Selected isotope fractionation factor – temperature equations of hydrogeological interest

$$10^3 \ln\alpha = a\,(10^6/T_K^2) + b\,(10^3/T_K) + c$$

Exchange Reaction	a	b	c	$10^3\ln\alpha$		Range (°C)	Reference
^2H							
Water—vapour	24.844	–76.248	52.612	76	@ 25°C	0–100	Majoube (1971)
"	2.408	64.55	–168.7	76	@ 25°C	10–40	Kakiuchi and Matsuo, 1979
Water—ice			19.3	19.3	@ 0°C	0	O'Neil (1968)
"			20.6	20.6	@ 0°C	0	Arnason (1969)
"			20.6	20.6	@ 0°C	0	Suzuoki and Kumura (1973)
Ice—vapour	24.844	–76.248	71.912	127	@ 0°C	0	combined i–w and w–v
Water vapour—H_2	0	467.6	–303.9	949	@ 100°C	80–200	Suess (1949)
"	13	389.61	–204.34	933	@ 100°C	0–700	Bottinga (1969)[1]
Water—H_2				1325	@ 25°C		combined w–v and v–H_2
CH_4—H_2	–8.949	181.264	–90.888	749	@ 100°C	100–600	Horibe and Craig (1975)
"	25	346	–223	1219	@ 25°C	0–700	Bottinga (1969)[1]
Water vapour—CH_4	–7.69	6.1	88.4	22	@ 25°C	10–250	Bottinga (1969)[1]
Water—CH_4				816	@ 25°C	0–100	combined w–v and v–CH_4
Water—H_2S	1	290.498	–127.9	858	@ 25°C	25–200	Galley et al., 1972)
Water—hornblende	0	23.9	–7.9	32	@ 500°C	450–850	Suzuoki and Epstein (1976)
Gypsum—water	0	2.1	-22	–15	@ 25°C	20–60	Fontes and Gonfiantini (1967)
^{18}O							
Water—vapour	1.137	–0.4156	–2.0667	9.3	@ 25°C	0–100	Majoube (1971)
"	1.534	–3.206	2.644	9.1	@ 25°C	0–100	Bottinga and Craig (1969)
"	5.9702	–32.801	52.227	9.4	@ 25°C	10–40	Kakiuchi and Matsuo (1979)
Water—ice			3.1	3.1	@ 0°C	0	O'Neil (1968)
"			2.8	2.8	@ 0°C	0	Suzuoki and Kumura (1973)
Ice—vapour	1.137	–0.4156	1.0333	14.7	@ 0°C	0	Majzoub (1971), O'Neil (1968)
$CO_{2(g)}$—water	–0.0206	17.9942	–19.97	40.1	@ 25°C	0–100	Bottinga (1968)
Calcite—water	2.78	0	–2.89	28.4	@ 25°C	0–500	O'Neil at al. (1969)
CO_2—calcite	–1.8034	10.611	–2.7798	12.5	@ 25°C	0–600	Bottinga (1968)
SO_4—water	3.25	0	–5.10	31.5	@ 25°C	0–500	Lloyd (1968)
"	2.88	0	–3.6	17.1	@ 100°C	110–200	Mitzutani and Rafter (1969)
Anhydrite—water	3.88	0	–2.9	25.0	@ 100°C	100–575	Lloyd (1968)
Gypsum—water	0	2.3	–3.7	4.0	@ 25°C	20–60	Fontes (1965)
$SiO_{2(gel)}$ —water	3.52	0	–4.35	29.4	@ 50°C	34–93	Kita et al.(1985) – (amorphous)
Quartz—water	1.9189	8.582	–18.977	26.0	@ 50°C	0–100	Kawabe (1978)
"	3.55	0	–2.57	13.3	@ 200°C	195–573	Shiro and Sakai (1972)
^{13}C							
$CO_{2(g)}$—$CO_{2(aq)}$	0	0.373	–0.19	1.1	@ 25°C	0–35	Vogel et al. (1970)
HCO_3^-—$CO_{2(g)}$	0	9.552	–24.10	7.9	@ 25°C	5–125	Mook et al. (1974)[2]
HCO_3^-—$CO_{2(aq)}$	0	9.866	–24.12	9.0	@ 25°C	5–125	Mook et al. (1974)
CO_3^{2-}—HCO_3^-	0	–0.867	2.52	–0.4	@ 25°C	5–125	Mook et al. (1974)
CO_3^{2-}—$CO_{2(g)}$	0.87	0	–3.4	6.4	@ 25°C	0–100	Deines et al. (1974)
CO_3^{2-}—$CO_{2(g)}$	0	9.037	–22.73	7.6	@ 25°C	0–100	Thode et al. (1965)
Calcite—HCO_3^-	0	–4.232	15.1	0.9	@ 25°C	0–35	Mook (1986)
$CO_{2(g)}$—calcite	–2.988	7.6663	–2.4612	–10.4	@ 25°C	0–100	Bottinga, (1968)
$CO_{2(g)}$—calcite	–4.3	12.1	–5.5	–4.0	@ 100°C	100–700	Bottinga, (1969)[1]
$CO_{2(g)}$—CH_4	2.28	15.176	–8.38	68.2	@ 25°C	0–700	Bottinga, (1969)[1]
^{34}S							
SO_4^{2-}—$SO_{2(g)}$	–1	9.2667	–7.4213	12.4	@ 25°C	25–1000	Sakai (1968)
SO_4^{2-}—$H_2S_{(aq)}$	3	14.009	–11.197	69.5	@ 25°C	25–1000	Sakai (1968)
SO_4^{2-}—$HS^-_{(aq)}$	3	15.67	–13.592	72.7	@ 25°C	25–1000	Sakai (1968)
SO_4^{2-}—$S^{2-}_{(aq)}$	3	19.359	–15.217	83.5	@ 25°C	25–1000	Sakai (1968)
$H_2S_{(g)}$ —$H_2S_{(aq)}$	0	4.80	–14.765	1.3	@ 25°C	11–30	Szaran (1996)

1 Regressed from values calculated for various temperatures by Bottinga (1969).

2 Modified in Friedman and O'Neil (1977).

3 This table can be down-loaded in spreadsheet format from <**www.science.uottawa.ca/~eih**>

Example: ^2H fractionation between water and vapour using the equation of Majzoub (1971):

$10^3\ln\alpha^2H_{water\text{-}vapour} = 24.844\,(10^6T^{-2}) - 76.248\,(10^3T^{-1}) + 52.612 = 76$ ‰ [for T = 298 K]