)OC^*CH=CHCOO^-$	-66.404	-1.40[b]	--	--	--	--	1.35×10^{10}
241	Monomethyl Fumarate	$CH_3OOCCH=CHCOO^-$		$CH_3OOCCH=CHCOO^- + e^- \rightarrow [CH_3OOCCH=CHCOO^-]^{*-}$	-64.429	-1.49[b]	--	--	--	--	1.30×10^{10}
242	2-Hydroxyethyl Acrylate	$CH_2=CHCOOCH_2CH_2OH$		$CH_2=CHCOOCH_2CH_2OH + e^- \rightarrow CH_2=CH^*CO(-)OCH_2CH_2OH$	-57.853	-1.77[b]	--	--	--	--	1.08×10^{10}
243	trans-Aconitate(3-)	$^-OOCCH=C(COO^-)CH_2COO^-$		$^-OOCCH=C(COO^-)CH_2COO^- + e^- \rightarrow [^-OOCCH=C(COO^-)CH_2COO^-]^{*-}$	-45.032	-2.33[b]	--	--	--	--	1.80×10^{8}
244	Acrylamide	$H_2C=CHCONH_2$		$H_2C=CHCONH_2 + e^- \rightarrow H_2C=CH^*CO(-)NH_2$	-51.891	-2.03[b]	--	--	--	--	3.81×10^{11}
245	Crotonamide	$CH_3CH=CHCONH_2$		$CH_3CH=CHCONH_2 + e^- \rightarrow CH_3CH=CH^*CO(-)NH_2$	-47.616	-2.22[b]	--	--	--	--	2.75×10^{10}
246	4-(Ethylamino)-4-oxobut-2-enoate	$C_2H_5NHCOCH=CHCOO^-$		$C_2H_5NHCOCH=CHCOO^- + e^- \rightarrow C_2H_5NH^*CO(-)CH=CHCOO^-$	-56.866	-1.81[b]	--	--	--	--	8.50×10^{9}
247	cis-Dimethyl Fumarate	$CH_3OOCCH=CHCOOCH_3$		$CH_3OOCCH=CHCOOCH_3 + e^- \rightarrow CH_3OOCCH=CH^*CO(-)OCH_3$	-73.513	-1.09[b]	--	--	--	--	3.20×10^{10}
248	4-Penten-2-OL	$H_2C=CHCH_2CH(OH)CH_3$		$H_2C=CHCH_2CH(OH)CH_3 + e^- \rightarrow [H_2C=CHCH_2CH(OH)CH_3]^{*-}$	-21.903	-3.33[b]	--	--	--	--	5.00×10^{5}
249	Guanidine	$H_2NC(=NH)NH_2$		$H_2NC(=NH)NH_2 + e^- \rightarrow [H_2NC(=NH)NH_2]^{*-}$	-4.978	-4.06[b]	--	--	--	--	2.02×10^{8}
250	Ethyl Acrylate	$H_2C=CHCOOC_2H_5$		$H_2C=CHCOOC_2H_5 + e^- \rightarrow H_2C=CH^*CO(-)OC_2H_5$	-57.326	-1.79[b]	--	--	--	--	1.34×10^{10}
251	Acetone Oxime	$(CH_3)_2C=NOH$		$(CH_3)_2C=NOH + e^- \rightarrow [(CH_3)_2C=NOH]$	-25.737	-3.16[b]	--	--	--	--	3.29×10^{8}

[a]M06-2X/cc-pVDZ
[b] structural optimization with M06-2X/cc-pVDZ and single point energy calculation with M06-2X/Aug-cc-pVTZ
[c]M06-2X/Aug-cc-pVTZ
[d]M06-2X/LANL2DZ

Table S5: Corrected experimental k_{chem} and calculated E_{red} overall results for dataset

Class	No.	Name	Chemical Formula	Molar Volume, V_b (cm^3/mol)	Diffusion Coefficient, D_l (cm^2/s)	k_D (M^{-1} s^{-1})	k_{chem} (M^{-1} s^{-1})	ln k_{chem}	$\Delta G°_{red,aq}$ (kcal/mol)	$E°_{red}$ (V vs SHE)	Upper Limit k_{exp} (M^{-1} s^{-1})	Lower Limit k_{exp} (M^{-1} s^{-1})
Alkane	1	Methane	CH_4	22.8	7.31×10^{-5}	2.49×10^{10}	1.00×10^{7}	16.12	25.97	-5.41	N/A	N/A
	2	Propane	$CH_3CH_2CH_3$	40.4	6.62×10^{-5}	2.44×10^{10}	2.10×10^{6}	14.56	23.74	-5.31	N/A	N/A
	3	Butane	C_4H_{10}	57.3	6.30×10^{-5}	2.45×10^{10}	2.40×10^{6}	14.69	22.77	-5.27	N/A	N/A
Carboxylate	4	Oxalate	$^{-}OOCCOO^{-}$	46.8	7.34×10^{-5}	2.77×10^{10}	2.28×10^{7}	16.94	-29.94	-2.98	4.60×10^{7}	1.00×10^{7}
	5	Formate	$HCOO^{-}$	38.5	7.41×10^{-5}	2.72×10^{10}	5.04×10^{5}	13.13	-9.93	-3.85	1.00×10^{6}	8.00×10^{3}
	6	Succinate	$^{-}OOC(CH_2)_2COO^{-}$	72.0	6.91×10^{-5}	2.79×10^{10}	1.59×10^{7}	16.58	-8.72	-3.90	3.10×10^{7}	7.00×10^{5}
	7	Acetate	CH_3COO^{-}	45.9	6.85×10^{-5}	2.58×10^{10}	1.05×10^{6}	13.86	-8.07	-3.93	1.10×10^{6}	1.00×10^{6}
	8	Hydrogen Oxalate	$HOOCCOO^{-}$	46.6	6.82×10^{-5}	2.57×10^{10}	3.65×10^{9}	22.02	-52.21	-2.02	N/A	N/A
	9	Malonate	$^{-}OOC\text{-}CH_2\text{-}COO^{-}$	79.6	7.05×10^{-5}	2.89×10^{10}	1.00×10^{7}	16.12	-9.07	-3.89	N/A	N/A
	10	Malonate(1-)	$HOOC\text{-}CH_2\text{-}COO^{-}$	68.4	--	--[a]	5.06×10^{8}	20.04	-35.93	-2.72	7.00×10^{8}	4.00×10^{8}
	11	Succinate(1-)	$HOOC(CH_2)_2COO^{-}$	86.8	--	--[a]	2.05×10^{8}	19.14	-32.74	-2.86	3.40×10^{8}	7.00×10^{7}
	12	Lactate	$CH_3CHOHCOO^{-}$	60.8	6.76×10^{-5}	2.65×10^{10}	1.00×10^{7}	16.12	-5.70	-4.03	N/A	N/A
	13	Glycolate	$HOCH_2COO^{-}$	47.9	--	--[a]	8.20×10^{6}	15.92	-6.61	-3.99	N/A	N/A
	14	Pyruvate	CH_3COCOO^{-}	61.5	--	--[a]	6.80×10^{9}	22.64	-50.94	-2.07	N/A	N/A
	15	CID_4134252	$HOCH_2(CHOH)_4COO^{-}$	145.8	--	--[a]	1.00×10^{6}	13.82	-13.59	-3.69	N/A	N/A
	16	Malate	$^{-}OOCCH_2CHOHCOO^{-}$	84.1	6.91×10^{-5}	2.86×10^{10}	6.01×10^{7}	17.91	-11.81	-3.77	N/A	N/A
Carboxylic Acid	17	Oxalic Acid	$HOOCCOOH$	57.9	6.29×10^{-5}	2.45×10^{10}	2.50×10^{10}	23.94[b]	-62.94	-1.55	N/A	N/A
	18	Formic Acid	$HCOOH$	28.1	7.02×10^{-5}	2.46×10^{10}	1.41×10^{8}	18.76	-39.00	-2.59	N/A	N/A
	19	Succinic Acid	$HOOC(CH_2)_2COOH$	98.0	5.92×10^{-5}	2.51×10^{10}	2.30×10^{8}	19.25	-35.30	-2.75	3.70×10^{8}	8.60×10^{7}
	20	Propionic Acid	CH_3CH_2COOH	64.9	6.20×10^{-5}	2.46×10^{10}	2.20×10^{7}	16.91	-35.03	-2.76	N/A	N/A
	21	Acetic Acid	CH_3COOH	50.2	6.41×10^{-5}	2.44×10^{10}	2.02×10^{8}	19.12	-32.16	-2.89	2.20×10^{8}	1.80×10^{8}
	22	Malonic Acid	$HOOC\text{-}CH_2\text{-}COOH$	55.8	6.32×10^{-5}	2.45×10^{10}	3.03×10^{9}	21.83	-40.83	-2.51	5.00×10^{9}	1.50×10^{9}
	23	Lactic Acid	$CH_3CH(OH)COOH$	60.2	6.26×10^{-5}	2.45×10^{10}	7.36×10^{8}	20.42	-38.23	-2.62	8.00×10^{8}	6.30×10^{8}
	24	Malic Acid	$HOOCCH_2CH(OH)COOH$	77.8	6.07×10^{-5}	2.48×10^{10}	3.41×10^{9}	21.95	-41.24	-2.49	N/A	N/A
	25	Glycolic acid	$HOCH_2COOH$	48.7	6.44×10^{-5}	2.44×10^{10}	4.38×10^{8}	19.90	-40.42	-2.53	N/A	N/A
Alcohol	26	Methanediol	$CH_2(OH)_2$	32.4	6.86×10^{-5}	2.45×10^{10}	1.00×10^{7}	16.12	-13.52	-3.69	N/A	N/A
	27	Tert-Butanol	$(CH_3)_3\text{-}C\text{-}OH$	71.7	6.12×10^{-5}	2.47×10^{10}	4.00×10^{5}	12.90	-6.33	-4.01	N/A	N/A
	28	Butane-1,2,3,4	$HOCH_2[CH(OH)]_2CH_2OH$	81.5	6.04×10^{-5}	2.48×10^{10}	5.00×10^{6}	15.43	-11.50	-3.78	N/A	N/A
	29	Mannitol	$HOCH_2[CH(OH)]_4CH_2OH$	132.4	5.75×10^{-5}	2.57×10^{10}	8.50×10^{6}	15.96	-16.74	-3.55	1.00×10^{7}	7.00×10^{6}
Ester	30	Methyl Acetate	CH_3COOCH_3	63.2	6.22×10^{-5}	2.46×10^{10}	8.73×10^{7}	18.28	-33.56	-2.82	N/A	N/A
	31	Methyl Propionate	$C_2H_5COOCH_3$	67.5	6.17×10^{-5}	2.46×10^{10}	9.03×10^{7}	18.32	-33.24	-2.84	N/A	N/A
	32	Ethyl Propionate	$C_2H_5COOC_2H_5$	97.9	5.92×10^{-5}	2.51×10^{10}	7.52×10^{7}	18.14	-33.22	-2.84	N/A	N/A
	33	Dimethyl Oxalate	$CH_3OOCCOOCH_3$	76.4	6.08×10^{-5}	2.48×10^{10}	1.04×10^{11}	25.37	-59.03	-1.72	N/A	N/A
	34	Tert-butyl Acetate	$(CH_3)_3CCOOCH_3$	90.5	5.97×10^{-5}	2.50×10^{10}	2.30×10^{7}	16.95	-30.20	-2.97	N/A	N/A
	35	2-Hydroxyethyl Acetate	$CH_3COOCH_2CH_2OH$	90.4	5.97×10^{-5}	2.50×10^{10}	2.60×10^{7}	17.07	-33.27	-2.84	N/A	N/A
	36	Di-tert-butyl Peroxide	$(CH_3)_3\text{-}COOC(CH_3)_3$	117.4	5.82×10^{-5}	2.55×10^{10}	1.41×10^{8}	18.76	44.93	-6.23	N/A	N/A
	37	Methylene glycol monoacetate	$HOCH_2COOCH_3$	59.5	6.27×10^{-5}	2.45×10^{10}	4.90×10^{8}	20.01	-37.37	-2.66	N/A	N/A
	38	Methyl methoxyacetate	$CH_3OCH_2COOCH_3$	68.3	6.16×10^{-5}	2.46×10^{10}	4.48×10^{8}	19.92	-38.04	-2.63	N/A	N/A
	39	Methyl trifluoroacetate	CF_3COOCH_3	62.0	6.23×10^{-5}	2.46×10^{10}	2.06×10^{9}	21.45	-55.22	-1.89	N/A	N/A
	40	Ethyl glycinate	$NH_2CH_2COOC_2H_5$	93.9	5.94×10^{-5}	2.51×10^{10}	8.58×10^{8}	20.57	-34.86	-2.77	N/A	N/A
	41	Acetoxymethylamine	$H_2NCH_2COOCH_3$	60.7	6.25×10^{-5}	2.45×10^{10}	3.14×10^{8}	19.56	-32.45	-2.87	3.30×10^{8}	2.90×10^{8}
Ether	42	Diethyl Ether	$(C_2H_5)_2O$	74.8	6.09×10^{-5}	2.47×10^{10}	1.00×10^{7}	16.12	-38.95	-2.59	N/A	N/A
Ketone	43	Acetone	CH_3COCH_3	49.1	6.43×10^{-5}	2.44×10^{10}	8.90×10^{9}	22.91	-38.95	-2.59	8.00×10^{9}	5.20×10^{9}
	44	Methyl Ethyl Ketone	$CH_3CH_2COCH_3$	72.3	6.12×10^{-5}	2.47×10^{10}	6.11×10^{9}	22.53	-38.72	-2.60	N/A	N/A
	45	2,3-Butanedione	$CH_3COCOCH_3$	60.9	6.25×10^{-5}	2.45×10^{10}	1.67×10^{10}	23.54	-69.05	-1.29	1.00×10^{10}	9.90×10^{9}
	46	Acetoin	$CH_3COCH(OH)CH_3$	57.2	6.30×10^{-5}	2.45×10^{10}	7.95×10^{9}	22.80	-43.76	-2.38	N/A	N/A
Aldehyde	47	Acetaldehyde	CH_3CHO	26.5	7.10×10^{-5}	2.47×10^{10}	6.11×10^{9}	22.53	-44.97	-2.33	5.40×10^{9}	4.40×10^{9}

	48	Propionaldehyde	CH_3CH_2CHO	60.7	6.25×10^{-5}	2.45×10^{10}	4.43×10^{9}	22.21	-44.42	-2.35	4.10×10^{9}	3.40×10^{9}
	49	*Chloroacetate*	*$ClCH_2COO^-$*	*59.3*	*6.90×10^{-5}*	*2.70×10^{10}*	*1.09×10^{9}*	*20.81*	*10.40*	*-4.73*	*1.20×10^{9}*	*8.90×10^{8}*
	50	*3-Chloropropanoate*	*$Cl(CH_2)_2COO^-$*	*63.5*	--	--[a]	*4.40×10^{8}*	*19.90*	*12.92*	*-4.84*	*N/A*	*N/A*
	51	*Bromoacetate*	*$BrCH_2COO^-$*	*69.2*	*6.78×10^{-5}*	*2.72×10^{10}*	*8.03×10^{9}*	*22.81*	*11.54*	*-4.78*	*N/A*	*N/A*
	52	*3-Bromopropanoate*	*$Br(CH_2)_2COO^-$*	*93.2*	--	--[a]	*2.70×10^{9}*	*21.72*	*15.24*	*-4.94*	*N/A*	*N/A*
	53	*Fluoroacetate*	*FCH_2COO^-*	*44.7*	*6.99×10^{-5}*	*2.62×10^{10}*	*1.20×10^{6}*	*14.00*	*66.82*	*-7.18*	*N/A*	*N/A*
Halocarboxylate	*54*	*2-Bromopropanoate*	*$CH_3CHBrCOO^-$*	*111.3*	--	--[a]	*5.30×10^{9}*	*22.39*	*6.18*	*-4.55*	*N/A*	*N/A*
	55	*2-Chloropropanoate*	*$CH_3CHClCOO^-$*	*78.6*	--	--[a]	*1.40×10^{9}*	*21.06*	*5.26*	*-4.51*	*N/A*	*N/A*
	56	*Trichloroacetate*	*Cl_3CCOO-*	*98.1*	*6.59×10^{-5}*	*2.80×10^{10}*	*1.22×10^{10}*	*23.23*	*1.91*	*-4.36*	*N/A*	*N/A*
	57	*2-Iodoacetate*	*ICH_2COO-*	*75.2*	--	--[a]	*1.20×10^{10}*	*23.21*	*5.89*	*-4.54*	*N/A*	*N/A*
	58	*2-Iodopropanoate*	*$CH_3CHICOO^-$*	*102.0*	--	--[a]	*6.60×10^{9}*	*22.61*	*-1.08*	*-4.23*	*N/A*	*N/A*
	59	*3-Iodanylpropanoate*	*$ICH_2CH_2COO^-$*	*76.9*	--	--[a]	*5.80×10^{9}*	*22.48*	*6.46*	*-4.56*	*N/A*	*N/A*
	60	Chloromethane	CH_3Cl	38.0	6.68×10^{-5}	2.44×10^{10}	8.33×10^{8}	20.54	-69.84	-1.25	1.20×10^{9}	4.60×10^{8}
	61	Dibromomethane	CH_2Br_2	51.1	6.39×10^{-5}	2.44×10^{10}	1.10×10^{11}	25.42	-73.00	-1.11	N/A	N/A
	62	Bromoform	$CHBr_3$	84.6	6.01×10^{-5}	2.49×10^{10}	1.67×10^{10}	23.54	-80.06	-0.81	N/A	N/A
	63	Bromoethane	CH_3CH_2Br	51.1	6.40×10^{-5}	2.44×10^{10}	1.89×10^{10}	23.66	-67.93	-1.33	1.20×10^{10}	8.00×10^{9}
	64	Bromopropane	$CH_3CH_2CH_2Br$	86.9	5.99×10^{-5}	2.49×10^{10}	1.47×10^{10}	23.41	-67.55	-1.35	1.00×10^{10}	8.50×10^{9}
	65	Chloropropane	$CH_3CH_2CH_2Cl$	67.3	6.17×10^{-5}	2.46×10^{10}	6.85×10^{8}	20.35	-70.86	-1.21	6.90×10^{8}	6.20×10^{8}
	66	Chloroethane	CH_3CH_2Cl	61.3	6.24×10^{-5}	2.45×10^{10}	7.21×10^{8}	20.40	-71.03	-1.20	N/A	N/A
	67	1-Bromo-2-chloroethane	CH_2ClCH_2Br	68.8	6.15×10^{-5}	2.46×10^{10}	1.18×10^{10}	23.20	-70.61	-1.22	N/A	N/A
	68	Halothane	$CF_3CHClBr$	76.5	6.08×10^{-5}	2.48×10^{10}	3.22×10^{10}	24.20	-79.44	-0.84	N/A	N/A
	69	1,1-Dichloroethane	CH_3CHCl_2	54.4	6.34×10^{-5}	2.45×10^{10}	1.42×10^{10}	23.38	-77.00	-0.94	N/A	N/A
	70	Diiodomethane	CH_2I_2	60.8	6.25×10^{-5}	2.45×10^{10}	3.40×10^{10}	24.25[b]	-80.13	-0.81	N/A	N/A
	71	Iodoethane	CH_3CH_2I	64.1	6.21×10^{-5}	2.46×10^{10}	3.85×10^{10}	24.37	-75.94	-0.99	N/A	N/A
	72	Dichloromethane	CH_2Cl_2	56.8	6.30×10^{-5}	2.45×10^{10}	7.95×10^{9}	22.80	-75.69	-1.00	N/A	N/A
	73	Chloroform	$CHCl_3$	83.6	6.02×10^{-5}	2.49×10^{10}	3.00×10^{10}	24.12[b]	-81.97	-0.73	N/A	N/A
	74	Trichlorofluoromethane	CCl_3F	60.5	6.25×10^{-5}	2.45×10^{10}	4.60×10^{10}	24.55	-82.75	-0.69	N/A	N/A
	75	Dichlorodifluoromethane	CF_2Cl_2	42.2	6.57×10^{-5}	2.44×10^{10}	3.28×10^{10}	24.21	-77.16	-0.93	N/A	N/A
	76	Chlorotrifluoromethane	$CClF_3$	55.7	6.32×10^{-5}	2.45×10^{10}	5.36×10^{9}	22.40	-71.19	-1.19	N/A	N/A
	77	Bromotrifluoromethane	CF_3Br	39.7	6.63×10^{-5}	2.44×10^{10}	3.93×10^{11}	26.70	-70.32	-1.23	N/A	N/A
Haloalkane	78	Carbon Tetrachloride	CCl_4	74.4	6.10×10^{-5}	2.47×10^{10}	7.61×10^{10}	25.06	-91.15	-0.33	2.40×10^{10}	1.30×10^{10}
	79	Chlorodifluoromethane	$CHClF_2$	48.9	6.43×10^{-5}	2.44×10^{10}	3.29×10^{9}	21.91	-70.22	-1.24	N/A	N/A
	80	1,1,2-Trichloroethane	$ClCH_2CHCl_2$	78.6	6.06×10^{-5}	2.48×10^{10}	1.27×10^{10}	23.27	-75.17	-1.02	N/A	N/A
	81	1,1,1-Trichloroethane	CH_3CCl_3	73.7	6.10×10^{-5}	2.47×10^{10}	9.24×10^{10}	25.25	-84.09	-0.63	2.50×10^{10}	1.40×10^{10}
	82	Hexachloroethane	CCl_3CCl_3	115.4	5.82×10^{-5}	2.54×10^{10}	3.90×10^{10}	24.39[b]	-89.80	-0.39	N/A	N/A
	83	2-Chlorobutane	$C_2H_5CH(Cl)CH_3$	65.7	6.19×10^{-5}	2.46×10^{10}	5.21×10^{8}	20.07	-71.79	-1.17	N/A	N/A
	84	1,2-Dibromoethane	$BrCH_2CH_2Br$	76.2	6.08×10^{-5}	2.48×10^{10}	2.74×10^{10}	24.03	-72.81	-1.12	1.40×10^{10}	1.20×10^{10}
	85	1,2-Dichloroethane	$ClCH_2CH_2Cl$	66.3	6.18×10^{-5}	2.46×10^{10}	1.91×10^{9}	21.37	-74.11	-1.07	2.90×10^{9}	6.40×10^{8}
	86	1,1,2-Trichloro-1,2,2-trifluoroethane	$ClCF_2CCl_2F$	94.5	5.94×10^{-5}	2.51×10^{10}	3.17×10^{10}	24.18	-80.52	-0.79	N/A	N/A
	87	1-Iodopropane	C_3H_7I	81.8	6.03×10^{-5}	2.48×10^{10}	2.73×10^{10}	24.03	-75.56	-1.00	N/A	N/A
	88	1-Iodobutane	$CH_3(CH_2)_3I$	102.4	5.89×10^{-5}	2.52×10^{10}	2.29×10^{10}	23.85	-75.50	-1.01	N/A	N/A
	89	1-Bromobutane	$CH_3(CH_2)_3Br$	64.8	6.20×10^{-5}	2.46×10^{10}	1.59×10^{10}	23.49	-67.54	-1.35	1.00×10^{10}	9.00×10^{9}
	90	1-Chlorobutane	$CH_3(CH_2)_3Cl$	81.5	6.04×10^{-5}	2.48×10^{10}	3.42×10^{8}	19.65	-70.83	-1.21	4.50×10^{8}	4.80×10^{7}
	91	1-Chloro-2-methylpropane	$(CH_3)_2CHCH_2Cl$	80.4	6.04×10^{-5}	2.48×10^{10}	5.21×10^{8}	20.07	-70.62	-1.22	N/A	N/A
	92	1-Bromopentane	$CH_3(CH_2)_4Br$	115.5	5.82×10^{-5}	2.54×10^{10}	1.17×10^{10}	23.18	-67.45	-1.36	N/A	N/A
	93	2-Bromo-2-methylpropane	$(CH_3)_3CBr$	67.9	6.16×10^{-5}	2.46×10^{10}	1.02×10^{10}	23.04	-70.36	-1.23	N/A	N/A
	94	2-Bromobutane	$CH_3CH_2CH(Br)CH_3$	81.9	6.03×10^{-5}	2.49×10^{10}	1.01×10^{10}	23.04	-69.18	-1.28	N/A	N/A
	95	Trifluoroiodomethane	CF_3I	53.4	6.36×10^{-5}	2.45×10^{10}	2.77×10^{10}	24.05	-77.06	-0.94	N/A	N/A
	96	Iodomethane	CH_3I	48.8	6.44×10^{-5}	2.44×10^{10}	4.64×10^{10}	24.56	-73.39	-1.10	N/A	N/A
	97	*Isoflurane*	*$CHF_2OCHClCF_3$*	*77.7*	*6.07×10^{-5}*	*2.48×10^{10}*	*5.80×10^{9}*	*22.48*	*0.87*	*-4.32*	*N/A*	*N/A*
Halooxygen	*98*	*1,1,1-Trifluoroacetone*	*CF_3COCH_3*	*40.8*	*6.61×10^{-5}*	*2.44×10^{10}*	*6.62×10^{7}*	*18.01*	*24.93*	*-5.36*	*N/A*	*N/A*
	99	*Fluoroacetone*	*CH_3COCH_2F*	*64.0*	*6.21×10^{-5}*	*2.46×10^{10}*	*9.77×10^{8}*	*20.70*	*19.34*	*-5.12*	*1.00×10^{9}*	*8.80×10^{8}*

	100	*Methoxyflurane*	*$CH_3OCF_2CHCl_2$*	*99.9*	*5.91×10^{-5}*	*2.52×10^{10}*	*3.16×10^{10}*	*24.18*	*1.31*	*-4.34*	*N/A*	*N/A*
	101	*2-Chloroethanol*	*$ClCH_2CH_2OH$*	*49.5*	*6.42×10^{-5}*	*2.44×10^{10}*	*5.34×10^{8}*	*20.10*	*15.25*	*-4.94*	*7.00×10^{8}*	*3.30×10^{8}*
	102	*2-Bromoethanol*	*$BrCH_2CH_2OH$*	*74.8*	*6.09×10^{-5}*	*2.47×10^{10}*	*1.71×10^{9}*	*21.26*	*18.64*	*-5.09*	*N/A*	*N/A*
	103	*Chloroacetic acid*	*$ClCH_2COOH$*	*62.0*	*6.23×10^{-5}*	*2.46×10^{10}*	*9.60×10^{9}*	*22.98*	*5.40*	*-4.51*	*N/A*	*N/A*
	104	*Chloral hydrate*	*$CCl_3CH(OH)_2$*	*87.4*	*5.99×10^{-5}*	*2.49×10^{10}*	*2.31×10^{10}*	*23.86*	*-0.79*	*-4.25*	*N/A*	*N/A*
	105	*Enflurane*	*CHF_2OCF_2CHClF*	*86.1*	*6.00×10^{-5}*	*2.49×10^{10}*	*3.03×10^{9}*	*21.83*	*4.14*	*-4.46*	*N/A*	*N/A*
Cyanide	106	Acetonitrile	CH_3CN	44.3	6.53×10^{-5}	2.44×10^{10}	3.74×10^{7}	17.44	-14.83	-3.64	4.40×10^{7}	3.00×10^{7}
	107	Succinonitrile	$NC(CH_2)_2CN$	64.6	6.20×10^{-5}	2.46×10^{10}	1.83×10^{9}	21.33	-21.84	-3.33	N/A	N/A
	108	Trichloroacetonitrile	CCl_3CN	86.2	6.00×10^{-5}	2.49×10^{10}	3.20×10^{10}	24.19[b]	-98.67	0.00	N/A	N/A
	109	Cyanamide	H_2NCN	36.9	6.71×10^{-5}	2.45×10^{10}	1.60×10^{9}	21.19	-21.23	-3.36	N/A	N/A
Amine	110	Methylamine	CH_3NH_2	31.3	6.89×10^{-5}	2.45×10^{10}	9.00×10^{5}	13.71	19.28	-5.12	N/A	N/A
	111	Butylamine	$CH_3(CH_2)_3NH_2$	70.1	6.14×10^{-5}	2.47×10^{10}	1.10×10^{6}	13.91	17.07	-5.02	N/A	N/A
	112	Propylamine	$CH_3CH_2CH_2NH_2$	73.5	6.11×10^{-5}	2.47×10^{10}	1.10×10^{6}	13.91	19.79	-5.14	N/A	N/A
	113	Ethylamine	$CH_3CH_2NH_2$	60.5	6.25×10^{-5}	2.45×10^{10}	1.00×10^{6}	13.82	20.42	-5.17	N/A	N/A
	114	Isobutylamine	$(CH_3)_2CHCH_2NH_2$	58.8	6.28×10^{-5}	2.45×10^{10}	1.10×10^{7}	16.21	18.63	-5.09	N/A	N/A
	115	Isoamylamine	$(CH_3)_2CHCH_2CH_2NH_2$	102.2	5.89×10^{-5}	2.52×10^{10}	1.00×10^{6}	13.82	20.07	-5.15	N/A	N/A
	116	1,2-Dimethylhydrazine	$CH_3NHNHCH_3$	62.4	6.23×10^{-5}	2.46×10^{10}	6.10×10^{6}	15.62	27.98	-5.49	N/A	N/A
	117	Methylhydrazine	CH_3NHNH_2	48.9	6.43×10^{-5}	2.44×10^{10}	6.50×10^{6}	15.69	12.20	-4.81	N/A	N/A
	118	Glycinate	$NH_2CH_2COO^-$	55.3	--	--[a]	1.70×10^{6}	14.35	-9.94	-3.85	N/A	N/A
	119	Ethanolamine	$H_2NCH_2CH_2OH$	39.4	6.64×10^{-5}	2.44×10^{10}	2.00×10^{7}	16.81	-0.27	-4.27	N/A	N/A
	120	Isopropylamine	$(CH_3)_2CHNH_2$	66.0	6.19×10^{-5}	2.46×10^{10}	1.50×10^{6}	14.22	18.20	-5.07	N/A	N/A
	121	Tert-Butylamine	$(CH_3)_3CNH_2$	84.1	6.01×10^{-5}	2.49×10^{10}	1.10×10^{6}	13.91	18.20	-5.07	N/A	N/A
	122	beta-Alaninate	$NH_2(CH_2)_2\text{-}COO^-$	80.0	--	--[a]	4.20×10^{6}	15.25	-9.80	-3.85	N/A	N/A
	123	N,N-Diethylhydroxylamine	$(C_2H_5)_2NOH$	90.9	5.96×10^{-5}	2.50×10^{10}	4.81×10^{7}	17.69	-2.51	-4.17	N/A	N/A
	124	N-Methyl-N-tritiohydroxylamine	CH_3NHOH	45.2	6.51×10^{-5}	2.44×10^{10}	2.42×10^{8}	19.31	-15.92	-3.59	N/A	N/A
	125	Amylamine	$CH_3(CH_2)_4NH_2$	85.8	6.00×10^{-5}	2.49×10^{10}	1.00×10^{6}	13.82	21.11	-5.20	N/A	N/A
	126	Trimethylhydrazine	$(CH_3)_2N\text{-}NHCH_3$	62.8	6.22×10^{-5}	2.46×10^{10}	1.00×10^{8}	18.42	-16.76	-3.55	N/A	N/A
	127	1,1-Dimethylhydrazine	$(CH_3)_2NNH_2$	56.5	6.31×10^{-5}	2.45×10^{10}	2.40×10^{7}	16.99	18.28	-5.07	N/A	N/A
Amide	128	Propionamide	$CH_3CH_2CONH_2$	71.2	6.13×10^{-5}	2.47×10^{10}	4.66×10^{7}	17.66	-23.71	-3.25	5.40×10^{7}	3.90×10^{7}
	129	N-Ethylacetamide	$CH_3CONHC_2H_5$	75.8	6.08×10^{-5}	2.48×10^{10}	1.40×10^{7}	16.46	-23.75	-3.25	N/A	N/A
	130	N-Methylacetamide	$CH_3CONHCH_3$	60.4	6.25×10^{-5}	2.45×10^{10}	2.30×10^{6}	14.65	-21.79	-3.34	N/A	N/A
	131	Acetamide	CH_3CONH_2	47.3	6.46×10^{-5}	2.44×10^{10}	3.84×10^{7}	17.46	-25.72	-3.16	4.50×10^{7}	3.50×10^{7}
	132	Urea	H_2NCONH_2	51.0	6.40×10^{-5}	2.44×10^{10}	3.10×10^{5}	12.64	-17.40	-3.53	3.20×10^{5}	3.00×10^{5}
	133	Glycinamide	$H_2NCH_2CONH_2$	55.9	6.32×10^{-5}	2.45×10^{10}	2.83×10^{8}	19.46	-27.34	-3.09	N/A	N/A
	134	Formamide	$HCONH_2$	37.9	6.68×10^{-5}	2.44×10^{10}	2.80×10^{7}	17.15	-28.17	-3.06	6.30×10^{7}	1.00×10^{6}
	135	*3-Chloropropionamide*	*$ClCH_2CH_2CONH_2$*	*63.2*	*6.22×10^{-5}*	*2.46×10^{10}*	*1.94×10^{9}*	*21.39*	*10.52*	*-4.74*	*N/A*	*N/A*
	136	(S)-2-Hydroxypropanamide	$CH_3CH(OH)CONH_2$	70.6	6.14×10^{-5}	2.47×10^{10}	1.91×10^{8}	19.07	-29.16	-3.02	N/A	N/A
	137	Aceturate	$CH_3CONHCH_2COO^-$	73.0	--	--[a]	1.13×10^{7}	16.24	-25.84	-3.16	2.00×10^{7}	2.60×10^{6}
	138	Pivalamide	$(CH_3)_3CCONH_2$	71.2	6.13×10^{-5}	2.47×10^{10}	1.50×10^{7}	16.52	-27.03	-3.11	N/A	N/A
	139	Malonamide	$H_2NCOCH_2CONH_2$	67.7	6.17×10^{-5}	2.46×10^{10}	1.15×10^{9}	20.86	-30.47	-2.96	N/A	N/A
	140	2-Hydroxyacetamide	$HOCH_2CONH_2$	52.3	6.37×10^{-5}	2.45×10^{10}	2.93×10^{8}	19.50	-29.10	-3.02	N/A	N/A
	141	Biuret	$H_2NCONHCONH_2$	68.3	6.16×10^{-5}	2.46×10^{10}	2.53×10^{8}	19.35	-26.98	-3.11	N/A	N/A
	142	*2-Chloropropionamide*	*$CH_3CH(Cl)CONH_2$*	*69.9*	*6.14×10^{-5}*	*2.47×10^{10}*	*7.58×10^{9}*	*22.75*	*0.91*	*-4.32*	*N/A*	*N/A*
	143	*Iodoacetamide*	*ICH_2CONH_2*	*77.7*	*6.07×10^{-5}*	*2.48×10^{10}*	*5.00×10^{10}*	*24.64[b]*	*-2.75*	*-4.16*	*N/A*	*N/A*
	144	Hydroxyurea	$HONHCONH_2$	40.7	6.61×10^{-5}	2.44×10^{10}	4.90×10^{8}	20.01	-27.45	-3.09	N/A	N/A
	145	Oxamate	$H_2NCOCOO^-$	53.4	--	--[a]	5.70×10^{9}	22.46	-44.35	-2.36	N/A	N/A
	146	Succinamide	$H_2NCOCH_2CH_2CONH_2$	85.9	6.00×10^{-5}	2.49×10^{10}	2.02×10^{8}	19.12	-26.23	-3.14	N/A	N/A
	147	Asparaginate	$H_2NCOCH_2CH(NH_2)COO^-$	90.6	--	--[a]	2.40×10^{7}	16.99	-26.51	-3.13	N/A	N/A
	148	N,N-Dimethylformamide	$HCON(CH_3)_2$	60.2	6.26×10^{-5}	2.45×10^{10}	3.08×10^{8}	19.55	-30.35	-2.96	4.60×10^{8}	5.20×10^{7}
	149	Methyl 2-acetamidoacetate	$CH_3CONHCH_2COOCH_3$	89.8	5.97×10^{-5}	2.50×10^{10}	3.34×10^{8}	19.63	-38.38	-2.62	N/A	N/A
	150	2-Formamidoacetate	$HCONHCH_2COO^-$	78.6	--	--[a]	2.90×10^{7}	17.18	-25.93	-3.16	N/A	N/A
	151	N-Methylformamide	$HCONHCH_3$	50.7	6.40×10^{-5}	2.44×10^{10}	4.31×10^{7}	17.58	-25.68	-3.17	7.10×10^{7}	1.50×10^{7}

	152	N-Tert-Butylacetamide	$CH_3CONHC(CH_3)_3$	122.7	5.79×10^{-5}	2.56×10^{10}	1.20×10^{7}	16.30	-21.69	-3.34	N/A	N/A
	153	Diacetamide	$(CH_3CO)_2NH$	73.2	6.11×10^{-5}	2.47×10^{10}	1.98×10^{10}	23.71	-43.29	-2.40	N/A	N/A
	154	N,N-Diethylacetamide	$CH_3CON(C_2H_5)_2$	93.8	5.95×10^{-5}	2.51×10^{10}	8.00×10^{6}	15.90	-23.89	-3.24	N/A	N/A
	155	N,N-Dimethylacetamide	$CH_3CON(CH_3)_2$	74.8	6.09×10^{-5}	2.47×10^{10}	1.50×10^{7}	16.52	-27.42	-3.09	2.10×10^{7}	9.00×10^{6}
	156		$(CH_3)_3CCON(CH_3)_2$	92.3	5.95×10^{-5}	2.50×10^{10}	1.20×10^{7}	16.30	-29.95	-2.98	N/A	N/A
Ammonium	157	Methyl Ammonium Hydride	$CH_3NH_3^+$	41.3	--	--[a]	1.85×10^{6}	14.43	-50.08	-2.11	1.90×10^{6}	1.80×10^{6}
	158	Ethylammonium	$C_2H_5NH_3^+$	41.3	--	--[a]	2.50×10^{6}	14.73	-51.52	-2.05	N/A	N/A
	159	Trideuterio(propyl)azanium	$CH_3(CH_2)_2NH_3^+$	58.7	--	--[a]	2.80×10^{6}	14.85	-50.99	-2.07	N/A	N/A
	160	Pentylazanium	$CH_3(CH_2)_4NH_3^+$	97.0	--	--[a]	2.70×10^{6}	14.81	-51.57	-2.04	N/A	N/A
	161	2-Methoxy-2-oxoethanaminium	$H_3COOCCH_2NH_3^+$	52.4	--	--[a]	6.80×10^{9}	22.64	-59.49	-1.70	N/A	N/A
	162	Methoxyazanium	$CH_3ONH_3^+$	34.4	--	--[a]	1.90×10^{10}	23.67	-96.51	-0.10	N/A	N/A
	163	Tert-butylammonium	$(CH_3)_3CNH_3^+$	87.1	--	--[a]	1.10×10^{6}	13.91	-53.40	-1.96	N/A	N/A
	164	2-Methylhydrazinium	$CH_3NHNH_3^+$	49.2	--	--[a]	1.40×10^{9}	21.06	-80.62	-0.78	N/A	N/A
	165	1,1-Dimethylhydrazinium	$(CH_3)_2NNH_3^+$	49.5	--	--[a]	5.80×10^{9}	22.48	-85.83	-0.56	N/A	N/A
	166	Tetramethylammonium	$(CH_3)_4N^+$	84.0	--	--[a]	5.60×10^{6}	15.54	-49.22	-2.15	N/A	N/A
	167	Tetraethylammonium	$(C_2H_5)_4N^+$	135.3	--	--[a]	1.20×10^{7}	16.30	-52.94	-1.98	N/A	N/A
Hydrogen Sulfide	168	Cysteaminium	$HSCH_2CH_2NH_3^+$	53.1	--	--[a]	2.25×10^{10}	23.84	-51.15	-2.06	3.00×10^{10}	1.50×10^{10}
	169	3-Sulfanylpropylazanium	$HS(CH_2)_3NH_3^+$	89.0	--	--[a]	1.70×10^{10}	23.56	-52.08	-2.02	N/A	N/A
Alkyne	170	Acetylene	HC triplet bond CH	27.0	7.07×10^{-5}	2.47×10^{10}	2.00×10^{7}	16.81	-21.82	-3.33	N/A	N/A
	171	Propargyl alcohol	HC triplet bond CCH_2OH	54.0	6.35×10^{-5}	2.45×10^{10}	2.12×10^{8}	19.17	-24.16	-3.23	N/A	N/A
Sulfate	172	Ethanesulfonate	$C_2H_5SO_3^-$	61.5	--	--[a]	3.50×10^{7}	17.37	7.65	-4.61	N/A	N/A
Sulfoxide	*173*	*Dibutyl sulphoxide*	*$[CH_3(CH_2)_3SO(CH_2)_3CH_3]$*	*154.7*	*5.68×10^{-5}*	*2.61×10^{10}*	*3.60×10^{6}*	*15.10*	*22.09*	*-5.24*	*N/A*	*N/A*
	174	*Di-tert-butyl sulfoxide*	*$[(CH_3)_3C]_2SO$*	*116.2*	*5.82×10^{-5}*	*2.55×10^{10}*	*1.50×10^{7}*	*16.52*	*-63.62*	*-1.52*	*N/A*	*N/A*
	175	*Methyl (methylsulfinyl)methyl sulfide*	*$CH_3SOCH_2SCH_3$*	*102.0*	*5.89×10^{-5}*	*2.52×10^{10}*	*1.31×10^{8}*	*18.69*	*22.05*	*-5.24*	*N/A*	*N/A*
Thiol	176	Methanethiol	CH_3SH	44.3	6.53×10^{-5}	2.44×10^{10}	1.08×10^{10}	23.11	-47.75	-2.21	N/A	N/A
	177	Thiolactate	$CH_3(CH)SHCOO^-$	86.2	--	--[a]	2.89×10^{9}	21.78	-58.46	-1.75	5.00×10^{9}	7.70×10^{8}
	178	2-Mercaptopropionic Acid	$CH_3CH(SH)COOH$	73.2	6.11×10^{-5}	2.47×10^{10}	4.08×10^{9}	22.13	-62.50	-1.57	N/A	N/A
	179	Methyl thioglycolate	$HSCH_2COOCH_3$	75.5	6.09×10^{-5}	2.47×10^{10}	1.12×10^{10}	23.14	-56.08	-1.85	1.40×10^{10}	1.40×10^{9}
	180	beta-Mercaptoethanol	$HS(CH_2)_2OH$	66.1	6.18×10^{-5}	2.46×10^{10}	1.73×10^{10}	23.57	-49.88	-2.12	1.20×10^{10}	8.30×10^{9}
	181	2-Methyl-2-propanethiol	$(CH_3)_3CSH$	103.2	5.89×10^{-5}	2.52×10^{10}	3.41×10^{9}	21.95	-54.27	-1.93	N/A	N/A
	182	3-Mercaptopropionic acid	$HS(CH_2)_2COOH$	76.9	6.07×10^{-5}	2.48×10^{10}	6.91×10^{9}	22.66	-50.10	-2.11	N/A	N/A
	183	Thioglycolate	$HSCH_2COO^-$	76.3	--	--[a]	3.03×10^{9}	21.83	-54.30	-1.93	5.50×10^{9}	5.60×10^{8}
	184		$H_2NC(=NH)NHCH_2CH_2SH$	84.6	6.01×10^{-5}	2.49×10^{10}	1.02×10^{11}	25.35	-51.25	-2.06	N/A	N/A
Sulfide/Disulfide	*185*	*Dimethylsulfide*	*CH_3SCH_3*	*53.6*	*6.35×10^{-5}*	*2.45×10^{10}*	*2.00×10^{7}*	*16.81*	*52.27*	*-6.55*	*N/A*	*N/A*
	186	*3,3'-Dithiodipropionate*	*$(SCH_2CH_2COO^-)_2$*	*131.5*	--	--[a]	*4.35×10^{9}*	*22.19*	*20.22*	*-5.16*	*4.40×10^{9}*	*4.30×10^{9}*
	187	*2,2'-Disulfanediyldiacetate*	*$(SCH_2COO^-)_2$*	*116.9*	--	--[a]	*4.30×10^{9}*	*22.18*	*25.32*	*-5.38*	*N/A*	*N/A*
	188	*2,2'-Sulfanediyldiacetate*	*$S(CH_2COO^-)_2$*	*109.2*	--	--[a]	*8.30×10^{7}*	*18.23*	*34.86*	*-5.79*	*N/A*	*N/A*
	189	*N-Acetylcysteamine*	*$CH_3CONHCH_2CH_2SH$*	*95.9*	*5.93×10^{-5}*	*2.51×10^{10}*	*1.43×10^{10}*	*23.38*	*29.28*	*-5.55*	*N/A*	*N/A*
	190	*Cystamine*	*$S_2(CH_2CH_2NH_2)_2$*	*147.2*	*5.70×10^{-5}*	*2.60×10^{10}*	*5.85×10^{10}*	*24.79*	*24.23*	*-5.33*	*N/A*	*N/A*
	191	*L-Cystine anion*	*$S_2[CH_2CH(NH_2)COO^-]_2$*	*139.8*	--	--[a]	*3.53×10^{9}*	*21.98*	*15.24*	*-4.94*	*5.00×10^{9}*	*1.50×10^{9}*
	192	*3,3'-Thiodipropanoate*	*$S(CH_2CH_2COO^-)_2$*	*135.6*	--	--[a]	*5.80×10^{7}*	*17.88*	*33.51*	*-5.73*	*N/A*	*N/A*
S-	193	2-Hydroxyethanethiolate	$HOCH_2CH_2S^-$	66.6	--	--[a]	1.80×10^{7}	16.71	-15.20	-3.62	N/A	N/A
	194	2-lambda1-Sulfanylethanamine	$H_2NCH_2CH_2S^-$	69.5	--	--[a]	9.55×10^{8}	20.68	-16.84	-3.55	1.50×10^{9}	4.10×10^{8}
	195	2-Acetamidoethanethiolate	$CH_3CONHCH_2CH_2S^-$	107.5	--	--[a]	1.90×10^{9}	21.37	-16.11	-3.58	N/A	N/A
CS	196	Carbon Disulfide	CS_2	48.0	6.45×10^{-5}	2.44×10^{10}	3.10×10^{10}	24.16[b]	-57.80	-1.77	N/A	N/A
	197	Thiourea	H_2NCSNH_2	54.1	6.35×10^{-5}	2.45×10^{10}	3.29×10^{9}	21.91	-18.12	-3.49	N/A	N/A
	198	Thiosemicarbazide	$H_2NNHCSNH_2$	51.2	6.39×10^{-5}	2.44×10^{10}	1.15×10^{9}	20.86	-19.10	-3.45	N/A	N/A
	199	N,N'-Diethylthiourea	$CH_3CH_2NHCSNHCH_2CH_3$	111.5	5.84×10^{-5}	2.54×10^{10}	5.10×10^{8}	20.05	-19.13	-3.45	N/A	N/A
Nitro	200	Nitromethane	CH_3NO_2	43.7	6.54×10^{-5}	2.44×10^{10}	1.80×10^{11}	25.92	-61.02	-1.63	2.20×10^{10}	2.10×10^{10}
	201	1-Nitropropane	$CH_3CH_2CH_2NO_2$	75.5	6.09×10^{-5}	2.47×10^{10}	2.70×10^{10}	24.02[b]	-60.85	-1.64	N/A	N/A
	202	Nitroethane	$CH_3CH_2NO_2$	55.8	6.32×10^{-5}	2.45×10^{10}	2.70×10^{10}	24.02[b]	-60.17	-1.67	N/A	N/A
	203	2-Methyl-2-nitrosopropane	$(CH_3)_3C(NO)$	84.7	6.01×10^{-5}	2.49×10^{10}	8.26×10^{9}	22.83	-63.46	-1.53	N/A	N/A

	204	*Trifluoroacetate*	*CF_3COO^-*	*61.6*	--	--[a]	*1.65×10^6*	*14.32*	*76.90*	*-7.61*	*1.90×10^6*	*1.40×10^6*
PFAS	*205*	*Perflurobutanoic Acid*	*$C_3F_7COO^-$*	*95.7*	--	--[a]	*7.10×10^6*	*15.78*	*57.88*	*-6.79*	*N/A*	*N/A*
	206	*Perflurooctanoic Acid*	*$C_7F_{15}COO^-$*	*186.5*	--	--[a]	*1.70×10^7*	*16.65*	*42.92*	*-6.14*	*N/A*	*N/A*
	207	Allylamine	$H_2C=CHCH_2NH_2$	42.7	6.56×10^{-5}	2.44×10^{10}	1.20×10^7	16.30	-23.13	-3.28	N/A	N/A
	208	Acrylonitrile	$H_2C=CHCN$	42.2	6.57×10^{-5}	2.44×10^{10}	2.78×10^{10}	24.05[b]	-53.94	-1.94	N/A	N/A
	209	Allyl alcohol	$H_2C=CHCH_2OH$	59.0	6.27×10^{-5}	2.45×10^{10}	3.47×10^7	17.36	-27.37	-3.09	7.20×10^7	1.20×10^7
	210	Acrylic acid	$H_2C=CHCOOH$	63.6	6.21×10^{-5}	2.46×10^{10}	1.03×10^{12}	27.66[b]	-59.27	-1.71	N/A	N/A
	211	Acrylate	$CH_2=CHCOO^-$	38.6	--	--[a]	5.30×10^9	22.39	-40.74	-2.51	N/A	N/A
	212	Methyl vinyl ketone	$H_2C=CHCOCH_3$	49.7	6.42×10^{-5}	2.44×10^{10}	2.78×10^9	21.75[b]	-63.32	-1.53	N/A	N/A
	213	Methyl acrylate	$H_2C=CHCOOCH_3$	71.7	6.12×10^{-5}	2.47×10^{10}	1.52×10^{10}	23.44[b]	-57.17	-1.80	N/A	N/A
	214	Senecioic acid amide	$(CH_3)_2C=CHCONH_2$	80.3	6.05×10^{-5}	2.48×10^{10}	7.23×10^9	22.70[b]	-44.00	-2.37	N/A	N/A
	215	*Vinyl chloride*	*$CH_2=CHCl$*	*45.8*	*6.49×10^{-5}*	*2.44×10^{10}*	*2.53×10^8*	*19.35*	*27.10*	*-5.45*	*N/A*	*N/A*
	216	Ethylene	$H_2C=CH_2$	27.3	7.06×10^{-5}	2.47×10^{10}	3.00×10^5	12.61	-24.75	-3.21	N/A	N/A
	217	Ethenesulfonate	$CH_2=CHSO_3^-$	60.1	--	--[a]	2.30×10^9	21.56	-37.67	-2.65	N/A	N/A
	218	*Tetrachloroethylene*	*$Cl_2C=CCl_2$*	*108.1*	*5.86×10^{-5}*	*2.53×10^{10}*	*2.67×10^{10}*	*24.01*	*15.17*	*-4.94*	*4.20×10^{10}*	*1.30×10^{10}*
	219	Crotonyl Alcohol	$CH_3CH=CHCH_2OH$	73.2	6.11×10^{-5}	2.47×10^{10}	5.51×10^7	17.83	-24.31	-3.23	N/A	N/A
	220	Crotonic Acid	$CH_3CH=CHCOOH$	73.7	6.10×10^{-5}	2.47×10^{10}	6.62×10^{10}	24.92[b]	-54.36	-1.92	N/A	N/A
	221	Dimethyl Fumarate	$CH_3OOCCH=CHCOOCH_3$	114.4	5.83×10^{-5}	2.54×10^{10}	3.30×10^{10}	24.22[b]	-76.95	-0.94	N/A	N/A
	222	Divinyl Sulfone	$(H_2C=CH)_2SO_2$	95.8	5.93×10^{-5}	2.51×10^{10}	1.66×10^{10}	23.53[b]	-55.62	-1.87	N/A	N/A
	223	Methacrylic Acid	$H_2C=C(CH_3)COOH$	70.9	6.13×10^{-5}	2.47×10^{10}	8.26×10^{10}	25.14[b]	-56.59	-1.83	N/A	N/A
	224	Methyl Methacrylate	$H_2C=C(CH_3)COOCH_3$	86.0	6.00×10^{-5}	2.49×10^{10}	2.72×10^{10}	24.03[b]	-54.41	-1.92	N/A	N/A
	225	*trans-1,2-Dichloroethylene*	*$ClCH=CHCl$*	*54.7*	*6.34×10^{-5}*	*2.45×10^{10}*	*1.08×10^{10}*	*23.10*	*22.70*	*-5.26*	*N/A*	*N/A*
	226	*Trichloroethylene*	*$ClCH=CCl_2$*	*69.3*	*6.15×10^{-5}*	*2.47×10^{10}*	*8.28×10^{10}*	*25.14*	*18.45*	*-5.08*	*N/A*	*N/A*
	227	*cis-1,2-Dichloroethylene*	*$H_2C=CCl_2$*	*52.5*	*6.37×10^{-5}*	*2.45×10^{10}*	*3.86×10^{11}*	*26.68*	*19.86*	*-5.14*	*N/A*	*N/A*
	228	1,3-Butadiene	$H_2C=CHCH=CH_2$	44.0	6.53×10^{-5}	2.44×10^{10}	1.19×10^{10}	23.20[b]	-42.65	-2.43	N/A	N/A
Alkene	229	Acetaldehyde Oxime	$CH_3CH=NOH$	60.5	6.25×10^{-5}	2.45×10^{10}	7.22×10^7	18.10	-30.63	-2.95	N/A	N/A
	230	N,N-Dimethylacrylamide	$CH_2=CHCON(CH_3)_2$	78.4	6.06×10^{-5}	2.48×10^{10}	4.51×10^{10}	24.53[b]	-51.04	-2.07	N/A	N/A
	231	Methacrylamide	$H_2C=C(CH_3)CONH_2$	81.3	6.04×10^{-5}	2.48×10^{10}	7.10×10^{11}	27.29[b]	-49.80	-2.12	N/A	N/A
	232	Cyanoguanidine	$NCN=C(NH_2)_2$	59.2	6.27×10^{-5}	2.45×10^{10}	1.96×10^{10}	23.70	-31.89	-2.90	N/A	N/A
	233	*Tetracyanoethylene*	*$(NC)_2C=C(CN)_2$*	*94.0*	*5.94×10^{-5}*	*2.51×10^{10}*	*3.74×10^{10}*	24.34	*36.90*	*-5.88*	*N/A*	*N/A*
	234	Methacrylate	$CH_2=C(CH_3)COO^-$	60.1	--	--[a]	4.50×10^9	22.23	-36.63	-2.69	N/A	N/A
	235	3-Buten-1-ol	$H_2C=CHCH_2CH_2OH$	74.5	6.10×10^{-5}	2.47×10^{10}	2.45×10^6	14.71	-22.99	-3.28	4.10×10^6	8.00×10^5
	236	3-Buten-2-OL	$H_2C=CHCH(OH)CH_3$	72.5	6.12×10^{-5}	2.47×10^{10}	5.91×10^7	17.90	-26.41	-3.13	N/A	N/A
	237	3-Methylbut-2-enoate	$(CH_3)_2C=CHCO_2^-$	104.6	--	--[a]	6.40×10^8	20.28	-31.71	-2.91	N/A	N/A
	238	3,3-Dimethylacrylic acid	$(CH_3)_2C=CHCOOH$	73.4	6.11×10^{-5}	2.47×10^{10}	2.53×10^{10}	23.95[b]	-50.40	-2.09	1.50×10^{10}	1.00×10^{10}
	239	Isocrotonate	$CH_3CH=CHCOO^-$	71.6	--	--[a]	1.30×10^9	20.99	-35.70	-2.73	N/A	N/A
	240	Hydrogen Fumarate	$HOOCCH=CHCOO^-$	64.8	--	--[a]	1.35×10^{10}	23.33[b]	-66.40	-1.40	1.80×10^{10}	9.00×10^9
	241	Monomethyl Fumarate	$CH_3OOCCH=CHCOO^-$	86.1	--	--[a]	1.30×10^{10}	23.29[b]	-64.43	-1.49	N/A	N/A
	242	2-Hydroxyethyl Acrylate	$CH_2=CHCOOCH_2CH_2OH$	65.9	6.19×10^{-5}	2.46×10^{10}	1.08×10^{10}	23.10[b]	-57.85	-1.77	N/A	N/A
	243	trans-Aconitate(3-)	$^-OOCCH=C(COO^-)CH_2COO^-$	119.2	--	--[a]	1.80×10^8	19.01	-45.03	-2.33	N/A	N/A
	244	Acrylamide	$H_2C=CHCONH_2$	54.7	6.34×10^{-5}	2.45×10^{10}	3.81×10^{11}	26.67[b]	-51.89	-2.03	3.30×10^{10}	1.50×10^{10}
	245	Crotonamide	$CH_3CH=CHCONH_2$	67.6	6.17×10^{-5}	2.46×10^{10}	2.75×10^{10}	24.04[b]	-47.62	-2.22	N/A	N/A
	246	4-(Ethylamino)-4-oxobut-2-enoate	$C_2H_5NHCOCH=CHCOO^-$	119.2	--	--[a]	8.50×10^9	22.86[b]	-56.87	-1.81	N/A	N/A
	247	cis-Dimethyl Fumarate	$CH_3OOCCH=CHCOOCH_3$	95.4	5.93×10^{-5}	2.51×10^{10}	3.20×10^{10}	24.19[b]	-73.51	-1.09	N/A	N/A
	248	4-Penten-2-OL	$H_2C=CHCH_2CH(OH)CH_3$	97.0	5.92×10^{-5}	2.51×10^{10}	5.00×10^5	13.12	-21.90	-3.33	N/A	N/A
	249	Guanidine	$H_2NC(=NH)NH_2$	57.9	6.29×10^{-5}	2.45×10^{10}	2.02×10^8	19.12	-4.98	-4.06	2.50×10^8	1.60×10^8
	250	Ethyl Acrylate	$H_2C=CHCOOC_2H_5$	89.2	5.98×10^{-5}	2.50×10^{10}	1.34×10^{10}	23.31[b]	-57.33	-1.79	N/A	N/A
	251	Acetone Oxime	$(CH_3)_2C=NOH$	64.5	6.20×10^{-5}	2.46×10^{10}	3.29×10^8	19.61	-25.74	-3.16	3.50×10^8	3.00×10^8

[a] D_I data not available in literature. Assumed $k_{exp} << k_D$.
[b] Reaction determined to be diffusion limited.
Association mechanism
Concerted mechanism
Stepwise mechanism

Table S6:

Mechanism	Class	No.	Name	Chemical Formula	Nearest Neighboring Functional Group(s)	Possible Taft Constant(s) of Nearest Functional Group		Sum of Taft Constants	Notes	$E°_{red}$ (V vs SHE)
Association with O	Carboxylate	8	Hydrogen Oxalate	HOOCCOO-	$-COO^-$ & -OH	0.75	1.37	2.12		-2.02
		10	Malonate(1-)	HOOC-CH_2-COO-	$-CH_2COO^-$ & -OH	-0.06	1.37	1.31		-2.72
		11	Succinate(1-)	HOOC$(CH_2)_2$COO-	$-(CH_2)_2COO^-$ & -OH	-0.06	1.37	1.31	Use Taft for CH2COO-	-2.86
		15	CID_4134252	$HOCH_2(CHOH)_4COO^-$	-(OH)CH & -O-	1.37	-1.5	-0.13	Use Taft for: CH(OH)2	-3.69
	Carboxylic Acid	17	Oxalic Acid	HOOCCOOH	-COOH, -OH	2.94	1.37	4.31		-1.55
		18	Formic Acid	HCOOH	-H, -OH	0.49	1.37	1.86		-2.59
		19	Succinic Acid	HOOC$(CH_2)_2$COOH	$-(CH_2)_2$, -OH	0	1.37	1.37	Use Taft for: CH_3	-2.75
		20	Propionic Acid	CH_3CH_2COOH	$-CH_2CH_3$, -OH	-0.1	1.37	1.27		-2.76
		21	Acetic Acid	CH_3COOH	$-CH_3$, -OH	0	1.37	1.37		-2.89
		22	Malonic Acid	HOOC-CH_2-COOH	$-CH_2COOH$, -OH	0.35	1.37	1.72	Use Taft for (CH2)2COOH	-2.51
		23	Lactic Acid	$CH_3CH(OH)COOH$	$-(OH)CHCH_3$, -OH	0.46	1.37	1.83		-2.62
		24	Malic Acid	$HOOCCH_2CH(OH)COOH$	$-(OH)CHCH_2$, -OH	0.46	1.37	1.83	Use Taft for: $OHCHCH_3$	-2.49

		25	Glycolic acid	$HOCH_2COOH$	$-CH_2OH$, -OH	0.56	1.37	1.93		-2.66
	Alcohol	26	Methanediol	$CH_2(OH)_2$	-CH2OH	0.56		0.56		-3.69
		27	Tert-Butanol	$(CH_3)_3$-C-OH	-C(CH3)3,	-0.3		-0.3		-4.01
		28	Butane-1,2,3,4	$HOCH_2[CH(OH)]_2CH_2OH$	-CH2CHOH	0.46		0.46	Use Taft for: $OHCHCH_3$	-3.78
		29	Mannitol	$HOCH_2[CH(OH)]_4CH_2OH$	-CH2CHOH	0.46		0.46	Use Taft for: $OHCHCH_3$	-3.55
	Ester	30	Methyl Acetate	CH_3COOCH_3	$-CH_3$ & $-OCH_3$	0	1.77	1.77		-2.82
		31	Methyl Propionate	$C_2H_5COOCH_3$	$-C_2H_5$ & $-OCH_3$	-0.1	1.77	1.67		-2.84
		32	Ethyl Propionate	$C_2H_5COOC_2H_5$	$-C_2H_5$ & $-OC_2H_5$	-0.1	1.68	1.58		-2.84
		33	Dimethyl Oxalate	$CH_3OOCCOOCH_3$	$-COOCH_3$ & $-OCH_3$	2	1.77	3.77		-1.72
		34	Tert-butyl Acetate	$(CH_3)_3CCOOCH_3$	$-OCH_3$ or $-C(CH_3)_3$	-0.3	1.77	1.47		-2.97
		35	2-Hydroxyethyl Acetate	$CH_3COOCH_2CH_2OH$	$-OCH_2CH_2$ or $-CH_3$	1.57	0	1.57	Use Taft for: $OCH_{2CH2}CH_3$	-2.84
		37	Methylene glycol monoacetate	$HOCH_2COOCH_3$	$-CH_2OH$ or $-OCH_3$	0.56	1.77	2.33		-2.66
		38	Methyl methoxyacetate	$CH_3OCH_2COOCH_3$	$-CH_2OCH_3$ or $-OCH_3$	0.52	1.77	2.29		-2.63
		40	Ethyl glycinate	$NH_2CH_2COOC_2H_5$	$-OC_2H_5$ or $-CH_2NH_2$	0.4	1.68	2.08		-2.77
		41	Acetoxymethylamine	$H_2NCH_2COOCH_3$	$-CH_3$ or $-OCH_2NH_2$	0	1.77	1.77	Use Taft for OCH3	-2.87
	Amide	128	Propionamide	$CH_3CH_2CONH_2$	$-NH_2$ & $-CH_2CH_3$	0.62	-0.1	0.52		-3.25
		129	N-Ethylacetamide	$CH_3CONHC_2H_5$	$-NHC_2H_5$ & $-CH_3$	0.94	0	0.94	Use Taft for: NHCH3	-3.25
		130	N-Methylacetamide	$CH_3CONHCH_3$	$-NHCH_3$ & $-CH_3$	0.94	0	0.94		-3.34
		131	Acetamide	CH_3CONH_2	$-NH_2$ & $-CH_3$	0.62	0	0.62		-3.16
		132	Urea	H_2NCONH_2	$-NH_2$ & -NH2	0.62	0.62	1.24		-3.53
		133	Glycinamide	$H_2NCH_2CONH_2$	$-NH_2$ & $-CH_2NH_2$	0.62	0.4	1.02		-3.09

134	Formamide	$HCONH_2$	$-NH_2$ & -H	0.62	0.49	1.11		-3.06
136	(S)-2-Hydroxypropanamide	$CH_3CH(OH)CONH_2$	$-NH_2$ & $-(OH)CHCH_3$	0.62	0.46	1.08		-3.02
137	Aceturate	$CH_3CONHCH_2COO^-$	$-CH_3$ & $-NHCH_2$	0	0.94	0.94	Use Taft for: NHCH3	-3.16
138	Pivalamide	$(CH_3)_3CCONH_2$	$-NH_2$ & $-C(CH_3)_3$	0.62	-0.3	0.32		-3.11
139	Malonamide	$H_2NCOCH_2CONH_2$	$-NH_2$ & -CH2CONH2	0.62	0.65	1.27		-2.96
140	2-Hydroxyacetamide	$HOCH_2CONH_2$	$-NH_2$ & $-CH_2OH$	0.62	0.56	1.18		-3.02
141	Biuret	$H_2NCONHCONH_2$	$-NH_2$ & -NHCONH2	0.62	1.31	1.93		-3.11
144	Hydroxyurea	$HONHCONH_2$	$-NH_2$ & -NHOH	0.62	0.3	0.92		-3.09
145	Oxamate	$H_2NCOCOO^-$	$-COO^-$ & $-NH_2$	0.75	0.62	1.37		-2.36
146	Succinamide	$H_2NCOCH_2CH_2CONH_2$	$-NH_2$ & -CH2CH2CONH2	0.62	0.19	0.81		-3.14
147	Asparaginate	$H_2NCOCH_2CH(NH_2)COO^-$	$-NH_2$ & $CH_2CH(NH_2)$	0.62	0.02	1.02	Use Taft for: CH_2NH_2	-3.13
148	N,N-Dimethylformamide	$HCON(CH_3)_2$	$-N(CH_3)_2$ & -H	1.02	0.49	1.51		-2.96
149	Methyl 2-acetamidoacetate	$CH_3CONHCH_2COOCH_3$	$-CH_3$ & $NHCH_2$	0	1.62	1.62	Use Taft for NHCHO	-2.62
150	2-Formamidoacetate	$HCONHCH_2COO^-$	-H & $NHCH_3$	0.49	0.94	1.43	Use Taft for NHCH3	-3.16
151	N-Methylformamide	$HCONHCH_3$	-H & $NHCH_3$	0.49	0.94	1.43		-3.17
152	N-Tert-Butylacetamide	$CH_3CONHC(CH_3)_3$	$-CH_3$ & $NHC(CH_3)_3$	0	1.08	1.08	Use Taft for: NH(CH2)3CH3	-3.34
153	Diacetamide	$(CH_3CO)_2NH$	-NHCOCH3 & $-CH_3$	1.62	0	1.62	Use Taft for NHCHO	-2.40
154	N,N-Diethylacetamide	$CH_3CON(C_2H_5)_2$	$-N(C_2H_5)_2$ & -CH3	1	0	1		-3.24
155	N,N-Dimethylacetamide	$CH_3CON(CH_3)_2$	$-N(CH_3)_2$ & -CH3	1.02	0	1.02		-3.09

		156		$(CH_3)_3CCON(CH_3)_2$	-$N(CH_3)_2$ & -C(CH3)3	1.02	0	1.02	Use Taft for CH3	-2.98
	Amine	124	N-Methyl-N-tritiohydroxylamine	CH3NHOH	-NCH3, -H	0.94		0.94		-3.59
Association with C=O	Carboxylate	4	Oxalate	$^-OOCCOO^-$	$-COO^-$ & $-O^-$	0.75	-2.78	-2.03		-2.98
		5	Formate	$HCOO^-$	-H & -O-	0.49	-2.78	-2.29		-3.85
		6	Succinate	$^-OOC(CH_2)_2COO^-$	$-(CH_2)_2COO^-$ & -O-	0.02	-2.78	-2.76		-3.90
		7	Acetate	CH_3COO^-	$-CH_3$ & -O-	0.00	-2.78	-2.78		-3.93
		12	Lactate	$CH_3CHOHCOO$-	$-(OH)CHCH_3$ & -O-	0.46	-2.78	-2.32		-4.03
		13	Glycolate	$HOCH_2COO^-$	$-CH_2OH$ & -O-	0.56	-2.78	-2.22		-3.99
		14	Pyruvate	CH_3COCOO^-	$-COO^-$ & $-CH_3$	0.75	0	0.75		-2.07
		16	Malate	$^-OOCCH_2CHOHCOO^-$	-(OH)CH & -O-	0.56	-2.78	-2.22	Use Taft for: CH2OH	-3.77
	Ketone	43	Acetone	CH_3COCH_3	$-CH_3$ & $-CH_3$	0	0	0		-2.59
		44	Methyl Ethyl Ketone	$CH_3CH_2COCH_3$	$-C_2H_5$ & $-CH_3$	-0.1	0	-0.1		-2.60
		45	2,3-Butanedione	$CH_3COCOCH_3$	$-COCH_3$ & $-CH_3$	1.65	0	1.65		-1.29
		46	Acetoin	$CH_3COCH(OH)CH_3$	$-CH_3$ & -$CH(OH)CH_3$	0	0.46	0.46		-2.38
	Aldehyde	47	Acetaldehyde	CH_3CHO	-H & $-CH_3$	0.49	0	0.49		-2.33
		48	Propionaldehyde	CH_3CH_2CHO	-H & $-CH_2CH_3$	0.49	-0.1	0.39		-2.35
	Amine	118	Glycinate	$NH_2CH_2COO^-$	-O-, $-CH_2NH_2$	-2.78	0.4	-2.38		-3.85
		122	beta-Alaninate	$NH_2(CH_2)_2$-COO^-	-O-, $-(CH_2)_2NH_2$	-2.78	0.4	-2.38	Use Taft for: CH_2NH_2	-3.85
Association with C=C	Alkene	207	Allylamine	$H_2C=CHCH_2NH_2$	-H, -CH2NH2		0.4	0.4		-3.28
		209	Allyl alcohol	$H_2C=CHCH_2OH$	-H, CH2OH		0.56	0.56		-3.09
		211	Acrylate	$CH_2=CHCOO^-$	-H, $-COO^-$		0.75	0.75		-2.51

		216	Ethylene	$H_2C=CH_2$	-H		0.49	0.49	Include one H Taft value to account for functional group.	-3.21
		219	Crotonyl Alcohol	$CH_3CH=CHCH_2OH$	-H, -CH3, -CH2OH		0.56	0.56		-3.23
		234	Methacrylate	$CH_2=C(CH_3)COO^-$	-H, -CH3, -COO-		0.75	0.75		-2.69
		235	3-Buten-1-ol	$H_2C=CHCH_2CH_2OH$	-H, -CH2CH2OH		0.56	0.56	Use Taft for CH2OH	-3.28
		236	3-Buten-2-OL	$H_2C=CHCH(OH)CH_3$	-H, -CH(OH)CH3		0.46	0.46	Use Taft for CH(OH)CH3	-3.13
		237	3-Methylbut-2-enoate	$(CH_3)_2C=CHCO_2^-$	-(CH3)2, -H, -CO2-		0.75	0.75		-2.91
		239	Isocrotonate	$CH_3CH=CHCOO^-$	-CH3, -H, -COO-		0.75	0.75		-2.73
		243	trans-Aconitate(3-)	$OOCCH=C(COO^-)CH_2COO^-$	-COO-, '-CH2COO-	0.75	-0.06	1.44		-2.33
		248	4-Penten-2-OL	$H_2C=CHCH_2CH(OH)CH_3$	-H, -CH2CH(OH)CH3		0.16	0.16		-3.33
Concerted C-Cl	*Haloalkane*	60	Chloromethane	CH_3Cl	$-CH_3$	0		0		-1.25
		65	Chloropropane	$CH_3CH_2CH_2Cl$	-CH2CH2CH3	-0.12		-0.12		-1.21
		66	Chloroethane	CH_3CH_2Cl	-CH2CH3	-0.1		-0.1		-1.20
		69	1,1-Dichloroethane	CH_3CHCl_2	-Cl & $-CHCH_3$	2.94	-0.19	2.75	Use Taft for CH2CH3	-0.94
		72	Dichloromethane	CH_2Cl_2	-Cl & $-CH_2$	0.98	2.8	3.78		-1.00
		73	Chloroform	$CHCl_3$	-CHCl2	2.01	5.88	7.89	Use Taft for CH3	-0.73
		74	Trichlorofluoromethane	CCl_3F	$-CCl_2$ & -F	1.1	5.88	6.98	Use Taft for CCl3	-0.69
		75	Dichlorodifluoromethane	CF_2Cl_2	-Cl & $-CF_2$	2.94	2.05	4.99		-0.93
		76	Chlorotrifluoromethane	$CClF_3$	$-CF_3$	2.56		2.56		-1.19
		78	Carbon Tetrachloride	CCl_4	$-CCl_3$	8.82		8.82		-0.33
		79	Chlorodifluoromethane	$CHClF_2$	$-CHF_2$	2.05		2.05		-1.24
		80	1,1,2-Trichloroethane	$ClCH_2CHCl_2$	$-CH_2CHCl_2$	2.01		2.01	Use Taft for CH2Cl	-1.02
		81	1,1,1-Trichloroethane	CH_3CCl_3	-CCl2 & $-CH_3$	5.88	0	5.88	Use Taft for CCl3	-0.63

		82	Hexachloroethane	CCl_3CCl_3	-CCl2 & -CCl_3	2.65	5.88	8.53	Use Taft for CCl3	-0.39
		83	2-Chlorobutane	$C_2H_5CH(Cl)CH_3$	-CH_3 & -CHC2H5	0.49	-0.1	0.39		-1.17
		85	1,2-Dichloroethane	$ClCH_2CH_2Cl$	-CH2CH2Cl	0.98	1.01	1.99	Use Taft for CH2Cl	-1.07
		86	1,1,2-Trichloro-1,2,2-trifluoroethane	$ClCF_2CCl_2F$	-CCl_2 & -CF_2	2.05	2.01	4.06	Use Taft for CCl3 & CF3	-0.79
		90	1-Chlorobutane	$CH_3(CH_2)_3Cl$	-(CH2)3CH3	-0.12		-0.12	Use Taft for CH2CH2CH3	-1.21
		91	1-Chloro-2-methylpropane	$(CH_3)_2CHCH_2Cl$	-CH2CH(CH3)2	-0.19		-0.19		-1.22
Stepwise C-Cl	*Halocarboxylate*	*49*	*Chloroacetate*	*$ClCH_2COO^-$*	*-H, -COO-*	*0.98*	*0.75*	*1.73*		*-4.73*
		50	*3-Chloropropanoate*	*$Cl(CH_2)_2COO^-$*	*-H, -CH2COO-*	*0.98*	*-0.06*	*0.92*	Use Taft for: CH_2CH_3	*-4.84*
		55	*2-Chloropropanoate*	*$CH_3CHClCOO^-$*	*-COO-, -H, -CH3*	*0.75*	*0.49*	*1.24*	Use Taft for: CH_2Cl	*-4.51*
		56	*Trichloroacetate*	*Cl_3CCOO^-*	*-Cl, -COO-*	*5.3*	*0.75*	*6.05*		*-4.36*
	Halooxygen	97	*Isoflurane*	*$CHF_2OCHClCF_3$*	*-CF3, -H, -OCHF2*	*3.05*	*2.81*	*5.86*	Use Taft for CHCl2	*-4.32*
		100	*Methoxyflurane*	*$CH_3OCF_2CHCl_2$*	*-Cl, -H, -CF2*	*3.43*	*2.56*	*5.99*	Use Taft for CF3	*-4.34*
		101	*2-Chloroethanol*	*$ClCH_2CH_2OH$*	*-H, -CH2OH*	*0.98*	*0.56*	*1.54*		*-4.94*
		103	*Chloroacetic acid*	*$ClCH_2COOH$*	*-H, -COOH*	*0.98*	*2.94*	*3.92*		*-4.51*
		104	*Chloral hydrate*	*$CCl_3CH(OH)_2$*	*-Cl, -CH(OH)2*	*5.88*	*1.37*	*7.25*		*-4.25*
		105	*Enflurane*	*CHF_2OCF_2CHClF*	*-F, -H, -CF2*	*2.54*	*2.56*	*5.1*	Use Taft for CF3	*-4.46*
Stepwise C=C-Cl	*Chloroalkene*	215	*Vinyl chloride*	*$CH_2=CHCl$*	*$CH=CH_2$, -Cl*	*2.94*	*0*	*2.94*		*-5.45*
		218	*Tetrachloroethylene*	*$Cl_2C=CCl_2$*	*-C=C-, Cl2*	*2.94*	*0*	*11.76*		*-4.94*
		225	*trans-1,2-Dichloroethylene*	*ClCH=CHCl*	*CH=CH, -Cl*	*2.94*	*0*	*5.88*		*-5.26*
		226	*Trichloroethylene*	*$ClCH=CCl_2$*	*CH=C, -Cl*	*2.94*	*0*	*8.82*		*-5.08*
		227	*cis-1,2-Dichloroethylene*	*$H_2C=CCl_2$*	*$C=CH_2$, -Cl2*	*2.94*	*0*	*5.88*		*-5.14*
Concerted C-NH3+	*Ammonium*	157	Methyl Ammonium Hydride	$CH_3NH_3^+$	-CH_3	0		0		-2.11

		158	Ethylammonium	$C_2H_5NH_3^+$	$-C_2H_5$	-0.1		-0.1		-2.05
		159	Trideuterio(propyl)azanium	$CH_3(CH_2)_2NH_3^+$	$-(CH_2)_2CH_3$	-0.12		-0.12		-2.07
		160	Pentylazanium	$CH_3(CH_2)_4NH_3^+$	$-(CH_2)_4CH_3$	-0.12		-0.12	Use Taft for: $(CH_2)_2CH_3$	-2.04
		162	Methoxyazanium	$CH_3ONH_3^+$	$-OCH_3$	1.77		1.77		-0.10
		163	Tert-butylammonium	$(CH_3)_3CNH_3^+$	$-C(CH_3)_3$	-0.3		-0.3		-1.96
		164	2-Methylhydrazinium	$CH_3NHNH_3^+$	$-NHCH_3$	0.94		0.94		-0.78
		165	1,1-Dimethylhydrazinium	$(CH_3)_2NNH_3^+$	$-N(CH_3)_2$	1.02		1.02		-0.56
Concerted C-SH	*Thiol*	176	Methanethiol	CH_3SH	-CH3	0	-	0		-2.21
		177	Thiolactate	$CH_3(CH)SHCOO^-$	-CH3(CH) & -COO-	0	0.75	0.75		-1.75
		178	2-Mercaptopropionic Acid	$CH_3CH(SH)COOH$	-CHCH3 & -COOH	-0.1	2.94	2.84	Use Taft for CH2CH3	-1.57
		179	Methyl thioglycolate	$HSCH_2COOCH_3$	-CH2COOCH3	0.7		0.7		-1.85
		180	beta-Mercaptoethanol	$HS(CH_2)_2OH$	-(CH2)2OH	0.56		0.56	Use Taft for CH2OH	-2.12
		181	2-Methyl-2-propanethiol	$(CH_3)_3CSH$	-C(CH3)3	-0.3		-0.3		-1.93
		182	3-Mercaptopropionic acid	$HS(CH_2)_2COOH$	-(CH2)2COOH	0.35		0.35		-2.11
		183	Thioglycolate	$HSCH_2COO^-$	-CH2COO-	-0.06		-0.06		-1.93
		184	-	$H_2NC(=NH)NHCH_2CH_2SH$	-CH2CH2NH	-0.1	-	-0.1	Use Taft for CH2CH3	-2.06
Stepwise S-S		186	*3,3'-Dithiodipropionate*	*$(SCH_2CH_2COO^-)_2$*	*-CH2CH2COO- & -SCH2CH2*	*-0.06*	*1.44*	*1.38*	Use Taft for SC2H5	*-5.16*
		187	*2,2'-Disulfanediyldiacetate*	*$(SCH_2COO^-)_2$*	*-CH2COO- & -SCH2*	*-0.06*	*1.44*	*1.38*	Use Taft for SC2H5	*-5.38*
		188	*2,2'-Sulfanediyldiacetate*	*$S(CH_2COO^-)_2$*	*-CH2COO- (x2)*	*-0.06*	*-0.06*	*-0.12*		*-5.79*
		189	*N-Acetylcysteamine*	*$CH_3CONHCH_2CH_2SH$*	*-CH2CH2NH*	*-0.1*		*-0.1*	Use Taft for CH2CH1	*-5.55*
		190	*Cystamine*	*$S_2(CH_2CH_2NH_2)_2$*	*-SCH2CH2 & -CH2CH2NH2*	*1.44*	*-0.1*	*1.34*	Use Taft for CH2CH2	*-5.33*
		191	*L-Cystine anion*	*$S_2[CH_2CH(NH_2)COO^-]_2$*	*-SCH2CH2 & -CH2CH(NH2)*	*1.44*	*-0.1*	*1.34*	Use Taft for CH2CH3	*-4.94*
		192	*3,3'-Thiodipropanoate*	*$S(CH_2CH_2COO^-)_2$*	*-CH2CH2COO- (x2)*	*-0.06*	*-0.06*	*-0.12*		*-5.73*

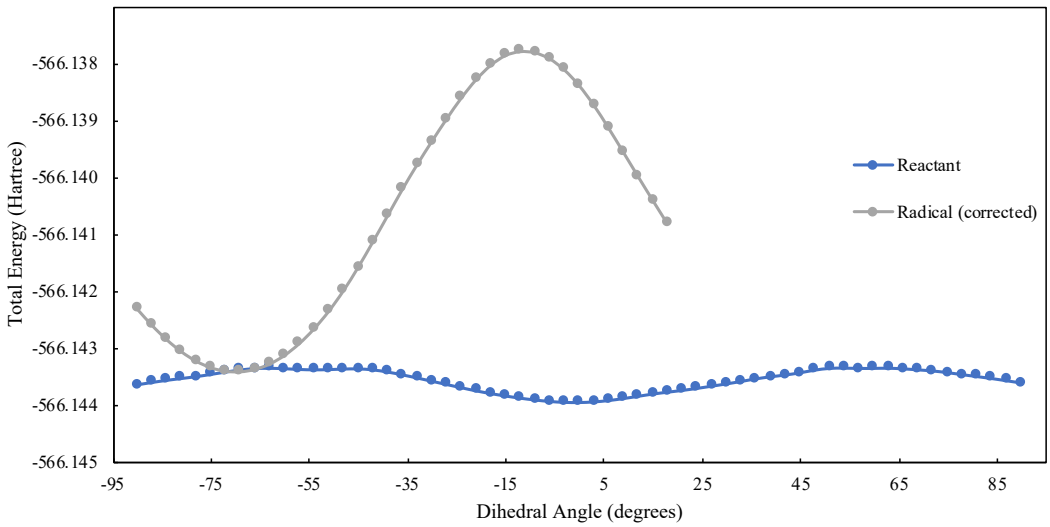


Figure S2: Potential energy surface of reactant and radical anion of methyl trifluoroacetate (No.39) as a function of dihedral angle with the corrected energy for radical anion based on.

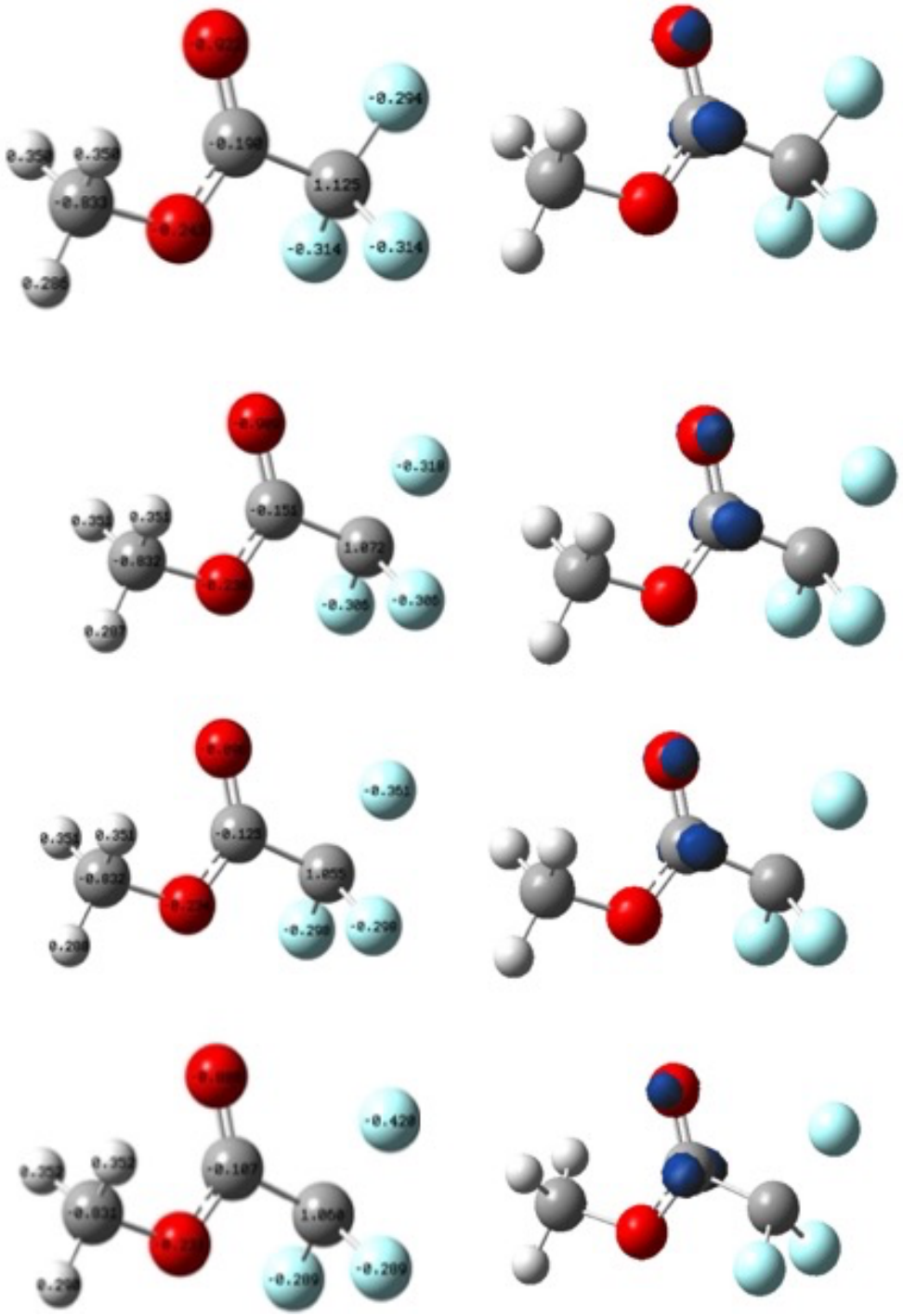


Figure S3: Distribution of charge (left) and spin density representing the blue shades on the atoms (right) of methyl trifluoroacetate (No.39) for different C-F bond lengths from top 1.324 Å (optimized); 1.431 Å, 1.538 Å, and 1.645 Å. The areas in blue indicate the high spin density.

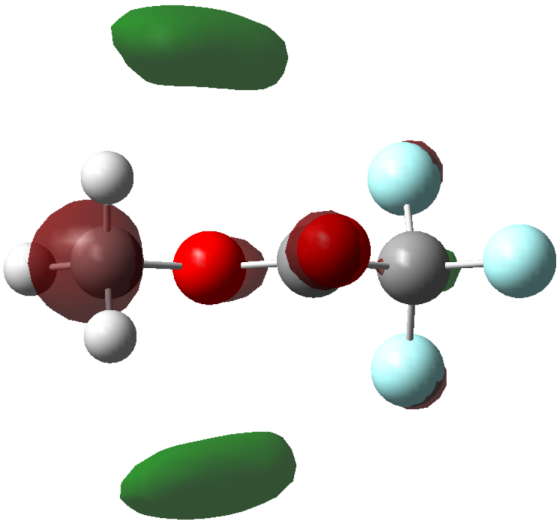


Figure S4: LUMO of trifluoroacetate

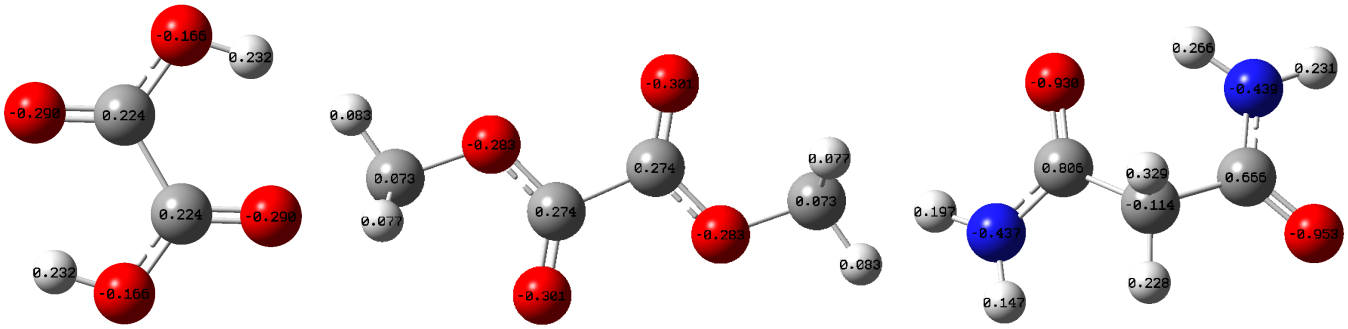


Figure S5: Charge distribution of oxalate, dimethylester, and acetamide.

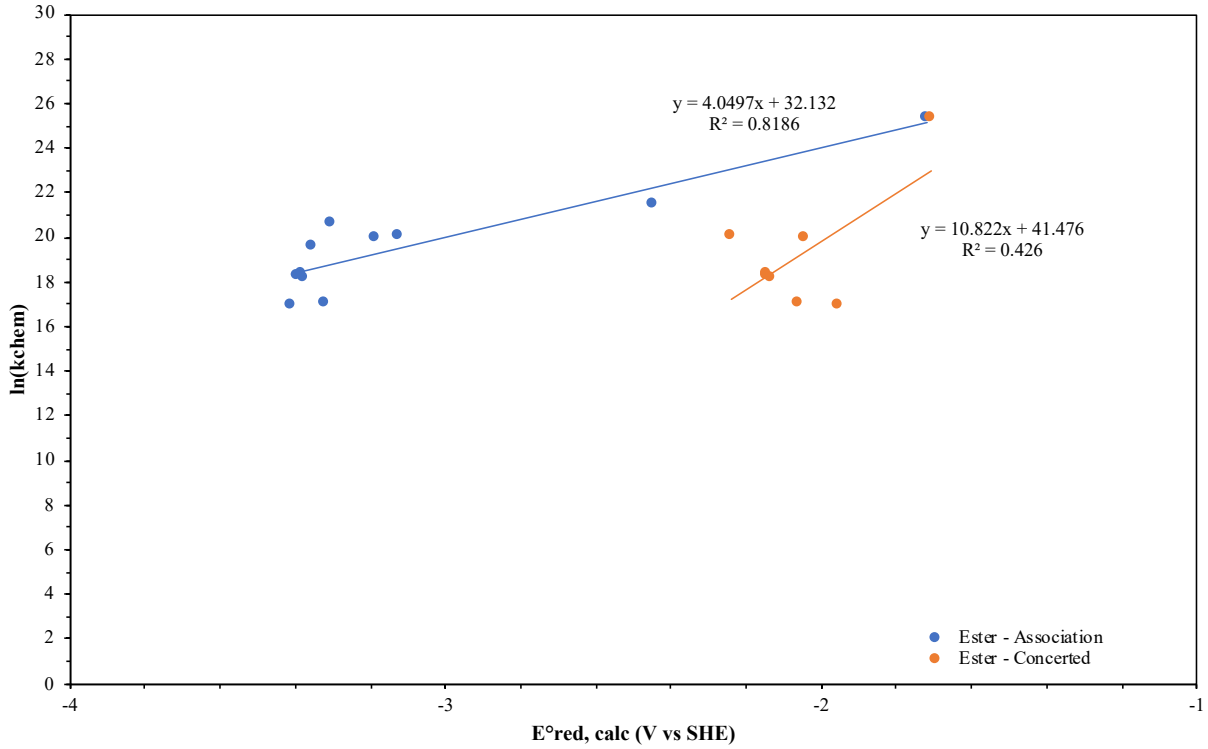


Figure S6: LFERs for ester via association and concerted C-O cleavage.

Figure S7: Spin density distribution of nitropropane

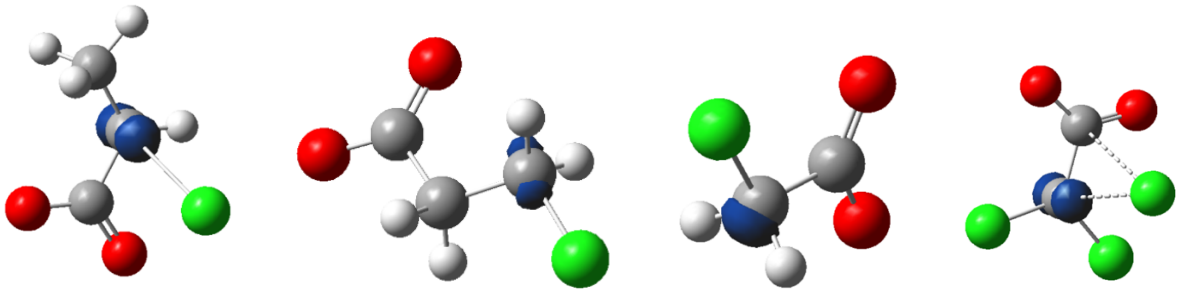


Figure S8: Spin density distribution of 2-chloropropanoate, 3-chloropropanoate, chloroacetate, and trichloroacetate

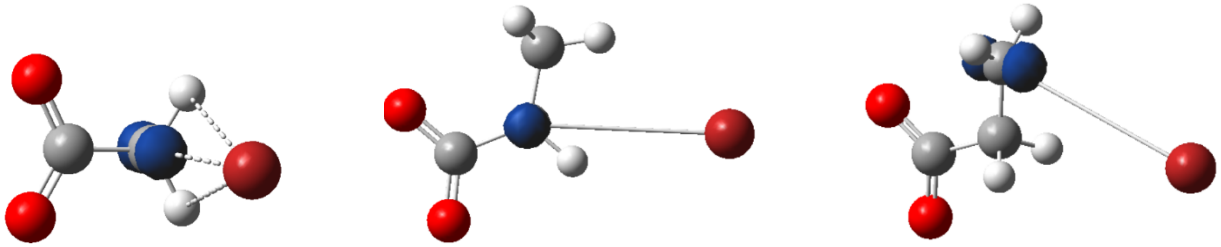


Figure S9: Spin density distribution of bromoacetate, 2-bromopropanoate, and 3-bromopropanoate

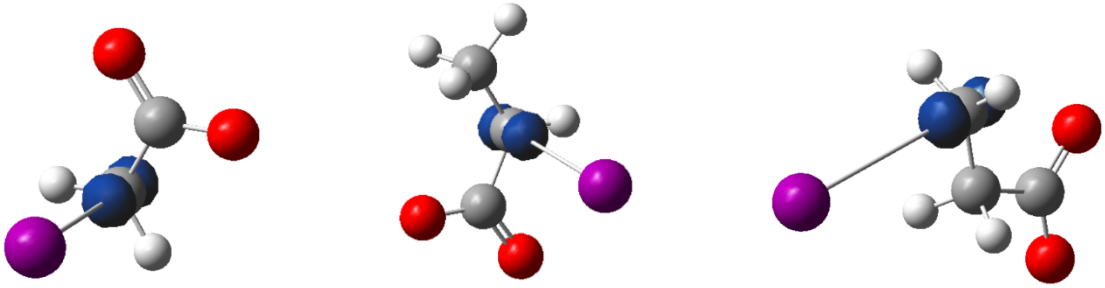


Figure S10: Spin density distribution of 2-iodoacetate, 2-iodopropanoate, and 3-iodanylpropanoate

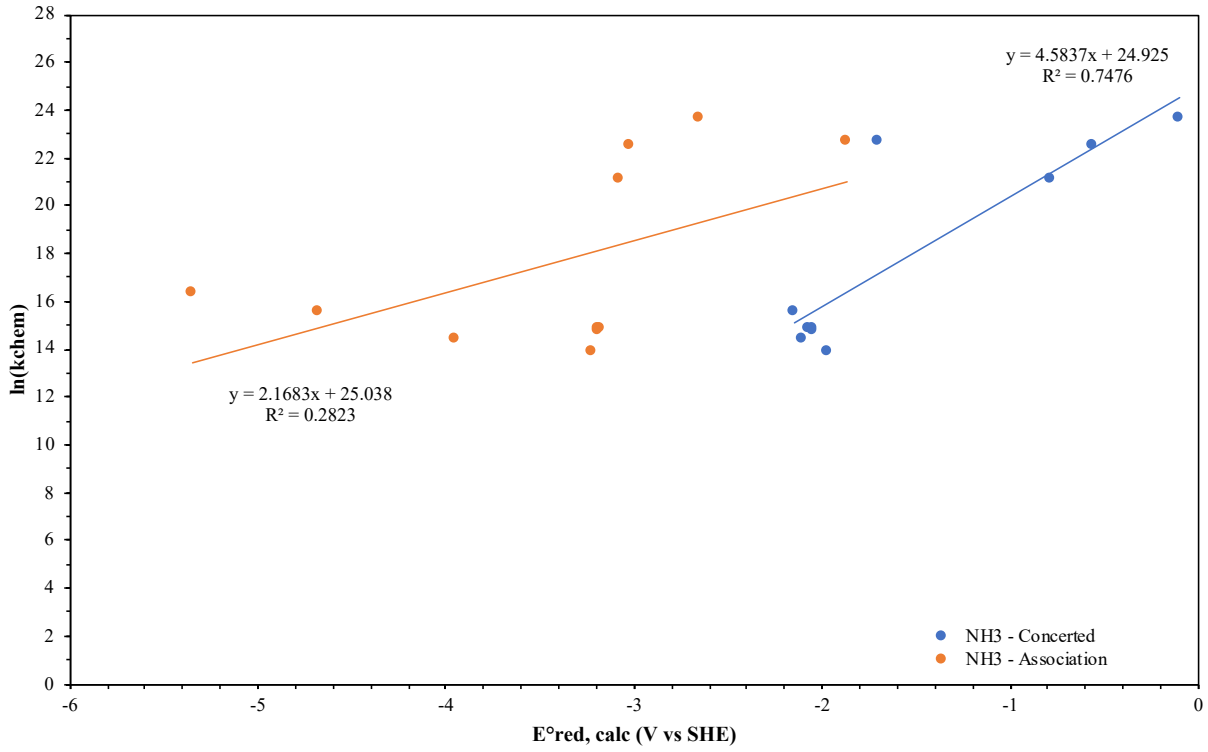


Figure S11: LEFRs for concerted and association mechanisms of C-NH_4^+ bond of ammonium compounds

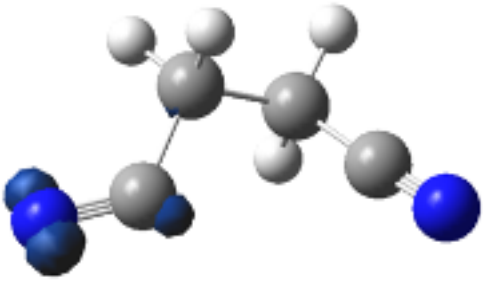


Figure S12: Spin density distribution of cyanide

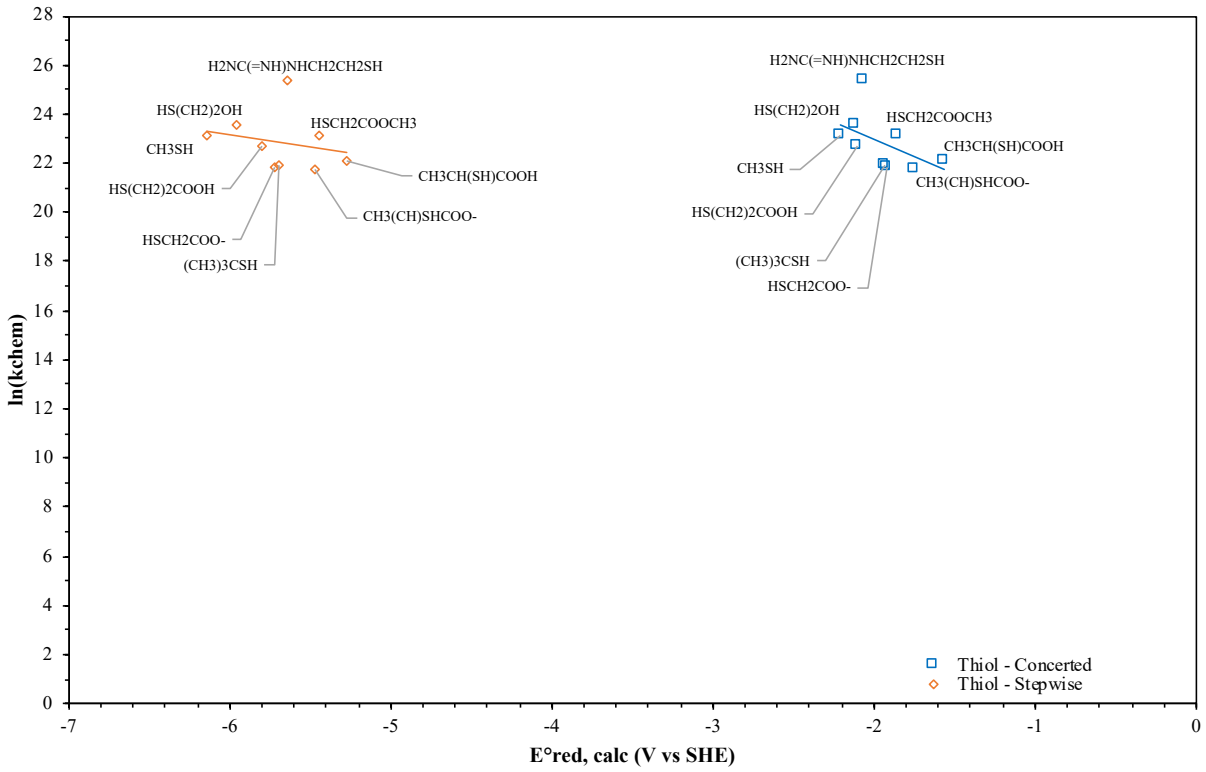


Figure S13: Linear free energy relationships for thiols undergoing stepwise (red dot) and concerted (blue dot) mechanisms

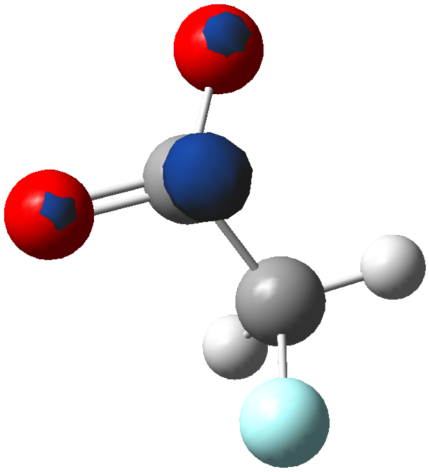


Figure S14: Spin density distribution of fluoroacetate

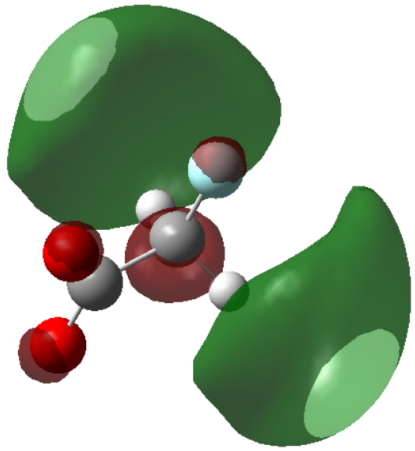


Figure S15: LUMO of fluoroacetate

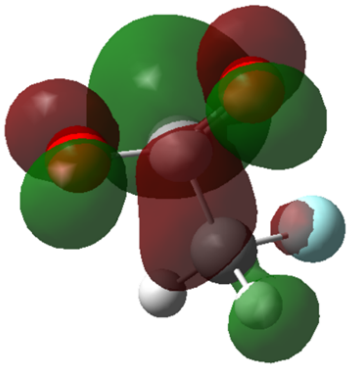


Figure S16: SOMO of fluoroacetate radical anion

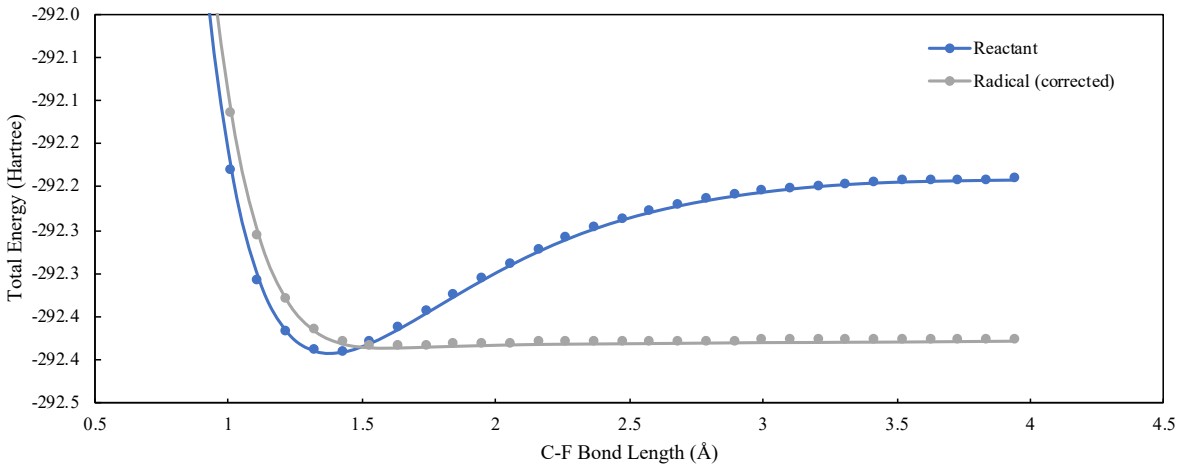


Figure S17: Potential energy surface of fluoroacetone as a function of C-F bond.

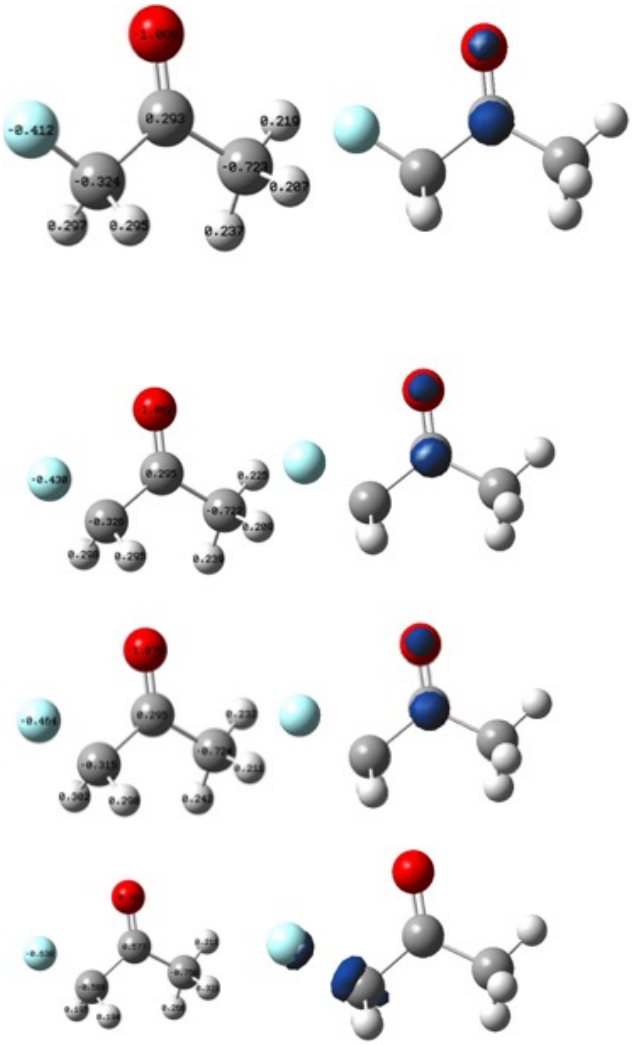


Figure S18: Distribution of charge and spin density of fluoroacetone (No. 99): C-F bond from 1.279 Å (optimized) (Top), 1.484 Å, 1.589 Å, and 1.694 Å (Bottom).

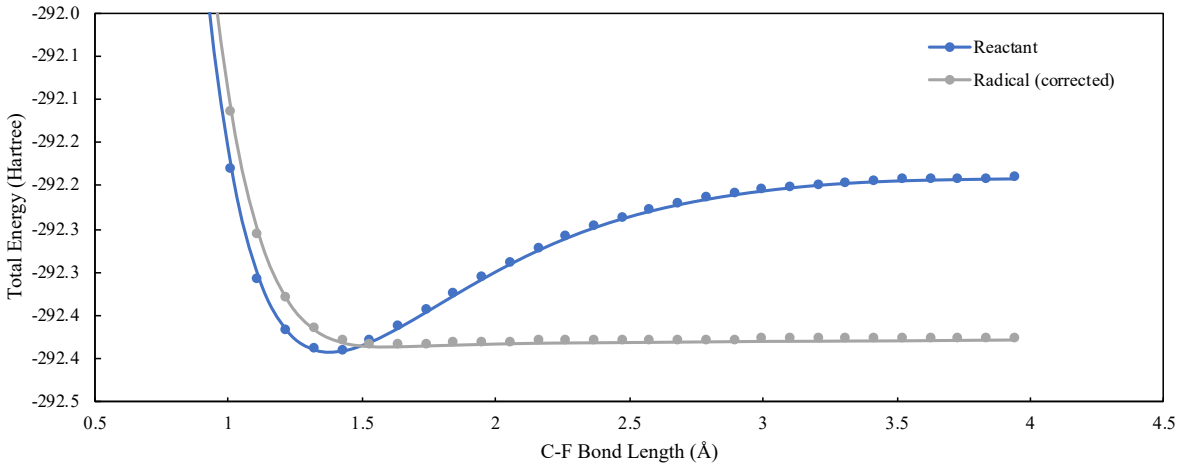


Figure S19: Potential energy surface of 1,1,1-trifluoroacetone as a function of one of C-F bonds

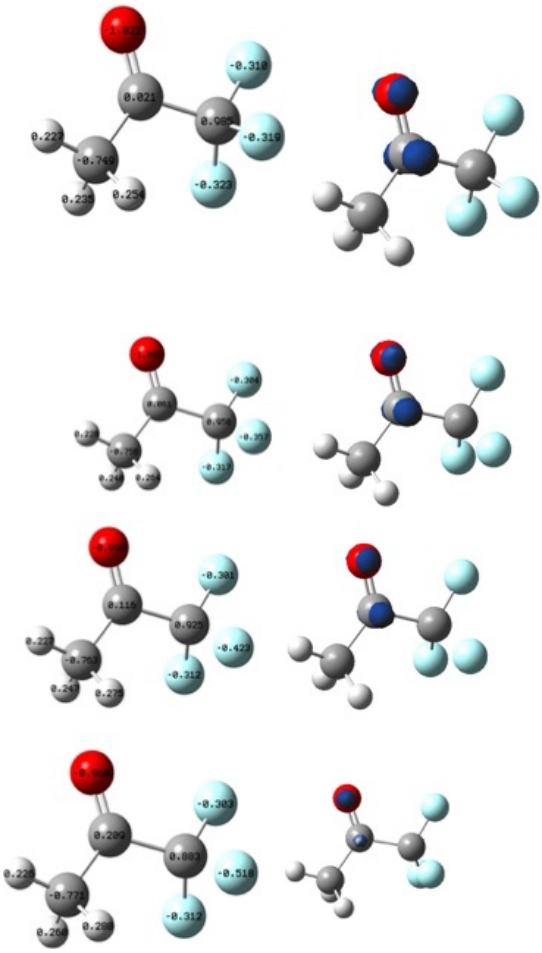


Figure S20: Distribution of charge and spin density of 1,1,1-trifluoroacetone (No. 98). C-F bond from 1.338 Å (optimized) (top), 1.444 Å, 1.551 Å, and 1.657 Å (bottom).

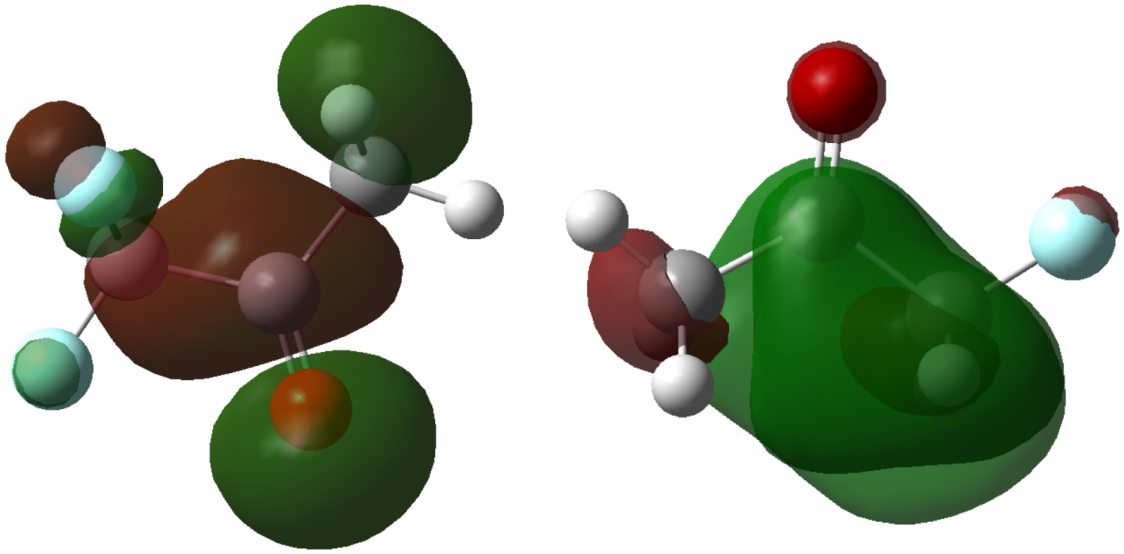


Figure S21: LUMO of 1,1,1-trifluoroacetone (No. 98) and fluoroacetone (No. 99)

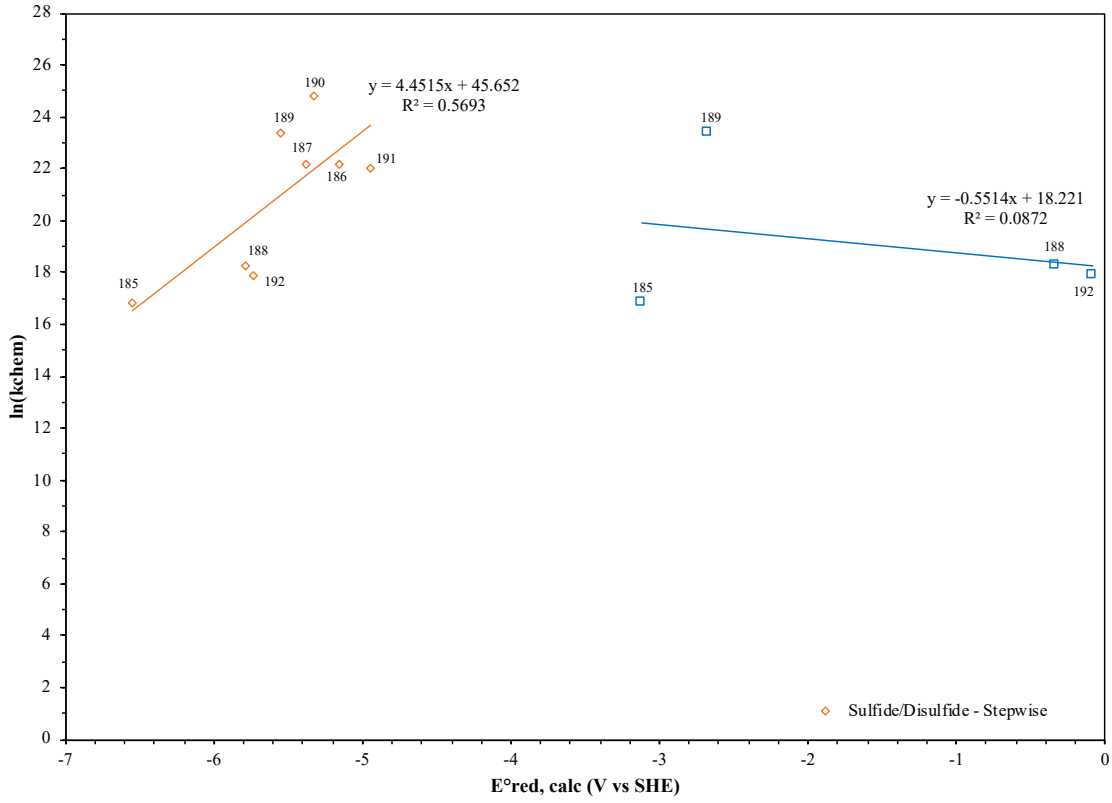
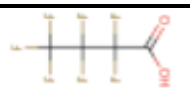
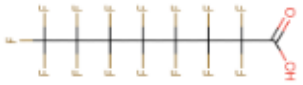


Figure S22: Linear free energy relationships for sulfides and disulfides undergoing stepwise (red dot) and concerted (blue dot) mechanisms

Table S7: Comparison of $E^0_{red,aq}$ values of representative PFASs calculated at M06-2X/cc-pVDZ and single point energy calculation at M06-2X/Aug-cc-pVTZ based on the optimized structure at M06-2X/cc-pVDZ

Class	Compound	Attacking Site	Chemical Structure	Stepwise Ered		
				opt + freq M06-2X/cc-pVDZ	single pt M06-2X/aug-cc-pVTZ	opt + freq M06-2X/aug-cc-pVTZ
PFCA	**Perfluorobutanoic acid (PFBA)**	**alpha**		**-6.79**	**-4.94**	-5.61
		beta		-7.06	-5.22	-5.61
		terminal		-7.39	-5.54	-5.61
	Perfluorooctanoic acid (PFOA)	**alpha**		**-6.14**	**-4.30**	-3.33
		beta		-6.28	-4.36	-3.33
		gamma		-6.25	-4.42	-3.33
		delta		-6.24	-4.40	-3.33
		epsilon		-6.30	-4.49	-3.33
		zeta		-6.30	-4.47	-3.33
		terminal		-6.66	-4.82	-3.33
PFSA	**Perfluorobutanesulfonic acid**	**alpha**		-6.69	-4.88	-3.33
		beta		-6.71	-4.87	-3.33
		gamma		**-6.60**	**-4.67**	-3.33
		terminal		-7.04	-5.08	-3.33
FTOH	**Heptafluorobutanol**	**alpha**		-7.11	-5.58	25253.07
		beta		**-7.10**	**-5.27**	25253.06
		terminal		-7.40	-5.90	2710.40

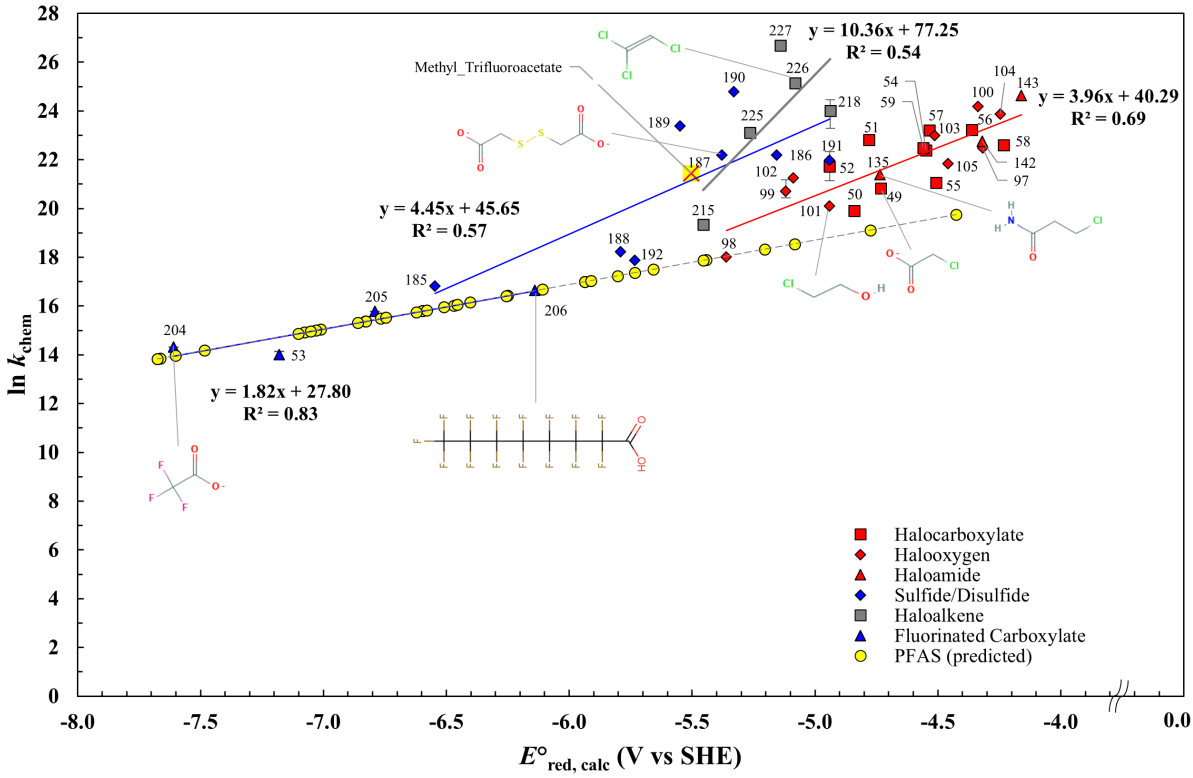


Figure S23: LFER for fluorinated compounds based on M06-2X/cc-pVDZ

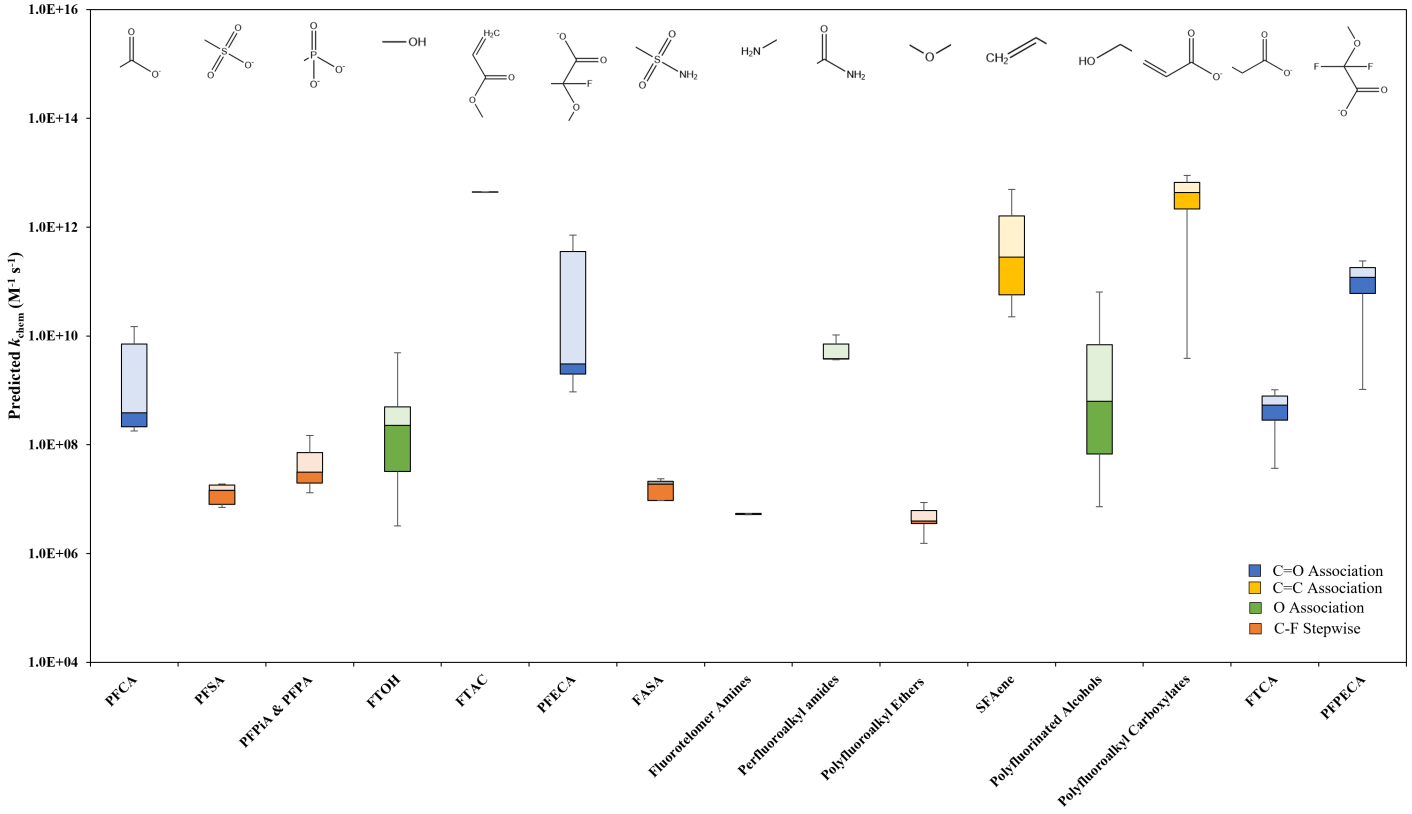


Figure S24: Predicted k_{chem} values for PFASs. The $E^{\circ}_{red,aq}$ values were calculated based on structural optimization at the level of M06-2X/cc-pVDZ and single point energy calculation at the level of M06-2X/Aug-cc-pVTZ and the LFER developed based on the same method and basis set.

Text S4: Description of an unsteady-state kinetic model and experimental condition used for simulating the fate of a model compound in the UV/sulfite process[125]

An unsteady-state kinetic model for UV/sulfite system was formulated by modifying our previously developed UV/H_2O_2 kinetic model[126]. The ordinary differential equations (ODEs) were written for all species involved in the reaction described below. The ODEs were solved with the given reaction rate constants using the Gear method to obtain the time-dependent concentration profiles of all species at the given experimental condition[127, 128]. The detailed evaluation of numerical solutions of ODEs was given in our previous publication.[126]

18W LPUV, I_0 = 3.85 Einstein/L/sec, b= 2.85 cm, 572 mL, $\Phi = 0.1$, ε=17.7 $M^{-1}cm^{-1}$, pH=9.5, 20℃, 10 mM of sulfite

$UV + HSO_3^-/SO_3^{2-} \rightarrow SO_3\cdot + e_{aq}^-$

$e_{aq}^- + R(PFAS) \rightarrow$ $\quad k_1 = 1.0\times 10^6\ M^{-1}s^{-1}$ with a difference of a factor of 1.2, 2, and 5

$SO_3\cdot + SO_3\cdot \rightarrow S_2O_6^{2-}$ $\quad 2k_2 = 1.0\times 10^6\ M^{-1}s^{-1}$

$SO_3\cdot + SO_3\cdot + H_2O \rightarrow SO_4^{2-} + H^+ + HSO_3^-$ $\quad k_3/k_2 = 0.37$

$e_{aq}^- + H^+ \rightarrow H\cdot$ $k_4 = 2.3 \times 10^{10}\ M^{-1}s^{-1}$

$e_{aq}^- + H\cdot + H_2O \rightarrow H_2 + OH^-$ $k_5 = 3.0 \times 10^{10}\ M^{-1}s^{-1}$

$e_{aq}^- + e_{aq}^- + 2H_2O \rightarrow H_2 + 2OH^-$ $2k_6 = 1.1 \times 10^{10}\ M^{-1}s^{-1}$

$e_{aq}^- + S_2O_6^{2-} \rightarrow SO_3^{2-} + SO_3\cdot$ $k_7 = 2.0 \times 10^{5}\ M^{-1}s^{-1}$

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