

Aquatic Chemistry

An Introduction Emphasizing
Chemical Equilibria in Natural Waters

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Appendix: Thermodynamic Properties; Table of G_f° , H_f° , and S° Values for Common Chemical Species in Aquatic Systems^a

Valid at 25°C, 1 atm Pressure and Standard States^b

Species	Formation from the Elements		Entropy	Reference ^c
	G_f° (kJ mol ⁻¹)	H_f° (kJ mol ⁻¹)	S° J mol ⁻¹ K ⁻¹	
Ag (Silver)				
Ag (metal)	0	0	42.6	NBS
Ag ⁺ (aq)	77.12	105.6	73.4	NBS
AgBr	-96.9	-100.6	107	NBS
AgCl	-109.8	-127.1	96	NBS
AgI	-66.2	-61.84	115	NBS
Ag ₂ S(α)	-40.7	-29.4	14	NBS
AgOH(aq)	-92	—	—	NBS
Ag(OH) ₂ ⁻ (aq)	-260.2	—	—	NBS
AgCl(aq)	-72.8	-72.8	154	NBS
AgCl ₂ ⁻ (aq)	-215.5	-245.2	231	NBS
Al (Aluminum)				
Al	0	0	28.3	R
Al ³⁺ (aq)	-489.4	-531.0	-308	R
AlOH ²⁺ (aq)	-698	—	—	S
Al(OH) ₂ ⁺ (aq)	-911	—	—	S
Al(OH) ₃ (aq)	-1115	—	—	S
Al(OH) ₄ ⁻ (aq)	-1325	—	—	S
Al(OH) ₃ (amorph)	-1139	—	—	R
Al ₂ O ₃ (corundum)	-1582	-1676	50.9	R
AlOOH (boehmite)	-922	-1000	17.8	R
Al(OH) ₃ (gibbsite)	-1155	-1293	68.4	R
Al ₂ Si ₂ (OH) ₄ (kaolinite)	-3799	-4120	203	R
KAl ₃ Si ₃ O ₁₀ (OH) ₂ (muscovite)	-1341	—	—	G

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$\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_8$ (chlorite)	-1962	—	—	R
$\text{CaAl}_2\text{Si}_2\text{O}_8$ (anorthite)	-4017.3	-4243.0	199	R
$\text{NaAlSiO}_3\text{O}_8$ (albite)	-3711.7	-3935.1	—	R
As (Arsenic)				
As (α metal)	0	0	35.1	NBS
$\text{H}_3\text{AsO}_4(\text{aq})$	-766.0	-898.7	206	NBS
$\text{H}_2\text{AsO}_4^-(\text{aq})$	-748.5	-904.5	117	NBS
$\text{HAsO}_4^{2-}(\text{aq})$	-707.1	-898.7	3.8	NBS
$\text{AsO}_4^{3-}(\text{aq})$	-636.0	-870.3	-145	NBS
$\text{H}_2\text{AsO}_3(\text{aq})$	-587.4	—	—	NBS
Ba (Barium)				
$\text{Ba}^{2+}(\text{aq})$	-560.7	-537.6	9.6	R
BaSO_4 (barite)	-1362	-1473	132	R
BaCO_3 (witherite)	-1132	-1211	112	R
Be (Beryllium)				
$\text{Be}^{2+}(\text{aq})$	-380	-382	-130	NBS
$\text{Be}(\text{OH})_2(\alpha)$	-815.0	-902	51.9	NBS
$\text{Be}_3(\text{OH})_3^{3+}$	-1802	—	—	NBS
B (Boron)				
$\text{H}_3\text{BO}_3(\text{aq})$	-968.7	-1072	162	NBS
$\text{B}(\text{OH})_4^-(\text{aq})$	-1153.3	-1344	102	NBS
Br (Bromide)				
$\text{Br}_2(\text{l})$	0	0	152	NBS
$\text{Br}_2(\text{aq})$	3.93	-2.59	130.5	NBS
$\text{Br}^-(\text{aq})$	-104.0	-121.5	82.4	NBS
$\text{HBrO}(\text{aq})$	-82.2	-113.0	147	NBS
$\text{BrO}^-(\text{aq})$	-33.5	-94.1	42	NBS
C (Carbon)				
C (graphite)	0	0	152	NBS
C (diamond)	3.93	-2.59	130.5	NBS
$\text{CO}_2(\text{g})$	-394.37	-393.5	213.6	NBS
$\text{H}_2\text{CO}_3^*(\text{aq})$	-623.2	-699.7	187.0	R
$\text{H}_2\text{CO}_3(\text{aq})$ ("true")	-607.1	—	—	S
$\text{HCO}_3^-(\text{aq})$	-586.8	-692.0	91.2	S
$\text{CO}_3^{2-}(\text{aq})$	-527.9	-677.1	-56.9	NBS
$\text{CH}_4(\text{g})$	-50.75	-74.80	186	NBS
$\text{CH}_4(\text{aq})$	-34.39	-89.04	83.7	NBS
$\text{CH}_3\text{OH}(\text{aq})$	-175.4	-245.9	133	NBS
$\text{HCOOH}(\text{aq})$	-372.3	-425.4	163	NBS
$\text{HCOO}^-(\text{aq})$	-351.0	-425.6	92	NBS
$\text{HCN}(\text{aq})$	119.7	107.1	124.6	NBS
$\text{CN}^-(\text{aq})$	172.4	150.6	94.1	NBS

$\text{CH}_3\text{COOH}(\text{aq})$	-396.6	-485.8	179	NBS
$\text{CH}_3\text{COO}^-(\text{aq})$	-369.4	-486.0	86.6	NBS
$\text{C}_2\text{H}_5\text{OH}(\text{aq})$	-181.8	-288.3	149	NBS
$\text{NH}_2\text{CH}_2\text{COOH}(\text{aq})$	-370.8	-514.0	158	NBS
$\text{NH}_2\text{CH}_2\text{COO}^-(\text{aq})$	-315.0	-469.8	119	NBS

Ca (Calcium)

$\text{Ca}^{2+}(\text{aq})$	-553.54	-542.83	-53	R
$\text{CaOH}^+(\text{aq})$	-718.4	—	—	NBS
$\text{Ca}(\text{OH})_2(\text{aq})$	-868.1	-1003	-74.5	NBS
$\text{Ca}(\text{OH})_2$ (portlandite)	-898.4	-986.0	83	R
CaCO_3 (calcite)	-1128.8	-1207.4	91.7	R
CaCO_3 (aragonite)	-1127.8	-1207.4	88.0	R
$\text{CaMg}(\text{CO}_3)_2$ (dolomite)	-2161.7	-2324.5	155.2	R
CaSiO_3 (wollastonite)	-1549.9	-1635.2	82.0	R
CaSO_4 (anhydrite)	-1321.7	-1434.1	106.7	R
$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ (gypsum)	-1797.2	-2022.6	194.1	R
$\text{Ca}_5(\text{PO}_4)_3\text{OH}$ (hydroxyapatite)	-6338.4	-6721.6	390.4	R

Cd (Cadmium)

Cd (γ metal)				
$\text{Cd}^{2+}(\text{aq})$	-77.58	-75.90	-73.2	R
$\text{CdOH}^+(\text{aq})$	-284.5			R
$\text{Cd}(\text{OH})_3^-(\text{aq})$	-600.8			R
$\text{Cd}(\text{OH})_4^{2-}(\text{aq})$	-758.5			R
$\text{Cd}(\text{OH})_2(\text{aq})$	-392.2			R
CdO (s)	-228.4	-258.1	54.8	
$\text{Cd}(\text{OH})_2$ (precip.)	-473.6	-560.6	96.2	R
$\text{CdCl}^+(\text{aq})$	-224.4	-240.6	43.5	R
$\text{CdCl}_2(\text{aq})$	-340.1	-410.2	39.8	R
$\text{CdCl}_3^-(\text{aq})$	-487.0	-561.0	203	R
CdCO_3 (s)	-669.4	-750.6	92.5	R

Cl (Chlorine)

$\text{Cl}^-(\text{aq})$	-131.3	-167.2	56.5	NBS
$\text{Cl}_2(\text{g})$	0	0	223.0	NBS
$\text{Cl}_2(\text{aq})$	6.90	-23.4	121	NBS
$\text{HClO}(\text{aq})$	-79.9	-120.9	142	NBS
$\text{ClO}^-(\text{aq})$	-36.8	-107.1	42	NBS
$\text{ClO}_2(\text{aq})$	117.6	74.9	173	NBS
$\text{ClO}_2^-(\text{aq})$	17.1	-66.5	101	NBS
$\text{ClO}_3^-(\text{aq})$	-3.35	-99.2	162	NBS
$\text{ClO}_4(\text{aq})$	-8.62	-129.3	182	NBS

Co (Cobalt)

Co (metal)	0	0	30.04	R
$\text{Co}^{2+}(\text{aq})$	-54.4	-58.2	-113	R
Co^{3+}	-134	-92	-305	R

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$\text{HCoO}_2^- (\text{aq})$	-407.5	—	—	NBS
$\text{Co}(\text{OH})_2 (\text{aq})$	-369	-518	134	NBS
$\text{Co}(\text{OH})_2$ (blue precip.)	-450	—	—	NBS
CoO	-214.2	-237.9	53.0	R
Co_3O_4 (cobalt spinel)	-725.5	-891.2	102.5	R

Cr (Chromium)

Cr (metal)	0	0	23.8	NBS
$\text{Cr}^{2+} (\text{aq})$	—	-143.5	—	NBS
$\text{Cr}^{3+} (\text{aq})$	-215.5	-256.0	308	NBS
Cr_2O_3 (eskolaite)	-1053	-1135	81	R
$\text{HCrO}_4^- (\text{aq})$	-764.8	-878.2	184	R
$\text{CrO}_4^{2-} (\text{aq})$	-727.9	-881.1	50	R
$\text{Cr}_2\text{O}_7^{2-} (\text{aq})$	-1301	-1490	262	R

Cu (Copper)

Cu (metal)	0	0	33.1	NBS
$\text{Cu}^+ (\text{aq})$	50.0	71.7	40.6	NBS
$\text{Cu}^{2+} (\text{aq})$	65.5	64.8	-99.6	NBS
$\text{Cu}(\text{OH})_2 (\text{aq})$	-249.1	-395.2	-121	NBS
$\text{HCuO}_2^- (\text{aq})$	-258	—	—	—
CuS (covellite)	-53.6	-53.1	66.5	NBS
Cu_2S (α)	-86.2	-79.5	121	NBS
CuO (tenorite)	-129.7	-157.3	43	NBS
$\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$ (malachite)	-893.7	-1051.4	186	NBS
$2\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$ (azurite)	—	-1632	—	NBS

F (Fluorine)

$\text{F}_2 (\text{g})$	0	0	202	NBS
$\text{F}^- (\text{aq})$	-278.8	-332.6	-13.8	NBS
$\text{HF} (\text{aq})$	-296.8	320.0	88.7	NBS
$\text{HF}_2^- (\text{aq})$	-578.1	-650	92.5	NBS

Fe (Iron)

Fe (metal)	0	0	27.3	NBS
$\text{Fe}^{2+} (\text{aq})$	-78.87	-89.10	-138	NBS
$\text{FeOH}^+ (\text{aq})$	-277.3	—	—	NBS
$\text{Fe}^{3+} (\text{aq})$	-4.60	-48.5	-316	NBS
$\text{FeOH}^{2+} (\text{aq})$	-229.4	-324.7	-29.2	NBS
$\text{Fe}(\text{OH})_2^+ (\text{aq})$	-438	—	—	NBS
$\text{Fe}(\text{OH})_2^- (\text{aq})$	-659	—	—	NBS
$\text{Fe}_2(\text{OH})_2^{4+} (\text{aq})$	-467.3	—	—	NBS
FeS_2 (pyrite)	-160.2	-171.5	52.9	R
FeS_2 (marcasite)	-158.4	-169.4	53.9	R
$\text{FeO} (\text{s})$	-251.1	-272.0	59.8	R
$\text{Fe}(\text{OH})_2$ (precip.)	-486.6	-569	87.9	NBS

$\alpha\text{-Fe}_2\text{O}_3$ (hematite) ^c	-742.7	-824.6	87.4	R
Fe_3O_4 (magnetite)	-1012.6	-1115.7	146	R
$\alpha\text{-FeOOH}$ (goethite) ^c	-488.6	-559.3	60.5	R
FeOOH (amorph) ^c	-462	—	—	S
$\text{Fe}(\text{OH})_3$ (amorph) ^c	-699(-712)	—	—	S
FeCO_3 (siderite)	-666.7	-737.0	105	R
Fe_2SiO_4 (fayalite)	-1379.4	-1479.3	148	R

H (Hydrogen)

$\text{H}_2(\text{g})$	0	0	130.6	NBS
$\text{H}_2(\text{aq})$	17.57	-4.18	57.7	NBS
$\text{H}^+(\text{aq})$	0	0	0	NBS
$\text{H}_2\text{O}(\text{l})$	-237.18	-285.83	69.91	NBS
$\text{H}_2\text{O}_2(\text{aq})$	-134.1	-191.1	144	NBS
$\text{HO}_2^-(\text{aq})$	-67.4	-160.3	23.8	NBS
$\text{H}_2\text{O}(\text{g})$	-228.57	-241.8	188.72	R

Hg (Mercury)

$\text{Hg}(\text{l})$	0	0	76.0	NBS
$\text{Hg}_2^{2+}(\text{aq})$	153.6	172.4	84.5	NBS
$\text{Hg}^{2+}(\text{aq})$	164.4	171.0	-32.2	NBS
Hg_2Cl_2 (calomel)	-210.8	265.2	192.4	NBS
HgO (red)	-58.5	-90.8	70.3	NBS
HgS (metacinnabar)	-43.3	-46.7	96.2	NBS
HgI_2 (red)	-101.7	-105.4	180	NBS
$\text{HgCl}^+(\text{aq})$	-5.44	-18.8	75.3	NBS
$\text{HgCl}_2(\text{aq})$	-173.2	-216.3	155	NBS
$\text{HgCl}_3^-(\text{aq})$	-309.2	-388.7	209	NBS
$\text{HgCl}_4^{2-}(\text{aq})$	-446.8	-554.0	293	NBS
$\text{HgOH}^+(\text{aq})$	-52.3	-84.5	71	NBS
$\text{Hg}(\text{OH})_2(\text{aq})$	-274.9	-355.2	142	NBS
$\text{HgO}_2^-(\text{aq})$	-190.3	—	—	NBS

I (Iodine)

I_2 (crystal)	0	0	116	NBS
$\text{I}_2(\text{aq})$	16.4	22.6	137	NBS
$\text{I}^-(\text{aq})$	-51.59	-55.19	111	NBS
$\text{I}_3^-(\text{aq})$	-51.5	-51.5	239	NBS
$\text{HIO}(\text{aq})$	-99.2	-138	95.4	NBS
$\text{IO}^-(\text{aq})$	-38.5	-107.5	-5.4	NBS
$\text{HIO}_3(\text{aq})$	-132.6	-211.3	167	NBS
IO_3^-	-128.0	-221.3	118	NBS

Mg (Magnesium)

Mg (metal)	0	0	32.7	R
$\text{Mg}^{2+}(\text{aq})$	-454.8	-466.8	-138	R
$\text{MgOH}^+(\text{aq})$	-626.8	—	—	S
$\text{Mg}(\text{OH})_2(\text{aq})$	-769.4	-926.8	-149	NBS
$\text{Mg}(\text{OH})_2$ (brucite)	-833.5	-924.5	63.2	R

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Mn (Manganese)

Mn (metal)	0	0	32.0	R
$\text{Mn}^{2+}(\text{aq})$	-228.0	-220.7	-73.6	R
$\text{Mn}(\text{OH})_2$ (precip.)	-616			S
Mn_3O_4 (hausmannite)	-1281			S
MnOOH (manganite)	-557.7			S
MnO_2 (manganate) (IV)				
($\text{MnO}_{1.7} - \text{MnO}_2$)	-453.1			S
MnO_2 (pyrolusite)	-465.1	-520.0	53	R
MnCO_3 (rhodochrosite)	-816.0	-889.3	100	R
MnS (albandite)	-218.1	-213.8	87	R
MnSiO_3 (rhodonite)	-1243	-1319	131	R

N (Nitrogen)

$\text{N}_2(\text{g})$	0	0	191.5	NBS
$\text{N}_2\text{O}(\text{g})$	104.2	82.0	220	NBS
$\text{NH}_3(\text{g})$	-16.48	-46.1	192	NBS
$\text{NH}_3(\text{aq})$	-26.57	-80.29	111	NBS
$\text{NH}_4^+(\text{aq})$	-79.37	-132.5	113.4	NBS
$\text{HNO}_2(\text{aq})$	-42.97	-119.2	153	NBS
$\text{NO}_2^-(\text{aq})$	-37.2	-104.6	140	NBS
$\text{HNO}_3(\text{aq})$	-111.3	-207.3	146.	NBS
$\text{NO}_3^-(\text{aq})$	-111.3	-207.3	146.4	NBS

Ni (Nickel)

$\text{Ni}^{2+}(\text{aq})$	-45.6	-54.0	-129	R
NiO (bunsenite)	-211.6	-239.7	38	R
NiS (millerite)	-86.2	-84.9	66	R

O (Oxygen)

$\text{O}_2(\text{g})$	0	0	205	NBS
$\text{O}_2(\text{aq})$	16.32	-11.71	111	NBS
$\text{O}_3(\text{g})$	163.2	142.7	239	NBS
$\text{OH}^-(\text{aq})$	-157.3	-230.0	-10.75	NBS

P (Phosphorus)

P (α , white)	0	0	41.1	
$\text{PO}_4^{3-}(\text{aq})$	-1018.8	-1277.4	-222	NBS
$\text{HPO}_4^{2-}(\text{aq})$	-1089.3	-1292.1	-33.4	NBS
$\text{H}_2\text{PO}_4^-(\text{aq})$	-1130.4	-1296.3	90.4	NBS
$\text{H}_3\text{PO}_4(\text{aq})$	-1142.6	-1288.3	158	NBS

Pb (Lead)

Pb (metal)	0	0	64.8	NBS
$\text{Pb}^{2+}(\text{aq})$	-24.39	-1.67	10.5	NBS
$\text{PbOH}^+(\text{aq})$	-226.3	—	—	NBS
$\text{Pb}(\text{OH})_3^-(\text{aq})$	-575.7			NBS
$\text{Pb}(\text{OH})_2$ (precip.)	-452.2			NBS
PbO (yellow)	-187.9	-217.3	68.7	NBS

PbO ₂	-217.4	-277.4	68.6	NBS
Pb ₃ O ₄	-601.2	-718.4	211	NBS
PbS	-98.7	-100.4	91.2	NBS
PbSO ₄	-813.2	-920.0	149	NBS
PbCO ₃ (cerussite)	-625.5	-699.1	131	NBS
S (Sulfur)				
S (rhombic)	0	0	31.8	NBS
SO ₂ (g)	-300.2	-296.8	248	NBS
SO ₃ (g)	-371.1	-395.7	257	NBS
H ₂ S(g)	-33.56	-20.63	205.7	NBS
H ₂ S(aq)	-27.87	-39.75	121.3	NBS
S ²⁻ (aq)	85.8	33.0	-14.6	NBS
HS ⁻ (aq)	12.05	-17.6	62.8	NBS
SO ₃ ⁻ (aq)	-486.6	-635.5	-29	NBS
HSO ₃ ⁻ (aq)	-527.8	-626.2	140	NBS
H ₂ SO ₃ [*] (aq)	-537.9	-608.8	232	NBS ^f
SO ₄ ²⁻ (aq)	-744.6	-909.2	20.1	NBS
HSO ₄ ⁻ (aq)	-756.0	-887.3	132	NBS
Se (Selenium)				
Se (black)	0	0	42.4	NBS
SeO ₃ ²⁻ (aq)	-369.9	-509.2	12.6	NBS
HSeO ₃ ⁻ (aq)	-431.5	-514.5	135	NBS
H ₂ SeO ₃ (aq)	-426.2	-507.5	208	NBS
SeO ₄ ²⁻ (aq)	-441.4	-599.1	54.0	NBS
HSeO ₄ ⁻ (aq)	-452.3	-581.6	149	NBS
Si (Silicon)				
Si (metal)	0	0	18.8	NBS
SiO ₂ (α, quartz)	-856.67	-910.94	41.8	NBS
SiO ₂ (α, cristobalite)	-855.88	-909.48	42.7	NBS
SiO ₂ (α, tridymite)	-855.29	-909.06	43.5	NBS
SiO ₂ (amorph)	-850.73	-903.49	46.9	NBS
H ₄ SiO ₄ (aq)	-1316.7	-1468.6	180	NBS
Sr (Strontium)				
Sr ²⁺ (aq)	-559.4	-545.8	-33	R
SrOH ⁺ (aq)	-721	—	—	NBS
SrCO ₃ (strontianite)	-1137.6	-1218.7	97	R
SrSO ₄ (celestite)	-1341.0	-1453.2	118	R
Zn (Zinc)				
Zn, metal	0	0	29.3	NBS
Zn ²⁺ (aq)	-147.0	-153.9	112	NBS
ZnOH ⁺ (aq)	-330.1	—	—	NBS
Zn(OH) ₂ (aq)	-522.3	—	—	NBS
Zn(OH) ₃ ⁻ (aq)	-694.3	—	—	NBS
Zn(OH) ₄ ²⁻ (aq)	-858.7	—	—	NBS

Zn(OH) ₂ (solid β)	-553.2	-641.9	81.2	R
ZnCl ⁺ (aq)	-275.3			NBS
ZnCl ₂ (aq)	-403.8			NBS
ZnCl ₃ ⁻ (aq)	-540.6			S
ZnCl ₄ ²⁻ (aq)	-666.1			NBS
ZnCO ₃ (smithsonite)	-731.6	-812.8	82.4	

^a The quality of the data is highly variable; the authors do not claim to have critically selected the "best" data. For information on precision of the data and for a more complete compendium which includes less common substances, the reader is referred to the references. For research work, the original literature should be consulted.

^b Thermodynamic properties taken from Robie, Hemingway, and Fisher are based on a reference state of the elements in their standard states at 1 bar (10^5 P = 0.987 atm). This change in reference pressure has a negligible effect upon the tabulated values for the condensed phases. [For gas phases only data from NBS (reference state = 1 atm) are given].

^c NBS: D. D. Wagman et al., Selected Values of Chemical Thermodynamic Properties, U.S. National Bureau of Standards, Technical Notes 270-3 (1968), 270-4 (1969), 270-5 (1971). R: R. A. Robie, B. S. Hemingway, and J. R. Fisher, *Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar (10^5 Pascals) Pressure and at Higher Temperatures*, Geological Survey Bulletin No. 1452, Washington D.C., 1978. S: Other sources (e.g., computed from data in *Stability Constants*).

^d $[\text{H}_2\text{CO}_3^*] = \text{CO}_2(\text{aq}) + \text{"true"} [\text{H}_2\text{CO}_3]$.

^e The thermodynamic stability of oxides, hydroxides, or oxyhydroxides of Fe(III) depends on mode of preparation, age, and molar surface. Reported solubility products ($K_{so} = \{\text{Fe}^{3+}\} \{\text{OH}^-\}^3$) range from $10^{-37.3}$ to $10^{-43.7}$. Correspondingly FeOOH may have G_f° values between -452 J mol^{-1} (freshly precipitated amorphous FeOOH) and -489 J mol^{-1} (aged goethite). If the precipitate is written as $\text{Fe}(\text{OH})_3$, its G_f° values vary from -692 to -729 J mol^{-1} . (See also Figure 5.23b).

^f $[\text{H}_2\text{SO}_3^*] = [\text{SO}_2(\text{aq})] + \text{"true"} [\text{H}_2\text{SO}_3]$.