

Supplementary Materials

A new look at physico-chemical causes of changing climate: Is strong acid production lowering the surface pH value the real cause of increasing $p\text{CO}_2$ in the Earth's atmosphere?

Ivan R. Kennedy^{1,2}, Angus N. Crossan², Migdat Hodzic³ and Raymond Ritchie⁴

¹School of Life and Environmental Sciences,

²Quick Test Technologies, c/- Sydney Institute of Agriculture
University of Sydney NSW 2006 Australia

³Faculty of Information Technologies, The Dzemal Bijedic University of Mostar
Bosnia and Herzegovina 88000

⁴Prince of Songkla University, Phuket, Thailand

Table S1, Data using CO2TIT1/Cal program for titration of seawater with strong acid and CO_2 at 278.15, 288.15 and 298.15 K.

Table S2 CO2TIT3/Cal program Titrate, I iterations, U -meq acid, A=alkalinity, T=meq alkalinity, P=pH value, K=temperature Kelvin, S=35 ‰;

Table S3. Program Code for CO2TIT1/Cal

Table S4 Program Code for CO2TIT3.

Table S5 Program Code for CO2TIT4

Table S6 Emerson (2012) inorganic carbon chemistry equations

Table S6

Chemical Oceanography and Marine Carbon Cycle

Steven Emerson

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Carbonate Chemistry

Emerson S. and Hedges pp. 101-133

Appendix 4.2 equations were employed in CO₂TIT1, CO₂TIT3, CO₂Tit4 to establish various constants for different temperature and salt concentrations.

TABLE S1: CO2TIT1 Astrocal Titration with strong acid and CO₂ at 278, 288 and 298 K

δmeq strong ac I=10,M=20,U=-66.5,A=2.17,P=8.15,K=278.15,S=35											
Years strong aci	0	10	20	30	40	50	60	70	80	90	100
a	14.802	15.844	16.887	17.93	18.972	20.015	21.057	22.1	23.143	24.185	25.228
b	1896.349	1858.072	1868.334	1773.018	1726.944	1678.879	1629.05	1577.648	1524.837	1470.759	1415.539
c	136.826	122.714	110.083	98.741	88.528	79.31	70.975	63.426	56.582	50.37	44.731
C	2047.976	1996.63	1943.804	1889.688	1834.444	1778.204	1721.082	1663.174	1604.561	1545.315	1485.497
Ac	2170	21035	2037	1970.5	1904	18375	1771	1704.5	1638	1580.376	1505
Ab	2239.945	2173.445	2106.945	2040.445	1973.945	1907.445	1840.945	1774.445	1707.945	1641.445	1574.945
Ksp	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07
K [Ca ²⁺][CO ₃ ²⁻]	2.71E-07	2.43E-07	2.18E-07	1.96E-07	1.75E-07	1.57E-07	1.41E-07	1.26E-07	1.12E-07	9.97E-08	8.86E-08
Ω	0.6287127	0.56387	0.505832	0.453715	0.406786	0.36443	0.32613	0.291443	0.259992	0.231451	0.205537
pH	8.15	8.1158	8.07416	8.03754	8.00155	7.96606	7.93092	7.896	7.8612	7.8264	7.7914
Temperature K	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15
Total pCO ₂ ppm	283.9	303.9	323.9	343.9	363.9	383.9	403.9	423.9	443.9	463.9	483.9
I=10,M=20,U=-66.5,A=2.17,P=8.15,K=288.15,S=35											
Years strong aci	0	10	20	30	40	50	60	70	80	90	100
a	10.767	11.516	12.265	13.014	13.763	14.513	15.262	16.011	16.76	17.509	18.259
b	1785.386	1755.748	1722.675	1686.56	1647.734	1606.481	1563.041	1517.624	1470.313	1421.457	1371.783
c	192.307	173.876	157.163	141.97	128.129	115.51	103.98	93.438	83.794	74.968	66.89
C	1988.46	1941.14	1892.102	1841.544	1789.626	1736.503	1682.282	1627.073	1570.966	1514.404	1456.369
Ac	2170	2103.5	2037	1970.5	1904	1837.5	1771	1704.5	1638	1571.5	1505
Ab	2258.78	2,192	2125.781	2059.281	1992.781	1926.281	1859.781	1793.281	1726.781	1660.281	1593.781
Ksp	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07	4.35E-07
K [Ca ²⁺][CO ₃ ²⁻]	3.81E-07	3.44E-07	3.11E-07	2.81E-07	2.54E-07	2.29E-07	2.06E+00	1.85E-07	1.66E-07	1.48E-07	1.32E-07
Ω	0.8824661	0.79789	0.721195	0.651479	0.587982	0.530056	0.477146	0.428772	0.384518	0.344016	0.306948
pH	8.15	8.11351	8.077884	8.04293	8.00851	7.97448	7.94071	7.9071	7.87351	7.839847	7.80599
Temperature K	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15
Total pCO ₂ ppm	287.4	307.4	327.4	347.4	367.4	387.4	407.4	427.4	447.4	467.4	487.4
I=10,M=20,U=-66.5,A=2.17,P=8.15,K=298.15,S=35											
Years strong aci	0	10	20	30	40	50	60	70	80	90	100
a	8.043	8.611	9.178	9.746	10.314	10.819	11.45	12.018	12.585	13.153	13.721
b	1652.623	1632.145	1607.864	1580.169	1549.388	1515.805	1479.665	1441.118	1400.542	1357.914	1313.444
c	258.688	235.678	214.568	195.165	177.306	160.847	145.668	131.66	118.729	106.793	95.778
C	1919.354	1910.744	1831.61	1785.08	1737.008	1687.534	1636.782	1584.858	1531.856	1477.86	1422.943
Ac	2170	2103.5	2037	1970.5	1904	1837.5	1771	1704.5	1638	1571.5	1505
Ab	2279.415	2277.727	2243.482	2209.867	2176.73	2143.938	2111.367	2078.901	2046.428	2,014	1981.022
Ksp	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07
K [Ca ²⁺][CO ₃ ²⁻]	5.12E-07	4.67E-07	4.25E-07	3.86E-07	3.51E-07	3.18E-07	2.88E-07	2.61E-07	2.35E-07	2.11E-07	1.90E-07
Ω	1.198879	1.092237	0.994404	0.904484	0.821715	0.74544	0.67509	0.61017	0.550244	0.494928	0.443879
pH	8.15	8.11495	8.08071	8.0471	8.01396	7.98117	7.94859	7.91613	7.88366	7.85107	7.818252
Temperature K	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15
Total pCO ₂ ppm	283.28	303.28	323.28	343.28	363.28	383.28	403.28	423.28	443.28	463.276	483.276
I=10,M=20,A=2.17,P=8.15,K=278.15,S=35											
Years CO ₂	0	10	20	30	40	50	60	70	80	90	100
a	14.802	15.844	16.887	17.93	18.97	20.014	21.057	22.1	23.143	24.185	25.228
b	1896.349	1910.52	1923.279	1934.827	1945.332	1954.929	1963.732	1971.837	1979.325	1986.264	1992.711
c	136.826	129.74	123.36	112.334	107.537	103.134	99.081	95.337	91.868	88.644	85.644
C	2047.977	2056.493	2063.526	2070.343	2076.638	2082.479	2087.923	2093.019	2097.805	2102.317	2106.584
Ac	2170	2170	2170	2170	2170	2170	2170	2170	2170	2170	2170
Ab	2239.945	2239.945	2239.945	2239.945	2239.945	2239.945	2239.945	2239.945	2239.945	2239.945	2239.945
Ksp	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07
K [Ca ²⁺][CO ₃ ²⁻]	2.71E-07	2.57E-07	2.44E-07	2.33E-07	2.22E-07	2.13E-07	2.04E-07	1.96E-07	1.89E-07	1.82E-07	1.76E-07
Ω	0.6287127	0.596152	0.56684	0.540309	0.516175	0.494126	0.4739	0.455277	0.438074	0.422133	0.407319
pH	8.15	8.12367	8.09888	8.07547	8.05327	8.03217	8.01207	7.992871	7.97745	7.95687	7.93996
Temperature K	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15	278.15
Total pCO ₂ ppm	283.392	303.932	323.932	343.932	363.931	383.932	403.932	423.932	443.932	463.932	483.932
I=10,M=20,A=2.17,P=8.15,K=288.15,S=35											
Years CO ₂	0	10	20	30	40	50	60	70	80	90	100
a	10.767	11.516	12.265	13.013	13.763	14.513	15.262	16.011	16.76	17.509	18.259
b	1785.386	1803.197	1819.39	1834.179	1847.745	1860.235	1871.775	1882.471	1892.414	1901.682	1910.343
c	192.307	183.401	175.305	167.91	161.128	154.883	149.113	143.765	138.793	134.159	129.828
C	1988.46	1998.115	2006.96	2015.104	2022.636	2029.63	2036.149	2042.247	2047.967	2053.351	2058.43
Ac	2170	2170	2170	2170	2170	2170	2170	2170	2170	2170	2170
Ab	2258.8	2258.781	2258.781	2258.781	2258.781	2258.781	2258.781	2258.781	2258.781	2258.781	2258.781
Ksp	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07	4.31E-07
K [Ca ²⁺][CO ₃ ²⁻]	3.81E-07	3.63E-07	3.47E-07	3.32E-07	3.19E-07	3.07E-07	2.95E-07	2.85E-07	2.75E-07	2.66E-07	2.57E-07
Ω	0.8824661	0.8416	0.804448	0.770514	0.73939	0.710732	0.684255	0.659713	0.6369	0.615634	0.59576
pH	8.15	8.1251	8.10161	8.07937	8.05827	8.03817	8.0189	8.00066	7.98309	7.96622	7.95
Temperature K	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15	288.15
Total pCO ₂ ppm	287.425	307.425	327.425	347.425	367.425	387.425	407.425	427.425	447.425	467.425	487.425
I=10,M=20A=2.17,P=8.15,K=298.15,S=35											
Years CO ₂	0	10	20	30	40	50	60	70	80	90	100
a	8.043	8.611	9.178	9.746	10.314	10.882	11.45	12.018	12.585	13.153	13.721
b	1652.623	1674.1	1693.779	1717.885	1728.607	1744.105	1758.512	1771.943	1784.498	1796.261	1807.308
c	258.688	247.95	238.111	229.058	220.696	212.948	205.744	199.028	192.751	186.869	181.346
C	1919.354	1930.661	1941.068	1950.689	1959.618	1967.934	1975.706	1982.989	1989.834	1996.284	2002.375
Ac	2170	2170	2170	2170	2170	2170	2170	2170	2170	2170	2170
Ab	2279.415	2279.416	2279.416	2279.416	2279.416	2279.416	2279.416	2279.416	2279.416	2279.416	2279.416
Ksp	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07	4.27E-07
K [Ca ²⁺][CO ₃ ²⁻]	5.12E-07	4.91E-07	4.71E-07	4.54E-07	4.37E-07	4.22E-07	4.07E-07	3.94E-07	3.82E-07	3.70E-07	3.59E-07
Ω	1.198879	1.149112	1.103512	1.061556	1.022806	0.986895	0.953511	0.922387	0.893295	0.866037	0.84044
pH	8.15	8.12598	8.10332	8.08187	8.0615	8.0421	8.02357	8.00586	7.98888	7.97257	7.95687
Temperature K	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15
Total pCO ₂ ppm	283.276	303.276	323.276	343.276	363.276	383.276	403.276	423.276	443.276	463.276	483.276

Table S1 **Table 3a** Effect of seawater temperature on long term titration with strong acid

Years	0	10	20	30	40	50	60	70	80	90	100
Initial pH 8.15, T=278.15, Ac=2.17, S=35, +0.0665 mequiv/kg acid											
K [Ca ²⁺][CO ₃ ²⁻]	2.71E-07	2.43E-07	2.18E-07	1.96E-07	1.75E-07	1.57E-07	1.41E-07	1.26E-07	1.12E-07	9.97E-08	8.86E-08
Ω	0.6287127	0.5638697	0.5058321	0.4537154	0.4067861	0.3644304	0.3261298	0.2914431	0.2599921	0.231451	0.2055366
pCO ₂ ppm	283.9	303.9	323.9	343.9	363.9	383.9	403.9	423.9	443.9	463.9	483.9
pH	8.15	8.11158	8.07416	8.03754	8.00155	7.96606	7.93092	7.896	7.8612	7.8264	7.7914
Initial pH 8.15, T=288.15, Ac=2.17, S=35, +0.0665 mequiv/kg acid									$K_{sp} = 4.309 \times 10^{-7}$		
K [Ca ²⁺][CO ₃ ²⁻]	3.81E-07	3.44E-07	3.11E-07	2.81E-07	2.54E-07	2.29E-07	2.06E+00	1.85E-07	1.66E-07	1.48E-07	1.32E-07
Ω	0.8824661	0.7978904	0.7211952	0.6514792	0.5879818	0.5300558	0.477146	0.4287723	0.3845175	0.3440164	0.3069479
pCO ₂ ppm	287.4	307.4	327.4	347.4	367.4	387.4	407.4	427.4	447.4	467.4	487.4
pH	8.15	8.11351	8.077838	8.04293	8.00851	7.97448	7.94071	7.9071	7.87351	7.8398469	7.80599
Initial pH 8.15, T=298.15, Ac=2.17, S=35, + 0.0665 mequiv/kg acid									$K_{sp} = 4.315 \times 10^{-7}$		
K [Ca ²⁺][CO ₃ ²⁻]	5.12E-07	4.67E-07	4.25E-07	3.86E-07	3.51E-07	3.18E-07	2.88E-07	2.61E-07	2.35E-07	2.11E-07	1.90E-07
Ω	1.198879	1.0922366	0.9944039	0.9044844	0.8217151	0.7454395	0.67509	0.6101697	0.5502439	0.4949277	0.4438793
pCO ₂ ppm	283.28	303.28	323.28	343.28	363.28	383.28	403.28	423.28	443.28	463.276	483.276
pH	8.15	8.11495	8.08071	8.0471	8.01396	7.98117	7.94859	7.91613	7.88366	7.85107	7.818252

Table 3b Effect of seawater temperature on long term titration with pCO₂

Years	0	10	20	30	40	50	60	70	80	90	100
Initial pH 8.15, T=278.15, Ac=2.17, S=35, +2 ppm CO ₂											
K [Ca ²⁺][CO ₃ ²⁻]	5.12E-07	4.67E-07	4.25E-07	3.86E-07	3.51E-07	3.18E-07	2.88E-07	2.61E-07	2.35E-07	2.11E-07	1.90E-07
Ω	0.6287127	0.5961523	0.5668404	0.5403085	0.5161751	0.4941258	0.4738995	0.4552774	0.4380744	0.4221332	0.4073189
pCO ₂ ppm	283.276	303.276	323.276	343.276	363.276	383.276	403.276	423.276	443.276	463.276	483.276
pH	8.15	8.11495	8.08071	8.0471	8.01396	7.98117	7.94859	7.91613	7.88366	7.85107	7.818252
Initial pH 8.15, T=288.15, Ac=2.17, S=35									$K_{sp} = 4.309 \times 10^{-7}$		
K [Ca ²⁺][CO ₃ ²⁻]	3.81E-07	3.63E-07	3.47E-07	3.32E-07	3.19E-07	3.07E-07	2.95E-07	2.85E-07	2.75E-07	2.66E-07	2.57E-07
Ω	0.8824661	0.8415998	0.8044478	0.7705144	0.7393898	0.7107323	0.6842546	0.6597128	0.6369	0.6156336	0.59576
pCO ₂ ppm	287.43	307.43	327.43	347.43	367.43	387.43	407.43	427.43	447.43	467.43	487.43
pH	8.15	8.1251	8.10161	8.07937	8.05827	8.03817	8.0189	8.00066	7.98309	7.96622	7.95
Initial pH 8.15, T=298.15, Ac=2.17, S=35									$K_{sp} = 4.315 \times 10^{-7}$		
K [Ca ²⁺][CO ₃ ²⁻]	5.12E-07	4.91E-07	4.71E-07	4.54E-07	4.37E-07	4.22E-07	4.07E-07	3.94E-07	3.82E-07	3.70E-07	3.59E-07
Ω	1.198879	1.1491118	1.1035124	1.0615562	1.0228062	0.9868949	0.9535107	0.9223872	0.8932954	0.866037	0.84044
Total pCO ₂ ppmv	283.276	303.276	323.276	343.276	363.276	383.276	403.276	423.276	443.276	463.276	483.276
pH	8.15	8.12598	8.10332	8.08187	8.0615	8.0421	8.02357	8.00586	7.98888	7.97257	7.956687

Table S2: Astrocal Titrant showing outputs for inputs. CO2TIT3

I=iterations,U=-meq acid, A=alkalinity, T= meq alkalinity, P=pH, K=temperature, S=35

TITRATE	Run 7A	I=11,U=-0.0166,T=0.00001,A=2.32,P=8.18,K=293.15,S=35										CO2TIT3												
Years strong acid + CO2																								
a		9.123	9.447	9.822	10.193	10.568	10.945	11.324	11.705	12.088	12.473	12.861	13.249											
b		1813.696	1814.149	1815.455	1815.789	1815.405	1814.321	1812.577	1810.208	1807.247	1803.725	1799.967	1795.113											
c		253.152	244.59	235.602	227.1	218.957	211.164	203.701	196.551	189.696	183.122	176.814	170.758											
C		2075.971	2068.186	2060.879	2053.082	2044.93	2036.43	2027.602	2018.464	2009.031	1999.32	1989.642	1979.12											
Ac		2320	2303.33	2286.66	2269.99	2253.32	2236.65	2219.98	2203.31	2186.64	2169.97	2153.3	2136.63											
Ab		2424.174	2404.822	2385.253	2365.831	2346.51	2327.288	2308.16	2289.121	2270.168	2251.296	2232.5	2213.779											
Ksp		4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07											
K [Ca ²⁺][CO ₃ ²⁻]		5.01E-07	4.84E-07	4.66E-07	4.50E-07	4.34E-07	4.18E-07	4.03E-07	3.89E-07	3.76E-07	3.63E-07	3.50E-07	3.38E-07											
Ω		1.165668	1.126244	1.084857	1.045709	1.008214	0.97233	0.937966	0.905041	0.873479	0.843208	0.814161	0.786276											
pH		8.18	8.16495	8.14838	8.13233	8.116568	8.10109	8.08588	8.07093	8.05622	8.04175	8.027507	8.013473											
Temperature K		293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15											
Total pCO2 ppmv		281.508	291.508	303.065	314.527	326.086	337.716	349.416	361.182	373.01	384.896	396.838	408.833											
TITRATE Run 7B I=11,U=0.0333,T=0.00001,A=2.32,P=8.18,K=293.15,S=35													CO2TIT3											
Years strong acid + C													0	10	20	30	40	50	60	70	80	90	100	110
a		9.123	9.447	9.911	10.362	10.821	11.283	11.748	12.219	12.692	13.168	13.648	14.131											
b		1813.696	1803.334	1796.251	1787.257	1777.021	1765.56	1752.953	1739.266	1724.564	1708.905	1692.343	1674.932											
c		253.152	241.683	228.574	216.421	204.89	193.97	183.624	173.817	164.518	155.698	147.328	139.384											
C		2075.971	2054.464	2034.736	2014.04	1992.732	1970.813	1948.325	1925.302	1901.774	1877.771	1853.319	1828.447											
Ac		2.32	2286.7	2253.4	2220.1	2186.8	2153.5	2120.2	2089.9	2053.6	2020.3	1987	1953.7											
Ab		2424.174	2387.734	2350.522	2313.578	2276.774	2240.115	2203.592	2167.199	2130.93	2094.777	2058.734	2022.8											
Ksp		4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07											
K [Ca ²⁺][CO ₃ ²⁻]		5.01E-07	4.79E-07	4.53E-07	4.29E-07	4.06E-07	3.84E-07	3.64E-07	3.44E-07	3.26E-07	3.08E-07	2.92E-07	2.76E-07											
Ω		1.165668	1.112856	1.052496	0.996538	0.943438	0.893157	0.845516	0.800359	0.755419	7.17E-01	0.678389	0.64181											
pH		8.18	8.16235	8.13984	8.11883	8.09701	8.07604	8.05534	8.03491	8.014717	7.99E+00	7.975	7.97554											
Temperature K		293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15											
Total pCO2 ppmv		281.508	291.508	305.809	319.755	333.894	348.156	362.54	377.037	391.642	4.06E+02	421.148	436.038											
TITRATE 7C I=11,U=0.0666,T=0.00001,A=2.32,P=8.18,K=293.15,S=35													CO2TIT3											
Years strong acid + C													0	10	20	30	40	50	60	70	80	90	100	110
a		9.123	9.447	10.089	10.704	11.333	11.971	12.617	13.271	13.934	14.602	15.277	15.957											
b		1813.696	1781.61	1757.096	1728.34	1696.855	1662.716	1626.123	1772.607	1719.862	1666.057	1458.48	1411.969											
c		253.152	235.895	214.852	195.93	178.373	162.142	147.138	133.276	120.474	108.658	97.76	87.716											
C		2075.971	2026.952	1982.037	1934.974	1886.561	1836.829	1785.878	1919.154	1854.27	1789.317	1571.517	1515.642											
Ac		2320	2253.4	2186.8	2120.2	2053.6	1987	1920.4	1853.8	1787.2	1720.6	1654	1587.4											
Ab		2424.174	2353.51	2280.986	2208.985	2137.227	2065.723	1994.456	1923.415	1852.585	1781.955	1711.513	1641.249											
Ksp		4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07											
K [Ca ²⁺][CO ₃ ²⁻]		5.01E-07	4.67E-07	4.25E-07	3.88E-07	3.53E-07	3.21E-07	2.91E-07	2.64E-07	2.39E-07	2.15E-07	1.94E-07	1.74E-07											
Ω		1.165668	1.086205	0.98931	0.902181	0.821337	0.7466	0.677515	0.613684	0.554736	0.50033	0.450147	0.403897											
pH		8.18	8.15709	8.12252	8.08965	8.05687	8.02426	7.991755	7.95929	7.9268	7.8942	7.86144	7.828435											
Temperature K		293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15											
Total pCO2 ppmv		281.508	291.508	311.312	330.295	349.708	369.39	389.337	409.527	429.432	450.571	471.394	492.399											
TITRATE 7D I=11,T=0.000005,A=2.32,P=8.18,K=293.15,S=35													CO2TIT3											
Years CO2													0	10	20	30	40	50	60	70	80	90	100	110
a		9.123	9.285	9.428	9.572	9.718	9.863	10.009	10.155	10.302	10.448	10.595	10.742											
b		1813.696	1819.398	1824.303	1829.199	1833.995	1838.705	1843.329	1847.869	1852.328	1856.709	1861.012	1865.239											
c		253.152	250.301	247.848	245.4	243.002	240.648	238.336	236.065	233.836	231.646	229.494	227.38											
C		2075.971	2078.984	2081.579	2084.171	2086.715	2089.216	2091.674	2094.089	2096.466	2098.803	2101.101	2103.361											
Ac		2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320											
Ab		2424.174	2423.049	2422.08	2421.112	2420.164	2419.231	24183.15	2417.414	2416.529	2415.659	2414.804	2413.396											
Ksp		4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07											
K [Ca ²⁺][CO ₃ ²⁻]		5.01E-07	4.96E-07	4.91E-07	4.86E-07	4.81E-07	4.76E+00	4.72E-07	4.67E-07	4.62E+00	4.59E-07	4.54E-07	4.50E-07											
Ω		1.165668	1.152539	1.141246	1.129974	1.108089	1.108089	1.097444	1.08699	1.076723	1.066639	1.056732	1.046999											
pH		8.17372	8.17372	8.16827	8.1628	8.15739	8.15205	8.14677	8.14154	8.13638	8.13126	8.12621	8.1212											
Temperature K		293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15											
Total pCO2 ppmv		281.508	286.508	290.906	295.387	299.868	304.359	308.859	313.368	317.884	322.409	326.942	331.482											

TITRATE 7E		I=11,T=0.00001,A=2.32,P=8.18,K=293.15,S=35										CO2TIT3	
Years CO2	0	10	20	30	40	50	60	70	80	90	100	110	
a	9.123	9.447	9.732	10.024	19.316	10.609	10.903	11.198	11.494	11.791	12.089	12.387	
b	1813.696	1824.968	1834.47	1843.786	1852.753	1861.408	1869.764	1877.835	1885.636	1893.318	1900.474	1907.536	
c	253.152	247.516	242.765	238.107	233.636	229.296	225.118	221.082	217.182	213.411	209.763	206.232	
C	2075.971	2081.931	2086.967	2091.917	2105.705	2101.313	2105.785	2110.115	2114.312	2118.52	2122.326	2126.155	
Ac	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	
Ab	2424.174	2421.941	2420.07	2418.224	2416.444	2414.725	2413.063	2,411	2409.899	2408.392	2406.933	2405.519	
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.90E-07	4.81E-07	4.71E-07	4.63E-07	4.54E-07	4.46E-07	4.38E-07	4.30E-07	4.23E-07	4.15E-07	4.08E-07	
Ω	1.165668	1.139716	1.11784	1.096392	1.075746	1.055819	1.036582	1.017999	1.00004	9.83E-08	0.965877	0.94962	
pH	8.18	8.16753	8.15686	8.14624	8.13588	8.12574	8.11581	8.10608	8.09654	8.09E+00	8.07805	8.06907	
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	
Total pCO2 ppmv	281.508	291.508	300.316	309.309	318.319	327.364	336.44	345.545	354.679	3.64E+02	373.026	382.237	
TITRATE 7F		I=11,T=0.00002,A=2.32,P=8.18,K=293.15,S=35										CO2TIT3	
Years CO2	0	10	20	30	40	50	60	70	80	90	100	110	
a	9.123	9.771	10.344	10.93	11.52	12.113	12.709	13.309	13.911	14.516	15.123	15.732	
b	1813.696	1835.726	1853.587	1870.517	1886.293	1901.053	1914.488	1927.867	1940.076	1951.574	1962.419	1972.665	
c	253.152	242.137	233.206	224.742	216.853	209.473	202.558	196.066	189.962	184.213	178.79	173.668	
C	2075.971	2087.634	2097.137	2106.189	2114.666	2122.639	2129.755	2137.242	2143.949	2150.303	2156.332	2162.065	
Ac	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	2320	
Ab	2424.174	2419.821	2416.279	2412.913	2409.767	2406.817	2404.046	2401.44	2398.983	2396.665	2394.475	2392.402	
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.79E-07	4.62E-07	4.45E-07	4.29E-07	4.15E-07	4.01E-07	3.88E-07	3.76E-07	3.65E-07	3.54E-07	3.44E+00	
Ω	1.165668	1.114946	1.073826	1.034848	0.998526	0.964545	0.932702	0.90281	0.874703	0.848231	0.82326	0.799672	
pH	8.18	8.15543	8.13491	8.1149	8.09574	8.07732	8.05959	8.04251	8.02603	8.01012	7.99473	7.97985	
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	
Total pCO2 ppmv	281.508	301.508	319.176	337.275	355.465	373.769	392.175	410.672	429.254	447.913	466.642	485.436	
TITRATE 7G		I=11,T=0.000005,U=-0.0444,A=2.32,P=8.18,K=293.15,S=35										CO2TIT3	
Years	0	10	20	30	40	50	60	70	80	90	100	110	
a	9.123	9.285	9.664	10.022	10.387	10.755	11.126	11.501	11.88	12.261	12.646	13.034	
b	1813.696	1790.677	1773.971	1755.178	1735.304	1714.295	1692.207	1669.083	1644.965	1619.894	1593.908	1567.046	
c	253.152	242.461	228.615	215.811	203.548	191.852	180.696	170.059	159.917	150.253	141.046	132.277	
C	2075.971	2042.423	2012.25	1981.011	1949.239	1916.902	1884.029	1850.643	1816.762	1782.408	1747.6	1712.357	
Ac	2320	2275.6	2231.2	2186.8	2142.4	2098	2053.6	2009.2	1964.8	1920.4	1876	1831.6	
Ab	2424.174	2377.42	2329.268	2281.39	2233.591	2185.889	2138.28	2090.759	2043.326	1995.977	1948.71	1,901,522	
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.80E-07	4.53E-07	4.27E-07	4.03E-07	3.80E-07	3.58E-07	3.37E-07	3.17E-07	2.98E-07	2.79E-07	2.62E-07	
Ω	1.165668	1.116439	1.052682	0.993726	0.93726	0.883406	0.832037	0.736358	0.736358	0.691858	0.649462	0.609085	
pH	8.18	8.16681	8.14534	8.12493	8.10447	8.08406	8.063679	8.0433	8.02292	8.00252	7.98207	7.96158	
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	
Total pCO2 ppmv	281.508	286.508	298.218	309.252	320.5	331.855	343.322	354.896	366.574	378.35	390.221	402.182	
TITRATE 7H		I=11,T=0.00001,U=-0.0666,L=0.0333,A=2.32,P=8.18,K=293.15,S=35										CO2TIT3	
Years	0	10	20	30	40	50	60	70	80	90	100	110	
a	9.123	9.447	10.089	10.56	11.052	11.545	12.042	12.54	13.04	13.543	14.047	14.552	
b	1813.696	1781.61	1801.635	1815.238	1828.591	1841.144	1853.013	1864.245	1874.889	1884.988	1894.58	1903.703	
c	253.152	235.895	225.882	219.081	212.404	206.128	200.194	194.577	189.255	184.206	179.41	174.849	
C	2075.971	2026.952	2037.606	2044.879	2052.047	2058.817	2065.249	2071.362	2077.184	2082.737	2088.037	2093.104	
Ac	2320	2253.4	2320	2253.4	2253.4	2320	2253.4	2253.4	2320	2253.4	2253.4	2320	
Ab	2424.174	2353.51	2349.422	2346.637	2343.897	2341.316	2338.871	2336.552	2334.35	2333.258	2330.267	2328.37	
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.67E-07	4.47E-07	4.34E-07	4.21E-07	4.08E-07	3.96E-07	3.85E-07	3.75E-07		3.55E-07	3.46E-07	
Ω	1.165668	1.086205	1.040101	1.008785	0.97804	0.94914	0.921814	0.895954	0.871448	0.848198	0.826113	0.80511	
pH	8.18	8.15709	8.13334	8.11685	8.10022	8.08423	8.06875	8.05377	8.03925	8.02518	8.01151	7.99825	
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	
Total pCO2 ppmv	281.508	291.508	311.312	325.841	341.047	356.273	371.579	386.953	402.39	417.885	433.435	449.035	

TITRATE 7I		I=11,T=0.00001,U=-0.0333,,A=2.32,P=8.18,K=293.15,S=35										
Years	0	10	20	30	40	50	60	70	80	90	100	110
a	9.123	9.447	9.911	10.362	10.821	11.283	11.748	12.219	12.692	13.169	13.648	14.131
b	1813.696	1803.334	1796.251	1787.257	1777.021	1765.559	1752.953	1739.266	1724.564	1708.904	1692.343	1674.932
c	253.152	241.683	228.574	216.422	204.89	193.97	183.624	173.817	164.518	155.698	147.328	139.384
C	2075.971	2054.464	2034.736	2014.041	1992.732	1970.812	1948.325	1925.302	1901.774	1877.771	1853.319	1828.447
Ac	2320	2286.7	2253.4	2220.1	2186.8	2153.5	2120.2	2086.9	2053.6	2020.3	1987	1953.7
Ab	2424.174	2387.734	2350.523	2313.578	2276.774	2203.592	2203.592	2167.199	2130.93	2094.777	2058.734	2022.797
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.79E-07	4.53E-07	4.29E-07	4.06E-07	3.84E-07	3.64E-07	3.44E-07	3.26E-07	3.08E-07	2.92E-07	2.76E-07
Ω	1.165668	1.112856	1.052496	0.996538	0.943438	0.893157	0.845516	0.80036	0.757542	0.716928	0.67839	0.64181
pH	8.18	8.16235	8.13984	8.1183	8.09701	8.07604	8.05534	8.03491	8.014717	7.99475	7.97498	7.9554
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15
Total pCO2 ppmv	281.508	291.508	305.81	319.755	333.894	348.156	362.54	377.037	391.642	406.348	421.148	436.038
TITRATE 7J		I=11,U=-0.0333,A=2.32,P=8.18,K=293.15,S=35										
Years	0	10	20	30	40	50	60	70	80	90	100	110
a	9.123	9.123	9.3	9.457	9.618	9.78	9.943	10.107	10.273	10.439	10.607	10.776
b	1813.696	1792.281	1776.767	1760.123	1743.18	1725.85	1708.147	1690.075	1671.637	1652.839	1633.684	1614.177
c	253.152	247.21	238.316	229.989	221.81	213.825	206.027	198.413	190.982	183.731	176.64	169.761
C	2075.971	2048.614	2024.383	1999.569	1974.608	1949.455	1924.117	1898.595	1872.892	1847.009	1821.931	1794.714
Ac	2320	2286.7	2253.4	2220.1	2186.8	2153.5	2120.2	2086.9	2053.6	2020.3	1987	1953.7
Ab	2424.174	2389.95	2354.496	2319.208	2283.919	2248.647	2213.392	2178.152	2142.937	2107.723	2072.532	2037.358
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.89E-07	4.72E-07	4.55E-07	4.39E-07	4.23E-07	4.08E-07	3.93E-07	3.78E-07	3.64E-07	3.50E-07	3.36E-07
Ω	1.165668	1.138304	1.097355	1.059009	1.02135	0.984582	0.948672	0.913614	0.879396	0.846009	0.813442	0.781685
pH	8.18	8.174842	8.16271	8.15135	8.13982	8.12824	8.11658	8.10485	8.09302	8.08113	8.06915	8.05707
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15
Total pCO2 ppmv	281.508	281.508	286.98	291.826	296.789	301.78	306.811	311.879	316.983	322.124	327.301	332.513
TITRATE 7K		I=11,U=-0.0666,A=2.32,P=8.18,K=293.15,S=35										
Years	0	10	20	30	40	50	60	70	80	90	100	110
a	9.123	9.123	9.478	9.795	10.122	10.453	10.789	11.129	11.474	11.823	12.176	12.538
b	1813.696	1770.775	1738.849	1703.964	1667.745	1630.061	1590.963	1550.483	1508.657	1465.52	1421.107	1375.453
c	253.152	241.312	223.976	208.118	192.927	178.469	164.719	151.659	139.272	127.54	116.447	105.974
C	2075.971	2021.21	1972.303	1921.877	1870.794	1818.983	1766.471	1713.271	1659.403	1604.883	1549.73	1493.965
Ac	2320	2253.4	2186.8	2120.2	2053.6	1987	1920.4	1853.8	1787.2	1720.6	1654	1587.4
Ab	2424.174	2355.716	2284.83	2214.303	2143.807	2073.379	2003.016	1932.717	1862.484	1792.315	1722.211	1652.171
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.78E-07	4.43E-07	4.12E-07	3.82E-07	3.53E-07	3.26E-07	3.00E-07	2.76E-07	2.53E-07	2.31E-07	2.10E-07
Ω	1.165668	1.111151	1.031213	0.958304	0.888356	0.821782	0.758466	0.698329	0.641292	0.587273	0.536191	0.487968
pH	8.18	8.1696	8.14512	8.12203	8.09844	8.07454	8.05027	8.02558	8.00045	7.97484	7.94868	7.92193
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15
Total pCO2 ppmv	281.508	281.508	292.46	302.242	312.327	322.544	332.906	343.408	354.048	364.822	375.726	386.756
TITRATE 7L		I=11,U=-0.0666,L=0.0333,A=2.32,P=8.18,K=293.15,S=35										
Years	0	10	20	30	40	50	60	70	80	90	100	110
a	9.123	9.123	9.4779	9.653	9.85	10.044	10.24	10.435	10.632	10.828	11.025	11.223
b	1813.696	1770.775	1782.615	1788.238	1794.38	1800.3	1806.085	1811.731	1817.242	1822.625	1827.882	1833.018
c	253.152	241.312	235.392	232.581	229.51	226.55	223.658	220.835	218.079	215.388	212.759	210.191
C	2075.971	2021.21	2027.485	2030.472	2033.74	2036.894	2039.983	2043.001	2045.953	2048.841	2051.666	2054.432
Ac	2320	2253.4	2320	2253.4	2186.8	2320	2186.8	2253.4	2320	2253.4	2186.8	2253.4
Ab	2424.174	2355.716	2353.305	2352.158	2350.09	2349.695	2348.512	2347.356	2346.226	2345.122	2344.043	2342.988
Ksp	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.30E-07	4.32E-07	4.30E-07	4.30E-07	4.30E-07
K [Ca ²⁺][CO ₃ ²⁻]	5.01E-07	4.78E-07	4.66E-07	4.61E-07	4.54E-07	4.49E-07	4.43E-07	4.37E-07	4.32E-07	4.26E-07	4.21E-07	4.16E-07
Ω	1.165668	1.111151	1.083891	1.070947	1.056806	1.043175	1.029856	1.016859	1.004169	0.991777	0.979673	0.967848
pH	8.18	8.1696	8.15592	8.14933	8.14207	8.135	8.12803	8.12116	8.11438	8.10771	8.10112	8.09463
Temperature K	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15	293.15
Total pCO2 ppmv	281.508	281.508	292.46	297.865	303.928	309.935	315.964	322.006	328.062	334.132	340.214	346.309

Oct 10 2020 TITRATE HN03 or CO2
 CO2TIT1
 Models Mauna Loa ti titration
 Inputs pH, pCO2 T to compute C and A
 Computes pCO2 from A, pH and Kelvin
 Varies H,K1,K2,Kw,Kc with T & salt S
 $C=[CO_2+HCO_3^-+CO_3^{2-}]$ total C mmoles/kg
 $A=[HCO_3^-+2CO_3^{2-}+OH^-+H^++B(OH_4)]^-$
 Alkalinity label
 167 moles CO2/m² dCO2=1=0.4175 m/m²
 Number increments A or pCO2
 To limit CO2, use Khx0.75 at 1353
 Omit M,T for dA; use U for dA

0520	096	LABEL
0521	073	I
0522	107	STO MEM
0523	048	0
0524	048	0
0525	119	print
0526	002	HALT

Margin, say 0.000001 for d(pCO2)

0567	096	LABEL
0568	077	M
0569	107	STO MEM
0570	057	9
0571	057	9
0572	119	print
0573	002	HALT

Input pCO2 trend 0.0000001 1 ppm

0614	096	LABEL
0615	084	T
0616	107	STO MEM
0617	055	7
0618	056	8
0619	119	print
0620	002	HALT

Add strong acid mmoles/kg -0.001

0661	096	LABEL
0662	085	U
0663	107	STO MEM
0664	056	8
0665	057	9
0666	119	print
0667	002	HALT

Alkalinity=[HCO3-]+2[CO32-]+B(OH+OH-)

0708	096	LABEL
0709	065	A
0710	107	STO MEM
0711	048	0
0712	049	1
0713	119	print
0714	002	HALT

Label C[CO2+HCO3-+CO32-] mmol/kg

0755	096	LABEL
0756	067	C
0757	107	STO MEM
0758	048	0
0759	056	8
0760	119	print
0761	002	HALT

Input pH value

0802	096	LABEL
0803	080	F
0804	107	STO MEM
0805	048	0
0806	051	3
0807	119	print
0808	002	HALT

Label pK1o

0849	096	LABEL
0850	078	N
0851	107	STO MEM
0852	048	0
0853	052	4
0854	119	print
0855	002	HALT

Label pK2o

0896	096	LABEL
0897	079	0
0898	107	STO MEM
0899	048	0
0900	053	5
0901	119	print
0902	002	HALT

Label Henry's constant Ho

0943	096	LABEL
0944	072	H
0945	107	STO MEM
0946	048	0
0947	054	6
0948	119	print
0949	002	HALT

Input temperature K

0990	096	LABEL
0991	075	K
0992	107	STO MEM
0993	053	5
0994	055	7
0995	119	print
0996	002	HALT

Input salinity S %o g/kg

1037	096	LABEL
1038	083	S
1039	107	STO MEM
1040	048	0
1041	057	9
1042	119	print
1043	002	HALT

Input pCO2 atmospheres

1084	096	LABEL
1085	090	Z
1086	107	STO MEM
1087	049	1
1088	056	8
1089	119	print
1090	002	HALT

Execute

1131	096	LABEL
1132	088	X
1133	040	(

1134	109	RCL MEM	1272	050	2
1135	053	5	1273	111	+/-
1136	055	7	1274	041)
1137	107	STD MEM	1275	110	LOG e
1138	048	0	1276	042	x
1139	055	7	1277	050	2
Get Bt =total borates			1278	051	3
1180	040	(1279	046	.
1181	048	0	1280	051	3
1182	046	.	1281	053	5
1183	052	4	1282	056	8
1184	049	1	1283	053	5
1185	054	6	1284	041)
1186	042	x	1285	043	+
1187	040	(1286	040	(
1188	109	RCL MEM	1287	109	RCL MEM
1189	048	0	1288	048	0
1190	057	9	1289	057	9
1191	047	/	1290	042	x
1192	051	3	1291	040	(
1193	053	5	1292	048	0
1194	041)	1293	046	.
1195	041)	1294	048	0
1196	119	print	1295	050	2
1197	107	STD MEM	1296	051	3
1198	056	8	1297	053	5
1199	056	8	1298	049	1
Get pK _a Henry's coefficient repC02			1299	055	7
1240	040	(1300	045	-
1241	048	0	1301	040	(
1242	045	-	1302	049	1
1243	054	6	1303	101	EE
1244	048	0	1304	050	2
1245	046	.	1305	111	+/-
1246	050	2	1306	042	x
1247	052	4	1307	109	RCL MEM
1248	048	0	1308	048	0
1249	057	9	1309	055	7
1250	043	+	1310	041)
1251	040	(1311	042	x
1252	057	9	1312	048	0
1253	051	3	1313	046	.
1254	052	4	1314	048	0
1255	053	5	1315	050	2
1256	046	.	1316	051	3
1257	049	1	1317	054	6
1258	055	7	1318	053	5
1259	047	/	1319	054	6
1260	109	RCL MEM	1320	043	+
1261	048	0	1321	040	(
1262	055	7	1322	049	1
1263	041)	1323	101	EE
1264	043	+	1324	050	2
1265	040	(1325	111	+/-
1266	109	RCL MEM	1326	042	x
1267	048	0	1327	109	RCL MEM
1268	055	7	1328	048	0
1269	042	x	1329	055	7
1270	049	1	1330	041)
1271	101	EE	1331	113	Square

1332	042	x
1333	048	0
1334	046	.
1335	048	0
1336	048	0
1337	052	4
1338	055	7
1339	048	0
1340	051	3
1341	054	6
1342	041)
1343	041)
1344	041)
Print lnK'o function;give rate factor		
1385	119	print
1386	064	Inverse
1387	110	LOG e
1388	042	x
1389	049	1
1390	101	EE
1391	051	3
1392	042	x
1393	049	1
1394	046	.
1395	048	0
1396	048	0
Print Ho' mM		
1437	061	=
1438	119	print
1439	107	STD MEM
1440	048	0
1441	054	6
Get pk1'		
1482	040	(
1483	040	(
1484	051	3
1485	054	6
1486	055	7
1487	048	0
1488	046	.
1489	055	7
1490	047	/
1491	109	RCL MEM
1492	048	0
1493	055	7
1494	045	-
1495	054	6
1496	050	2
1497	046	.
1498	048	0
1499	048	0
1500	056	8
1501	043	+
1502	040	(
1503	109	RCL MEM
1504	048	0
1505	055	7
1506	110	LOG e
1507	042	x
1508	057	9

1509	046	.
1510	055	7
1511	057	9
1512	052	4
1513	052	4
1514	041)
1515	045	-
1516	040	(
1517	048	0
1518	046	.
1519	048	0
1520	049	1
1521	049	1
1522	056	8
1523	042	x
1524	109	RCL MEM
1525	048	0
1526	057	9
1527	041)
1528	043	+
1529	040	(
1530	109	RCL MEM
1531	048	0
1532	057	9
1533	113	Square
1534	042	x
1535	048	0
1536	046	.
1537	048	0
1538	048	0
1539	048	0
1540	049	1
1541	049	1
1542	054	6
1543	041)
1544	041)
Print pk1'		
1585	119	print
1586	107	STD MEM
1587	048	0
1588	052	4
Get pk2'		
1629	040	(
1630	040	(
1631	049	1
1632	051	3
1633	057	9
1634	052	4
1635	046	.
1636	055	7
1637	047	/
1638	109	RCL MEM
1639	048	0
1640	055	7
1641	041)
1642	043	+
1643	052	4
1644	046	.
1645	055	7
1646	055	7

1647	055	7	1785	045	-
1648	045	-	1786	040	(
1649	048	0	1787	109	RCL MEM
1650	046	.	1788	048	0
1651	048	0	1789	055	7
1652	049	1	1790	110	LOG e
1653	056	8	1791	042	x
1654	052	4	1792	050	2
1655	042	x	1793	051	3
1656	109	RCL MEM	1794	046	.
1657	048	0	1795	054	6
1658	057	9	1796	053	5
1659	043	+	1797	050	2
1660	040	(1798	049	1
1661	109	RCL MEM	1799	041)
1662	048	0	1800	043	+
1663	057	9	1801	040	(
1664	113	Square	1802	040	(
1665	042	x	1803	040	(
1666	048	0	1804	049	1
1667	046	.	1805	049	1
1668	048	0	1806	056	8
1669	048	0	1807	046	.
1670	048	0	1808	054	6
1671	049	1	1809	055	7
1672	049	1	1810	047	/
1673	056	8	1811	109	RCL MEM
1674	041)	1812	048	0
1675	041)	1813	055	7
Print pk2'			1814	041)
1716	119	print	1815	045	-
1717	107	STD MEM	1816	053	5
1718	048	0	1817	046	.
1719	053	5	1818	057	9
Get water dissociation lnKw			1819	055	7
1760	040	(1820	055	7
1761	049	1	1821	043	+
1762	052	4	1822	040	(
1763	056	8	1823	109	RCL MEM
1764	046	.	1824	048	0
1765	057	9	1825	055	7
1766	054	6	1826	110	LOG e
1767	053	5	1827	042	x
1768	048	0	1828	049	1
1769	050	2	1829	046	.
1770	045	-	1830	048	0
1771	040	(1831	052	4
1772	049	1	1832	057	9
1773	051	3	1833	053	5
1774	056	8	1834	041)
1775	052	4	1835	041)
1776	055	7	1836	042	x
1777	046	.	1837	109	RCL MEM
1778	050	2	1838	048	0
1779	054	6	1839	057	9
1780	047	/	1840	064	Inverse
1781	109	RCL MEM	1841	113	Square
1782	048	0	1842	041)
1783	055	7	1843	041)
1784	041)	1844	045	-

1845	048	0	2022	109	RCL MEM
1846	046	.	2023	048	0
1847	048	0	2024	055	7
1848	049	1	2025	041)
1849	054	6	2026	045	-
1850	049	1	2027	040	(
1851	053	5	2028	109	RCL MEM
1852	042	x	2029	048	0
1853	109	RCL MEM	2030	055	7
1854	048	0	2031	108	LOG 10
1855	057	9	2032	042	x
1856	041)	2033	055	7
Print ln Kw			2034	049	1
1897	119	print	2035	046	.
1898	107	STO MEM	2036	053	5
1899	048	0	2037	057	9
1900	050	2	2038	053	5
1901	064	Inverse	2039	041)
1902	110	LOG e	2040	043	+
Print Kw			2041	040	(
1943	119	print	2042	048	0
1944	107	STO MEM	2043	046	.
1945	054	6	2044	055	7
1946	049	1	2045	055	7
Get calcite pKs for solubility product			2046	055	7
1987	040	(2047	049	1
1988	049	1	2048	050	2
1989	055	7	2049	045	-
1990	049	1	2050	040	(
1991	046	.	2051	048	0
1992	057	9	2052	046	.
1993	048	0	2053	048	0
1994	054	6	2054	048	0
1995	053	5	2055	050	2
1996	043	+	2056	056	8
1997	040	(2057	052	4
1998	048	0	2058	050	2
1999	046	.	2059	054	6
2000	048	0	2060	042	x
2001	055	7	2061	109	RCL MEM
2002	055	7	2062	048	0
2003	057	9	2063	055	7
2004	057	9	2064	041)
2005	051	3	2065	045	-
2006	042	x	2066	040	(
2007	109	RCL MEM	2067	049	1
2008	048	0	2068	055	7
2009	055	7	2069	056	8
2010	041)	2070	046	.
2011	045	-	2071	051	3
2012	040	(2072	052	4
2013	050	2	2073	047	/
2014	056	8	2074	109	RCL MEM
2015	051	3	2075	048	0
2016	057	9	2076	055	7
2017	046	.	2077	041)
2018	051	3	2078	041)
2019	049	1	2079	042	x
2020	057	9	2080	040	(
2021	047	/	2081	109	RCL MEM

2082	048	0	2259	045	-
2083	057	9	2260	056	8
2084	064	Inverse	2261	057	9
2085	113	Square	2262	054	6
2086	041)	2263	054	6
2087	041)	2264	046	.
2088	043	+	2265	057	9
2089	040	(2266	048	0
2090	048	0	2267	045	-
2091	046	.	2268	109	RCL MEM
2092	048	0	2269	048	0
2093	055	7	2270	057	9
2094	055	7	2271	064	Inverse
2095	049	1	2272	113	Square
2096	049	1	2273	042	x
2097	042	x	2274	050	2
2098	109	RCL MEM	2275	056	8
2099	048	0	2276	057	9
2100	057	9	2277	048	0
2101	041)	2278	046	.
2102	045	-	2279	053	5
2103	040	(2280	051	3
2104	048	0	2281	045	-
2105	046	.	2282	109	RCL MEM
2106	048	0	2283	048	0
2107	048	0	2284	057	9
2108	052	4	2285	042	x
2109	049	1	2286	055	7
2110	050	2	2287	055	7
2111	052	4	2288	046	.
2112	057	9	2289	057	9
2113	042	x	2290	052	4
2114	040	(2291	050	2
2115	109	RCL MEM	2292	043	+
2116	048	0	2293	109	RCL MEM
2117	057	9	2294	048	0
2118	091	Exponent	2295	057	9
2119	049	1	2296	091	Exponent
2120	046	.	2297	049	1
2121	053	5	2298	046	.
2122	041)	2299	053	5
2123	041)	2300	042	x
2124	041)	2301	049	1
Print pKs calcite			2302	046	.
2165	119	print	2303	055	7
2166	107	STD MEM	2304	050	2
2167	049	1	2305	056	8
2168	054	6	2306	045	-
2169	111	+/-	2307	109	RCL MEM
2170	064	Inverse	2308	048	0
2171	108	LOG 10	2309	057	9
Print Ks calcite solubility product			2310	113	Square
2212	119	print	2311	042	x
2213	107	STD MEM	2312	048	0
2214	049	1	2313	046	.
2215	055	7	2314	048	0
Get lnKb boric acid			2315	057	9
2256	040	(2316	057	9
2257	040	(2317	054	6
2258	048	0	2318	041)

2319	047	/	2379	056	8
2320	109	RCL MEM	2380	053	5
2321	048	0	2381	043	+
2322	055	7	2382	109	RCL MEM
2323	043	+	2383	048	0
2324	049	1	2384	057	9
2325	052	4	2385	042	x
2326	056	8	2386	048	0
2327	046	.	2387	046	.
2328	048	0	2388	050	2
2329	050	2	2389	052	4
2330	052	4	2390	055	7
2331	056	8	2391	052	4
2332	043	+	2392	041)
2333	109	RCL MEM	2393	042	x
2334	048	0	2394	040	(
2335	057	9	2395	109	RCL MEM
2336	064	Inverse	2396	048	0
2337	113	Square	2397	055	7
2338	042	x	2398	110	LOG e
2339	049	1	2399	041)
2340	051	3	2400	043	+
2341	055	7	2401	109	RCL MEM
2342	046	.	2402	048	0
2343	049	1	2403	055	7
2344	057	9	2404	042	x
2345	052	4	2405	109	RCL MEM
2346	050	2	2406	048	0
2347	043	+	2407	057	9
2348	109	RCL MEM	2408	064	Inverse
2349	048	0	2409	113	Square
2350	057	9	2410	042	x
2351	042	x	2411	048	0
2352	049	1	2412	046	.
2353	046	.	2413	048	0
2354	054	6	2414	053	5
2355	050	2	2415	051	3
2356	049	1	2416	049	1
2357	052	4	2417	048	0
2358	050	2	2418	053	5
2359	045	-	2419	041)
2360	040	(Print lnkb		
2361	050	2	2460	119	print
2362	052	4	2461	047	/
2363	046	.	2462	049	1
2364	052	4	2463	048	0
2365	051	3	2464	110	LOG e
2366	052	4	2465	041)
2367	052	4	2466	111	+/-
2368	043	+	Print pkb		
2369	109	RCL MEM	2507	119	print
2370	048	0	2508	107	STD MEM
2371	057	9	2509	049	1
2372	064	Inverse	2510	057	9
2373	113	Square	Get R= [HCO3-]/[CO2] lnlg(pH-pK1)		
2374	042	x	2551	040	(
2375	050	2	2552	109	RCL MEM
2376	053	5	2553	048	0
2377	046	.	2554	051	3
2378	048	0	2555	045	-

```

2556 109 RCL MEM
2557 048 0
2558 052 4
2559 041 )
2560 119 print
2561 064 Inverse
2562 108 LOG 10
2563 119 print
2564 107 STO MEM
2565 049 1
2566 049 1
Get [C032-]/HC03-]=S
2607 040 (
2608 109 RCL MEM
2609 048 0
2610 051 3
2611 045 -
2612 109 RCL MEM
2613 048 0
2614 053 5
2615 041 )
2616 119 print
2617 064 Inverse
2618 108 LOG 10
Print S
2659 119 print
2660 107 STO MEM
2661 049 1
2662 050 2
Get B(OH)4-
2703 040 (
2704 040 (
2705 049 1
2706 043 +
2707 040 (
2708 040 (
2709 109 RCL MEM
2710 049 1
2711 057 9
2712 045 -
2713 109 RCL MEM
2714 048 0
2715 051 3
2716 041 )
2717 064 Inverse
2718 108 LOG 10
2719 041 )
2720 041 )
2721 114 1/x
2722 042 x
2723 109 RCL MEM
2724 056 8
2725 056 8
2726 041 )
Print B(OH)4-
2767 119 print
2768 107 STO MEM
2769 056 8
2770 055 7
2771 052 4

```

```

Get c from A and pH
c=A/([H+]/K2 +2)
2852 040 (
2853 109 RCL MEM
2854 048 0
2855 049 1
2856 047 /
2857 040 (
2858 040 (
2859 111 +/-
2860 109 RCL MEM
2861 048 0
2862 051 3
2863 111 +/-
2864 064 Inverse
2865 108 LOG 10
2866 047 /
2867 040 (
2868 109 RCL MEM
2869 048 0
2870 053 5
2871 111 +/-
2872 064 Inverse
2873 108 LOG 10
2874 041 )
2875 041 )
2876 043 +
2877 050 2
2878 041 )
2879 041 )
Print and stow c=[C032-]
2920 119 print
2921 107 STO MEM
2922 049 1
2923 053 5
Get b=[HC03-]=c[H+]/K2
2964 040 (
2965 040 (
2966 109 RCL MEM
2967 049 1
2968 053 5
2969 042 x
2970 040 (
2971 109 RCL MEM
2972 048 0
2973 051 3
2974 111 +/-
2975 064 Inverse
2976 108 LOG 10
2977 041 )
2978 041 )
2979 047 /
2980 040 (
2981 109 RCL MEM
2982 048 0
2983 053 5
2984 111 +/-
2985 064 Inverse
2986 108 LOG 10
2987 041 )

```

```

2988 041 )
Print and stow b
3029 119 print
3030 107 STO MEM
3031 049 1
3032 052 4
Get a=[CO2]=b[H+]/K1
3073 040 (
3074 040 (
3075 109 RCL MEM
3076 049 1
3077 052 4
3078 042 x
3079 040 (
3080 109 RCL MEM
3081 048 0
3082 051 3
3083 111 +/-
3084 064 Inverse
3085 108 LOG 10
3086 041 )
3087 041 )
3088 047 /
3089 040 (
3090 109 RCL MEM
3091 048 0
3092 052 4
3093 111 +/-
3094 064 Inverse
3095 108 LOG 10
3096 041 )
3097 041 )
Print and stow a
3138 119 print
3139 107 STO MEM
3140 049 1
3141 051 3
Get pCO2 atm
3182 040 (
3183 109 RCL MEM
3184 049 1
3185 051 3
3186 047 /
3187 109 RCL MEM
3188 048 0
3189 054 6
3190 041 )
Print and stow pCO2
3231 119 print
3232 107 STO MEM
3233 049 1
3234 056 8
Compute [CO2] from pCO2 and H
[CO2] = Ho'xZ
3315 040 (
3316 109 RCL MEM
3317 048 0
3318 054 6
3319 042 x
3320 109 RCL MEM

```

```

3321 049 1
3322 056 8
3323 041 )
Print [CO2] mmoles/kg
3364 119 print
3365 107 STO MEM
3366 049 1
3367 051 3
Compute [HCO3-] = [CO2]xR
3408 040 (
3409 109 RCL MEM
3410 049 1
3411 049 1
3412 042 x
3413 109 RCL MEM
3414 049 1
3415 051 3
3416 041 )
Print HCO3-
3457 119 print
3458 107 STO MEM
3459 049 1
3460 052 4
Compute CO32- = [HCO3-]xS
3501 040 (
3502 109 RCL MEM
3503 049 1
3504 050 2
3505 042 x
3506 109 RCL MEM
3507 049 1
3508 052 4
3509 041 )
Print [CO32-]
3550 119 print
3551 107 STO MEM
3552 049 1
3553 053 5
Get pH
3594 040 (
3595 040 (
3596 109 RCL MEM
3597 048 0
3598 052 4
3599 043 +
3600 040 (
3601 109 RCL MEM
3602 049 1
3603 052 4
3604 047 /
3605 109 RCL MEM
3606 049 1
3607 051 3
3608 041 )
3609 108 LOG 10
3610 041 )
3611 041 )
Print and stow pH
3652 119 print
3653 107 STO MEM

```

```

3654 048 0
3655 051 3
Get CaxCO32-
3696 040 (
3697 040 (
3698 049 1
3699 046 .
3700 057 9
3701 056 8
3702 101 EE
3703 051 3
3704 111 +/-
3705 042 x
3706 109 RCL MEM
3707 049 1
3708 053 5
3709 042 x
3710 049 1
3711 101 EE
3712 051 3
3713 111 +/-
3714 041 )
Print calcite product
3755 119 print
3756 047 /
3757 109 RCL MEM
3758 049 1
3759 055 7
3760 041 )
Print Omega
3801 119 print
Compute C=[CO2]+[HCO3-]+[CO32-]
3842 040 (
3843 109 RCL MEM
3844 049 1
3845 051 3
3846 043 +
3847 109 RCL MEM
3848 049 1
3849 052 4
3850 043 +
3851 109 RCL MEM
3852 049 1
3853 053 5
3854 041 )
Print total carbon C
3895 119 print
3896 107 STD MEM
3897 048 0
3898 056 8
Compute alkalinity including borate
3939 040 (
3940 109 RCL MEM
3941 049 1
3942 052 4
3943 043 +
3944 040 (
3945 050 2
3946 042 x
3947 109 RCL MEM

```

```

3948 049 1
3949 053 5
3950 041 )
3951 043 +
3952 109 RCL MEM
3953 056 8
3954 055 7
3955 043 +
3956 040 (
3957 109 RCL MEM
3958 048 0
3959 050 2
3960 111 +/-
3961 064 Inverse
3962 110 LOG e
Print Kw
4003 119 print
4004 114 1/x
4005 042 x
4006 040 (
4007 109 RCL MEM
4008 048 0
4009 052 4
4010 111 +/-
4011 064 Inverse
4012 108 LOG 10
4013 041 )
4014 041 )
4015 045 -
4016 040 (
4017 109 RCL MEM
4018 048 0
4019 052 4
4020 111 +/-
4021 064 Inverse
4022 108 LOG 10
4023 041 )
4024 041 )
Print alkalinity = Ac+Ab
4065 119 print
4066 107 STD MEM
4067 056 8
4068 051 3
Get new pCO2
4109 096 LABEL
4110 104 Hyperbol
4111 040 (
4112 109 RCL MEM
4113 057 9
4114 057 9
4115 043 +
4116 109 RCL MEM
4117 055 7
4118 056 8
4119 043 +
4120 109 RCL MEM
4121 049 1
4122 056 8
4123 041 )
Print and stow next pCO2

```

```

4164 119 print
4165 107 STO MEM
4166 049 1
4167 056 8
Get new A=[b+2c-U) Titrate strong acid
4208 040 (
4209 109 RCL MEM
4210 048 0
4211 049 1
4212 043 +
4213 109 RCL MEM
4214 056 8
4215 057 9
4216 041 )
4217 119 print
4218 107 STO MEM
4219 048 0
4220 049 1
Get next [CO2] = a using KH
4261 040 (
4262 109 RCL MEM
4263 048 0
4264 054 6
4265 042 x
4266 109 RCL MEM
4267 049 1
4268 056 8
4269 041 )
Print next [CO2] = a
4310 119 print
4311 107 STO MEM
4312 049 1
4313 051 3
Compute z=K2/(K1a)=c/b^2; b=HCO3-, c=CO3
Solve xb^2+b-y=0 equating c's
x=-b+- (b^2-4ac)^0.5/2a x=b
4434 040 (
4435 040 (
4436 109 RCL MEM
4437 048 0
4438 053 5
4439 111 +/-
4440 064 Inverse
4441 108 LOG 10
4442 041 )
4443 047 /
4444 040 (
4445 109 RCL MEM
4446 048 0
4447 052 4
4448 111 +/-
4449 064 Inverse
4450 108 LOG 10
4451 041 )
4452 041 )
4453 047 /
4454 109 RCL MEM
4455 049 1
4456 051 3
4457 041 )

```

```

Print z
4498 119 print
4499 107 STO MEM
4500 057 9
4501 056 8
Get Alkalinity change
4542 040 (
4543 109 RCL MEM
4544 049 1
4545 052 4
4546 043 +
4547 050 2
4548 042 x
4549 109 RCL MEM
4550 049 1
4551 053 5
4552 043 +
4553 109 RCL MEM
4554 056 8
4555 057 9
4556 041 )
4557 119 print
4558 107 STO MEM
4559 055 7
4560 057 9
Solve c=Zb^2=(Ac-b)/2
So 2Zb^2+b-A=0 to solve
4641 040 (
4642 040 (
4643 049 1
4644 043 +
4645 040 (
4646 056 8
4647 042 x
4648 109 RCL MEM
4649 057 9
4650 056 8
4651 042 x
4652 109 RCL MEM
4653 055 7
4654 057 9
4655 041 )
4656 041 )
4657 064 Inverse
4658 113 Square
4659 045 -
4660 049 1
4661 041 )
4662 047 /
4663 040 (
4664 052 4
4665 042 x
4666 109 RCL MEM
4667 057 9
4668 056 8
4669 041 )
4670 041 )
Print and stow b
4711 119 print
4712 107 STO MEM

```

4713	049	1	
4714	052	4	
Compute $y=C-a=b+c$			
4755	040	(
4756	109	RCL MEM	
4757	048	0	
4758	056	8	
4759	045	-	
4760	109	RCL MEM	
4761	049	1	
4762	051	3	
4763	041)	
Print $y=b+c=C-a$			
4804	119	print	
4805	107	STO MEM	
4806	057	9	
4807	055	7	
Compute pH			
4848	040	(
4849	040	(
4850	109	RCL MEM	
4851	048	0	
4852	052	4	
4853	043	+	
4854	040	(
4855	109	RCL MEM	
4856	049	1	
4857	052	4	
4858	047	/	
4859	109	RCL MEM	
4860	049	1	
4861	051	3	
4862	041)	
4863	108	LOG 10	
4864	041)	
4865	041)	
Print and stow pH			
4906	119	print	
4907	107	STO MEM	
4908	048	0	
4909	051	3	
Compute $c=[CO_3^{2-}]$			
4950	040	(
4951	109	RCL MEM	
4952	049	1	
4953	052	4	
4954	113	Square	
4955	042	x	
4956	109	RCL MEM	
4957	057	9	
4958	056	8	
4959	041)	
Print c			
5000	119	print	
5001	107	STO MEM	
5002	049	1	
5003	053	5	
Get new R			
5044	040	(
5045	109	RCL MEM	
5046	048	0	
5047	051	3	
5048	045	-	
5049	109	RCL MEM	
5050	048	0	
5051	052	4	
5052	041)	
5053	119	print	
5054	064	Inverse	
5055	108	LOG 10	
5056	119	print	
5057	107	STO MEM	
5058	049	1	
5059	049	1	
Get new $a = b/R$			
5100	040	(
5101	109	RCL MEM	
5102	049	1	
5103	052	4	
5104	047	/	
5105	109	RCL MEM	
5106	049	1	
5107	049	1	
5108	041)	
5109	119	print	
5110	107	STO MEM	
5111	049	1	
5112	051	3	
Get new pCO_2 atm			
5153	040	(
5154	109	RCL MEM	
5155	049	1	
5156	051	3	
5157	047	/	
5158	109	RCL MEM	
5159	048	0	
5160	054	6	
5161	041)	
Print and stow pCO_2			
5202	119	print	
5203	107	STO MEM	
5204	049	1	
5205	056	8	
Compute $C=a+b+c$			
5246	040	(
5247	109	RCL MEM	
5248	049	1	
5249	051	3	
5250	043	+	
5251	109	RCL MEM	
5252	049	1	
5253	052	4	
5254	043	+	
5255	109	RCL MEM	
5256	049	1	
5257	053	5	
5258	041)	
Print and stow C			
5299	119	print	
5300	107	STO MEM	

```

5301 048 0
5302 056 8
Compute A=b+2c
5343 040 (
5344 109 RCL MEM
5345 049 1
5346 052 4
5347 043 +
5348 040 (
5349 050 2
5350 042 x
5351 109 RCL MEM
5352 049 1
5353 053 5
5354 041 )
5355 041 )
Print alkalinity Ac
5396 119 print
5397 107 STO MEM
5398 048 0
5399 049 1
Compute and print Ac+Ab
Get B(OH)4-
5480 040 (
5481 109 RCL MEM
5482 056 8
5483 055 7
5484 107 STO MEM
5485 056 8
5486 054 6
5487 040 (
5488 049 1
5489 043 +
5490 040 (
5491 040 (
5492 109 RCL MEM
5493 049 1
5494 057 9
5495 045 -
5496 109 RCL MEM
5497 048 0
5498 051 3
5499 041 )
5500 064 Inverse
5501 108 LOG 10
5502 041 )
5503 041 )
5504 114 1/x
5505 042 x
5506 109 RCL MEM
5507 056 8
5508 056 8
5509 041 )
5510 119 print
5511 107 STO MEM
5512 056 8
5513 055 7
5514 041 )
5515 040 (
5516 109 RCL MEM

```

```

5517 056 8
5518 055 7
5519 045 -
5520 109 RCL MEM
5521 056 8
5522 054 6
5523 041 )
5524 117 SUM MEM
5525 056 8
5526 053 5
5527 109 RCL MEM
5528 056 8
5529 053 5
Print extra acid needed
5570 119 print
Get Ab
5611 040 (
5612 109 RCL MEM
5613 048 0
5614 049 1
5615 043 +
5616 109 RCL MEM
5617 056 8
5618 055 7
5619 041 )
5620 119 print
Get [Ca2+][CO32-] product
5661 040 (
5662 049 1
5663 046 .
5664 057 9
5665 056 8
5666 101 EE
5667 051 3
5668 111 +/-
5669 042 x
5670 109 RCL MEM
5671 049 1
5672 053 5
5673 042 x
5674 049 1
5675 101 EE
5676 051 3
5677 111 +/-
5678 041 )
5679 119 print
5680 107 STO MEM
5681 057 9
5682 054 6
5683 040 (
5684 109 RCL MEM
5685 057 9
5686 054 6
5687 047 /
5688 109 RCL MEM
5689 049 1
5690 055 7
5691 041 )
Print Omega solubility
5732 119 print

```

5733	109	RCL	MEM
5734	048	0	
5735	048	0	

5736	039	Dec	JPNZ
5737	104	Hyperbol	
5738	002	HALT	

CO2TIT3/CAL TITRATE with HNO3 or CO2
 28/10/20 pCO2 ex pH and Alkalinity
 Inputs Iterations, Margins, Uacid, A,
 Inputs PH, Kemperature, Salt
 Computes pCO2 from A, pH and Kelvin
 Varies H,K1,K2,Kw,Kc with T & salt S
 $C=[CO_2+HCO_3^-+CO_3^{2-}]$ total C mmoles/kg
 $A=[HCO_3^-+2CO_3^{2-}+OH^-+H^++B(OH)_4^-]$
 Alkalinity label=Ac plus Ab borate
 $167 \text{ moles CO}_2/\text{m}^2 \text{ dCO}_2=1=0.4175 \text{ m}/\text{m}^2$
 I increments with M dpCO2 atm
 To limit CO2 uptake, KawxX @ 1353
 Omit M,T for dA; use U for dA
 Check 5616 change 66600kg/atm 2×10^{-4}
 Iterations

0600	096	LABEL
0601	073	I
0602	107	STO MEM
0603	048	0
0604	048	0
0605	119	print
0606	002	HALT
Margin, atm 0.000001 for d(pCO2)		
0647	096	LABEL
0648	077	M
0649	107	STO MEM
0650	057	9
0651	057	9
0652	119	print
0653	002	HALT
Input pCO2 trend 0.000001, 1 ppm		
0694	096	LABEL
0695	084	T
0696	107	STO MEM
0697	055	7
0698	056	8
0699	119	print
0700	002	HALT
Add strong acid mmoles/kg eg. -0.0033		
0741	096	LABEL
0742	085	U
0743	107	STO MEM
0744	056	8
0745	057	9
0746	119	print
0747	002	HALT
Ac = [a+2b]		
0788	096	LABEL
0789	065	A
0790	107	STO MEM
0791	048	0
0792	049	1
0793	119	print
0794	002	HALT
Liming meq C, dA=2dC mmoles/kg		
0835	096	LABEL
0836	076	L
0837	107	STO MEM
0838	054	6
0839	051	3

0840	119	print
0841	002	HALT
Label C[CO2+HCO3^-+CO3^{2-}] mmol/kg a+b+c		
0882	096	LABEL
0883	067	C
0884	107	STO MEM
0885	048	0
0886	056	8
0887	119	print
0888	002	HALT
Input pH value		
0929	096	LABEL
0930	080	F
0931	107	STO MEM
0932	048	0
0933	051	3
0934	119	print
0935	002	HALT
Label pK1'		
0976	096	LABEL
0977	078	N
0978	107	STO MEM
0979	048	0
0980	052	4
0981	119	print
0982	002	HALT
Label pK2'		
1023	096	LABEL
1024	079	O
1025	107	STO MEM
1026	048	0
1027	053	5
1028	119	print
1029	002	HALT
Label Henry's constant Ho		
1070	096	LABEL
1071	072	H
1072	107	STO MEM
1073	048	0
1074	054	6
1075	119	print
1076	002	HALT
Input temperature K		
1117	096	LABEL
1118	075	K
1119	107	STO MEM
1120	053	5
1121	055	7
1122	119	print
1123	002	HALT
Input salinity S ‰ g/kg		
1164	096	LABEL
1165	083	S
1166	107	STO MEM
1167	048	0
1168	057	9
1169	119	print
1170	002	HALT
Input pCO2 atmospheres		
1211	096	LABEL

Input pCO2 atmospheres			1387	109	RCL MEM
1211	096	LABEL	1388	048	0
1212	090	Z	1389	055	7
1213	107	STD MEM	1390	041)
1214	049	1	1391	043	+
1215	056	8	1392	040	(
1216	119	print	1393	109	RCL MEM
1217	002	HALT	1394	048	0
Execute			1395	055	7
1258	096	LABEL	1396	042	x
1259	088	X	1397	049	1
1260	040	(1398	101	EE
1261	109	RCL MEM	1399	050	2
1262	053	5	1400	111	+/-
1263	055	7	1401	041)
1264	107	STD MEM	1402	110	LOG e
1265	048	0	1403	042	x
1266	055	7	1404	050	2
Get Bt =total borates			1405	051	3
1307	040	(1406	046	.
1308	048	0	1407	051	3
1309	046	.	1408	053	5
1310	052	4	1409	056	8
1311	049	1	1410	053	5
1312	054	6	1411	041)
1313	042	x	1412	043	+
1314	040	(1413	040	(
1315	109	RCL MEM	1414	109	RCL MEM
1316	048	0	1415	048	0
1317	057	9	1416	057	9
1318	047	/	1417	042	x
1319	051	3	1418	040	(
1320	053	5	1419	048	0
1321	041)	1420	046	.
1322	041)	1421	048	0
1323	119	print	1422	050	2
1324	107	STD MEM	1423	051	3
1325	056	8	1424	053	5
1326	056	8	1425	049	1
Get pK _o Henry's coefficient repCO2			1426	055	7
1367	040	(1427	045	-
1368	048	0	1428	040	(
1369	045	-	1429	049	1
1370	054	6	1430	101	EE
1371	048	0	1431	050	2
1372	046	.	1432	111	+/-
1373	050	2	1433	042	x
1374	052	4	1434	109	RCL MEM
1375	048	0	1435	048	0
1376	057	9	1436	055	7
1377	043	+	1437	041)
1378	040	(1438	042	x
1379	057	9	1439	048	0
1380	051	3	1440	046	.
1381	052	4	1441	048	0
1382	053	5	1442	050	2
1383	046	.	1443	051	3
1384	049	1	1444	054	6
1385	055	7	1445	053	5
1386	047	/	1446	054	6

1447	043	+	1624	046	.
1448	040	(1625	048	0
1449	049	1	1626	048	0
1450	101	EE	1627	056	8
1451	050	2	1628	043	+
1452	111	+/-	1629	040	(
1453	042	x	1630	109	RCL MEM
1454	109	RCL MEM	1631	048	0
1455	048	0	1632	055	7
1456	055	7	1633	110	LOG e
1457	041)	1634	042	x
1458	113	Square	1635	057	9
1459	042	x	1636	046	.
1460	048	0	1637	055	7
1461	046	.	1638	057	9
1462	048	0	1639	052	4
1463	048	0	1640	052	4
1464	052	4	1641	041)
1465	055	7	1642	045	-
1466	048	0	1643	040	(
1467	051	3	1644	048	0
1468	054	6	1645	046	.
1469	041)	1646	048	0
1470	041)	1647	049	1
1471	041)	1648	049	1
Print lnK'o function;give rate factor			1649	056	8
1512	119	print	1650	042	x
1513	064	Inverse	1651	109	RCL MEM
1514	110	LOG e	1652	048	0
1515	042	x	1653	057	9
1516	049	1	1654	041)
1517	101	EE	1655	043	+
1518	051	3	1656	040	(
1519	042	x	1657	109	RCL MEM
1520	049	1	1658	048	0
1521	046	.	1659	057	9
1522	048	0	1660	113	Square
1523	048	0	1661	042	x
Print Kaw mM, stow m06			1662	048	0
1564	061	=	1663	046	.
1565	119	print	1664	048	0
1566	107	STD MEM	1665	048	0
1567	048	0	1666	048	0
1568	054	6	1667	049	1
Get pk1'			1668	049	1
1609	040	(1669	054	6
1610	040	(1670	041)
1611	051	3	1671	041)
1612	054	6	Print pk1', stow m04		
1613	055	7	1712	119	print
1614	048	0	1713	107	STD MEM
1615	046	.	1714	048	0
1616	055	7	1715	052	4
1617	047	/	Get pk2'		
1618	109	RCL MEM	1756	040	(
1619	048	0	1757	040	(
1620	055	7	1758	049	1
1621	045	-	1759	051	3
1622	054	6	1760	057	9
1623	050	2	1761	052	4

1762	046	.	1900	051	3
1763	055	7	1901	056	8
1764	047	/	1902	052	4
1765	109	RCL MEM	1903	055	7
1766	048	0	1904	046	.
1767	055	7	1905	050	2
1768	041)	1906	054	6
1769	043	+	1907	047	/
1770	052	4	1908	109	RCL MEM
1771	046	.	1909	048	0
1772	055	7	1910	055	7
1773	055	7	1911	041)
1774	055	7	1912	045	-
1775	045	-	1913	040	(
1776	048	0	1914	109	RCL MEM
1777	046	.	1915	048	0
1778	048	0	1916	055	7
1779	049	1	1917	110	LOG e
1780	056	8	1918	042	x
1781	052	4	1919	050	2
1782	042	x	1920	051	3
1783	109	RCL MEM	1921	046	.
1784	048	0	1922	054	6
1785	057	9	1923	053	5
1786	043	+	1924	050	2
1787	040	(1925	049	1
1788	109	RCL MEM	1926	041)
1789	048	0	1927	043	+
1790	057	9	1928	040	(
1791	113	Square	1929	040	(
1792	042	x	1930	040	(
1793	048	0	1931	049	1
1794	046	.	1932	049	1
1795	048	0	1933	056	8
1796	048	0	1934	046	.
1797	048	0	1935	054	6
1798	049	1	1936	055	7
1799	049	1	1937	047	/
1800	056	8	1938	109	RCL MEM
1801	041)	1939	048	0
1802	041)	1940	055	7
Print pk2', stow m05			1941	041)
1843	119	print	1942	045	-
1844	107	STD MEM	1943	053	5
1845	048	0	1944	046	.
1846	053	5	1945	057	9
Get water dissociation lnKw			1946	055	7
1887	040	(1947	055	7
1888	049	1	1948	043	+
1889	052	4	1949	040	(
1890	056	8	1950	109	RCL MEM
1891	046	.	1951	048	0
1892	057	9	1952	055	7
1893	054	6	1953	110	LOG e
1894	053	5	1954	042	x
1895	048	0	1955	049	1
1896	050	2	1956	046	.
1897	045	-	1957	048	0
1898	040	(1958	052	4
1899	049	1	1959	057	9

1960	053	5	2137	041)
1961	041)	2138	045	-
1962	041)	2139	040	(
1963	042	x	2140	050	2
1964	109	RCL MEM	2141	056	8
1965	048	0	2142	051	3
1966	057	9	2143	057	9
1967	064	Inverse	2144	046	.
1968	113	Square	2145	051	3
1969	041)	2146	049	1
1970	041)	2147	057	9
1971	045	-	2148	047	/
1972	048	0	2149	109	RCL MEM
1973	046	.	2150	048	0
1974	048	0	2151	055	7
1975	049	1	2152	041)
1976	054	6	2153	045	-
1977	049	1	2154	040	(
1978	053	5	2155	109	RCL MEM
1979	042	x	2156	048	0
1980	109	RCL MEM	2157	055	7
1981	048	0	2158	108	LOG 10
1982	057	9	2159	042	x
1983	041)	2160	055	7
Print lnKw, stow m02			2161	049	1
2024	119	print	2162	046	.
2025	107	STD MEM	2163	053	5
2026	048	0	2164	057	9
2027	050	2	2165	053	5
2028	064	Inverse	2166	041)
2029	110	LOG e	2167	043	+
Print Kw			2168	040	(
2070	119	print	2169	048	0
2071	107	STD MEM	2170	046	.
2072	054	6	2171	055	7
2073	049	1	2172	055	7
Get calcite pKs for solubility product			2173	055	7
2114	040	(2174	049	1
2115	049	1	2175	050	2
2116	055	7	2176	045	-
2117	049	1	2177	040	(
2118	046	.	2178	048	0
2119	057	9	2179	046	.
2120	048	0	2180	048	0
2121	054	6	2181	048	0
2122	053	5	2182	050	2
2123	043	+	2183	056	8
2124	040	(2184	052	4
2125	048	0	2185	050	2
2126	046	.	2186	054	6
2127	048	0	2187	042	x
2128	055	7	2188	109	RCL MEM
2129	055	7	2189	048	0
2130	057	9	2190	055	7
2131	057	9	2191	041)
2132	051	3	2192	045	-
2133	042	x	2193	040	(
2134	109	RCL MEM	2194	049	1
2135	048	0	2195	055	7
2136	055	7	2196	056	8

2197	046	.	2296	111	+/-
2198	051	3	2297	064	Inverse
2199	052	4	2298	108	LOG 10
2200	047	/			Print Ks calcite sol. product, sto m17
2201	109	RCL MEM	2339	119	print
2202	048	0	2340	107	STO MEM
2203	055	7	2341	049	1
2204	041)	2342	055	7
2205	041)			Get lnKb boric acid
2206	042	x	2383	040	(
2207	040	(2384	040	(
2208	109	RCL MEM	2385	048	0
2209	048	0	2386	045	-
2210	057	9	2387	056	8
2211	064	Inverse	2388	057	9
2212	113	Square	2389	054	6
2213	041)	2390	054	6
2214	041)	2391	046	.
2215	043	+	2392	057	9
2216	040	(2393	048	0
2217	048	0	2394	045	-
2218	046	.	2395	109	RCL MEM
2219	048	0	2396	048	0
2220	055	7	2397	057	9
2221	055	7	2398	064	Inverse
2222	049	1	2399	113	Square
2223	049	1	2400	042	x
2224	042	x	2401	050	2
2225	109	RCL MEM	2402	056	8
2226	048	0	2403	057	9
2227	057	9	2404	048	0
2228	041)	2405	046	.
2229	045	-	2406	053	5
2230	040	(2407	051	3
2231	048	0	2408	045	-
2232	046	.	2409	109	RCL MEM
2233	048	0	2410	048	0
2234	048	0	2411	057	9
2235	052	4	2412	042	x
2236	049	1	2413	055	7
2237	050	2	2414	055	7
2238	052	4	2415	046	.
2239	057	9	2416	057	9
2240	042	x	2417	052	4
2241	040	(2418	050	2
2242	109	RCL MEM	2419	043	+
2243	048	0	2420	109	RCL MEM
2244	057	9	2421	048	0
2245	091	Exponent	2422	057	9
2246	049	1	2423	091	Exponent
2247	046	.	2424	049	1
2248	053	5	2425	046	.
2249	041)	2426	053	5
2250	041)	2427	042	x
2251	041)	2428	049	1
		Print pKs calcite, stow m16	2429	046	.
2292	119	print	2430	055	7
2293	107	STO MEM	2431	050	2
2294	049	1	2432	056	8
2295	054	6	2433	045	-

2434	109	RCL MEM	2494	052	4
2435	048	0	2495	043	+
2436	057	9	2496	109	RCL MEM
2437	113	Square	2497	048	0
2438	042	x	2498	057	9
2439	048	0	2499	064	Inverse
2440	046	.	2500	113	Square
2441	048	0	2501	042	x
2442	057	9	2502	050	2
2443	057	9	2503	053	5
2444	054	6	2504	046	.
2445	041)	2505	048	0
2446	047	/	2506	056	8
2447	109	RCL MEM	2507	053	5
2448	048	0	2508	043	+
2449	055	7	2509	109	RCL MEM
2450	043	+	2510	048	0
2451	049	1	2511	057	9
2452	052	4	2512	042	x
2453	056	8	2513	048	0
2454	046	.	2514	046	.
2455	048	0	2515	050	2
2456	050	2	2516	052	4
2457	052	4	2517	055	7
2458	056	8	2518	052	4
2459	043	+	2519	041)
2460	109	RCL MEM	2520	042	x
2461	048	0	2521	040	(
2462	057	9	2522	109	RCL MEM
2463	064	Inverse	2523	048	0
2464	113	Square	2524	055	7
2465	042	x	2525	110	LOG e
2466	049	1	2526	041)
2467	051	3	2527	043	+
2468	055	7	2528	109	RCL MEM
2469	046	.	2529	048	0
2470	049	1	2530	055	7
2471	057	9	2531	042	x
2472	052	4	2532	109	RCL MEM
2473	050	2	2533	048	0
2474	043	+	2534	057	9
2475	109	RCL MEM	2535	064	Inverse
2476	048	0	2536	113	Square
2477	057	9	2537	042	x
2478	042	x	2538	048	0
2479	049	1	2539	046	.
2480	046	.	2540	048	0
2481	054	6	2541	053	5
2482	050	2	2542	051	3
2483	049	1	2543	049	1
2484	052	4	2544	048	0
2485	050	2	2545	053	5
2486	045	-	2546	041)
2487	040	(Print Inkb, stow m19		
2488	050	2	2587	119	print
2489	052	4	2588	047	/
2490	046	.	2589	049	1
2491	052	4	2590	048	0
2492	051	3	2591	110	LOG e
2493	052	4	2592	041)

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2593 111 +/-
Print pKb, stow m19
2634 119 print
2635 107 STO MEM
2636 049 1
2637 057 9
Get R= [HCO3-]/[CO2] Inlg(pH-pK1)
2678 040 (
2679 109 RCL MEM
2680 048 0
2681 051 3
2682 045 -
2683 109 RCL MEM
2684 048 0
2685 052 4
2686 041 )
2687 119 print
2688 064 Inverse
2689 108 LOG 10
Print R, stow m11
2730 119 print
2731 107 STO MEM
2732 049 1
2733 049 1
Get [CO32-]/HCO3-]=S
2774 040 (
2775 109 RCL MEM
2776 048 0
2777 051 3
2778 045 -
2779 109 RCL MEM
2780 048 0
2781 053 5
2782 041 )
Print S, stow m12
2823 119 print
2824 064 Inverse
2825 108 LOG 10
Print S
2866 119 print
2867 107 STO MEM
2868 049 1
2869 050 2
Get B(OH)4-
2910 040 (
2911 040 (
2912 049 1
2913 043 +
2914 040 (
2915 040 (
2916 109 RCL MEM
2917 049 1
2918 057 9
2919 045 -
2920 109 RCL MEM
2921 048 0
2922 051 3
2923 041 )
2924 064 Inverse
2925 108 LOG 10

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2926 041 )
2927 041 )
2928 114 1/x
2929 042 x
2930 109 RCL MEM
2931 056 8
2932 056 8
2933 041 )
Print B(OH)4-, stow m87
2974 119 print
2975 107 STO MEM
2976 056 8
2977 055 7
Get c from A and pH
c=A/([H+]/K2 +2)
3058 040 (
3059 109 RCL MEM
3060 048 0
3061 049 1
3062 047 /
3063 040 (
3064 040 (
3065 111 +/-
3066 109 RCL MEM
3067 048 0
3068 051 3
3069 111 +/-
3070 064 Inverse
3071 108 LOG 10
3072 047 /
3073 040 (
3074 109 RCL MEM
3075 048 0
3076 053 5
3077 111 +/-
3078 064 Inverse
3079 108 LOG 10
3080 041 )
3081 041 )
3082 043 +
3083 050 2
3084 041 )
3085 041 )
Print [CO32-]=c, stow m15
3126 119 print
3127 107 STO MEM
3128 049 1
3129 053 5
Get b=[HCO3-]=c[H+]/K2
3170 040 (
3171 040 (
3172 109 RCL MEM
3173 049 1
3174 053 5
3175 042 x
3176 040 (
3177 109 RCL MEM
3178 048 0
3179 051 3
3180 111 +/-

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3183	041)	3438	107	STO MEM
3184	041)	3439	049	1
3185	047	/	3440	056	8
3186	040	(Compute [CO2] from pCO2 and Kaw		
3187	109	RCL MEM	[CO2] = KawxZ		
3188	048	0	3521	040	(
3189	053	5	3522	109	RCL MEM
3190	111	+/-	3523	048	0
3191	064	Inverse	3524	054	6
3192	108	LOG 10	3525	042	x
3193	041)	3526	109	RCL MEM
3194	041)	3527	049	1
Print and stow b, m14			3528	056	8
3235	119	print	3529	041)
3236	107	STO MEM	Print [CO2] mmol/kg		
3237	049	1	3570	119	print
3238	052	4	3571	107	STO MEM
Get a=[CO2]=b[H+]/K1			3572	049	1
3279	040	(3573	051	3
3280	040	(Compute [HCO3-] = [CO2]xR		
3281	109	RCL MEM	3614	040	(
3282	049	1	3615	109	RCL MEM
3283	052	4	3616	049	1
3284	042	x	3617	049	1
3285	040	(3618	042	x
3286	109	RCL MEM	3619	109	RCL MEM
3287	048	0	3620	049	1
3288	051	3	3621	051	3
3289	111	+/-	3622	041)
3290	064	Inverse	Print HCO3- = b		
3291	108	LOG 10	3663	119	print
3292	041)	3664	107	STO MEM
3293	041)	3665	049	1
3294	047	/	3666	052	4
3295	040	(Compute CO32- = [HCO3-]xS		
3296	109	RCL MEM	3707	040	(
3297	048	0	3708	109	RCL MEM
3298	052	4	3709	049	1
3299	111	+/-	3710	050	2
3300	064	Inverse	3711	042	x
3301	108	LOG 10	3712	109	RCL MEM
3302	041)	3713	049	1
3303	041)	3714	052	4
Print and stow a, m13			3715	041)
3344	119	print	Print [CO32-]		
3345	107	STO MEM	3756	119	print
3346	049	1	3757	107	STO MEM
3347	051	3	3758	049	1
Get pCO2 atm			3759	053	5
3388	040	(Get pH		
3389	109	RCL MEM	3800	040	(
3390	049	1	3801	040	(
3391	051	3	3802	109	RCL MEM
3392	047	/	3803	048	0
3393	109	RCL MEM	3804	052	4
3394	048	0	3805	043	+
3395	054	6	3806	040	(
3396	041)	3807	109	RCL MEM
Print and stow pCO2			3808	049	1
3437	119	print	3809	052	4

3808	049	1		4102	107	STO MEM
3809	052	4		4103	048	0
3810	047	/		4104	056	8
3811	109	RCL MEM		Compute	alkalinity	including borate
3812	049	1		4145	040	(
3813	051	3		4146	109	RCL MEM
3814	041)		4147	049	1
3815	108	LOG 10		4148	052	4
3816	041)		4149	043	+
3817	041)		4150	040	(
Print and stow	pH, m03			4151	050	2
3858	119	print		4152	042	x
3859	107	STO MEM		4153	109	RCL MEM
3860	048	0		4154	049	1
3861	051	3		4155	053	5
Get CaxCO32-				4156	041)
3902	040	(4157	043	+
3903	040	(4158	109	RCL MEM
3904	049	1		4159	056	8
3905	046	.		4160	055	7
3906	057	9		4161	043	+
3907	056	8		4162	040	(
3908	101	EE		4163	109	RCL MEM
3909	051	3		4164	048	0
3910	111	+/-		4165	050	2
3911	042	x		4166	111	+/-
3912	109	RCL MEM		4167	064	Inverse
3913	049	1		4168	110	LOG e
3914	053	5		Print Kw		
3915	042	x		4209	119	print
3916	049	1		4210	114	1/x
3917	101	EE		4211	042	x
3918	051	3		4212	040	(
3919	111	+/-		4213	109	RCL MEM
3920	041)		4214	048	0
Print calcite ionic product				4215	052	4
3961	119	print		4216	111	+/-
3962	047	/		4217	064	Inverse
3963	109	RCL MEM		4218	108	LOG 10
3964	049	1		4219	041)
3965	055	7		4220	041)
3966	041)		4221	045	-
Print Omega				4222	040	(
4007	119	print		4223	109	RCL MEM
Compute C=[CO2]+[HCO3-]+[CO32-]				4224	048	0
4048	040	(4225	052	4
4049	109	RCL MEM		4226	111	+/-
4050	049	1		4227	064	Inverse
4051	051	3		4228	108	LOG 10
4052	043	+		4229	041)
4053	109	RCL MEM		4230	041)
4054	049	1		Print alkalinity = Ac+Ab, stow m83		
4055	052	4		4271	119	print
4056	043	+		4272	107	STO MEM
4057	109	RCL MEM		4273	056	8
4058	049	1		4274	051	3
4059	053	5		Get new pCO2		
4060	041)		4315	096	LABEL
Print total carbon C, stow m08				4316	104	Hyperbol
4101	092	Root		4317	040	(

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4318 109 RCL MEM
4319 057 9
4320 057 9
4321 043 +
4322 109 RCL MEM
4323 055 7
4324 056 8
4325 043 +
4326 109 RCL MEM
4327 049 1
4328 056 8
4329 041 )
Print pCO2 atm stow m18
4370 119 print
4371 107 STO MEM
4372 049 1
4373 056 8
Get new A=[b+2c-U), stoq m01 mm/kg
4414 040 (
4415 109 RCL MEM
4416 048 0
4417 049 1
4418 043 +
4419 109 RCL MEM
4420 056 8
4421 057 9
4422 041 )
4423 119 print
4424 107 STO MEM
4425 048 0
4426 049 1
Get next [CO2] = a using Kaw
4467 040 (
4468 109 RCL MEM
4469 048 0
4470 054 6
4471 042 x
4472 109 RCL MEM
4473 049 1
4474 056 8
4475 041 )
Print next [CO2] = a, stow m14
4516 119 print
4517 107 STO MEM
4518 049 1
4519 051 3
Compute z=K2/(K1a)=c/b^2; b=HCO3-, c=CO3
Solve xb^2+b-y=0 equating c's
x=-b+- (b^2-4ac)^0.5/2a x=b
4640 040 (
4641 040 (
4642 109 RCL MEM
4643 049 1
4644 051 3
4645 114 1/x
4646 042 x
4647 040 (
4648 040 (
4649 109 RCL MEM
4650 048 0

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4651 053 5
4652 111 +/-
4653 064 Inverse
4654 108 LOG 10
4655 041 )
4656 047 /
4657 040 (
4658 109 RCL MEM
4659 048 0
4660 052 4
4661 111 +/-
4662 064 Inverse
4663 108 LOG 10
4664 041 )
4665 041 )
4666 041 )
Print z
4707 119 print
4708 107 STO MEM
4709 057 9
4710 056 8
Solve c=Zb^2=(Ac-b)/2
So 2Zb^2+b-A=0 to solve
4791 040 (
4792 040 (
4793 049 1
4794 043 +
4795 040 (
4796 056 8
4797 042 x
4798 109 RCL MEM
4799 057 9
4800 056 8
4801 042 x
4802 109 RCL MEM
4803 048 0
4804 049 1
4805 041 )
4806 041 )
4807 064 Inverse
4808 113 Square
4809 045 -
4810 049 1
4811 041 )
4812 047 /
4813 040 (
4814 052 4
4815 042 x
4816 109 RCL MEM
4817 057 9
4818 056 8
4819 041 )
4820 041 )
Print and stow b, m14
4861 119 print
4862 107 STO MEM
4863 049 1
4864 052 4
Compute y=C-a=b+c
4905 040 (

```

4906	109	RCL MEM	5200	048	0
4907	048	0	5201	052	4
4908	056	8	5202	041)
4909	045	-	5203	119	print
4910	109	RCL MEM	5204	064	Inverse
4911	049	1	5205	108	LOG 10
4912	051	3	5206	119	print
4913	041)	5207	107	STO MEM
Print y=b+c=C-a			5208	049	1
4954	119	print	5209	049	1
4955	107	STO MEM	Get new a = b/R		
4956	057	9	5250	040	(
4957	055	7	5251	109	RCL MEM
Compute pH			5252	049	1
4998	040	(5253	052	4
4999	040	(5254	047	/
5000	109	RCL MEM	5255	109	RCL MEM
5001	048	0	5256	049	1
5002	052	4	5257	049	1
5003	043	+	5258	041)
5004	040	(5259	119	print
5005	109	RCL MEM	5260	107	STO MEM
5006	049	1	5261	049	1
5007	052	4	5262	051	3
5008	047	/	Get new pCO2 atm		
5009	109	RCL MEM	5303	040	(
5010	049	1	5304	109	RCL MEM
5011	051	3	5305	049	1
5012	041)	5306	051	3
5013	108	LOG 10	5307	047	/
5014	041)	5308	109	RCL MEM
5015	041)	5309	048	0
Print and stow pH, m03			5310	054	6
5056	119	print	5311	041)
5057	107	STO MEM	Print and stow pCO2 atm, stow m18		
5058	048	0	5352	119	print
5059	051	3	5353	107	STO MEM
Compute c=[CO32-]			5354	049	1
5100	040	(5355	056	8
5101	109	RCL MEM	Store C and get new C=a+b+c		
5102	049	1	5396	040	(
5103	052	4	5397	109	RCL MEM
5104	113	Square	5398	048	0
5105	042	x	5399	056	8
5106	109	RCL MEM	5400	107	STO MEM
5107	057	9	5401	054	6
5108	056	8	5402	056	8
5109	041)	5403	040	(
Print c, stow m15			5404	109	RCL MEM
5150	119	print	5405	049	1
5151	107	STO MEM	5406	051	3
5152	049	1	5407	043	+
5153	053	5	5408	109	RCL MEM
Get new R			5409	049	1
5194	040	(5410	052	4
5195	109	RCL MEM	5411	043	+
5196	048	0	5412	109	RCL MEM
5197	051	3	5413	049	1
5198	045	-	5414	053	5
5199	109	RCL MEM	5415	041)

Print and stow C, mOB in M

5456 119 print
5457 107 STO MEM
5458 048 0
5459 056 8
5460 040 (
5461 040 (
5462 109 RCL MEM
5463 054 6
5464 056 8
5465 045 -
5466 109 RCL MEM
5467 048 0
5468 056 8
5469 041)

Print dPCO2/period, stow m99

Adjust kg water 33K 10e-44or 66K 2x

5550 119 print
5551 042 x
5552 048 0
5553 046 .
5554 048 0
5555 048 0
5556 048 0
5557 050 2
5558 041)

Print, stow mmoles CO2/per in m99

5599 119 print
5600 107 STO MEM
5601 057 9
5602 057 9
Compute A=b+2c
5643 040 (
5644 109 RCL MEM
5645 049 1
5646 052 4
5647 043 +
5648 040 (
5649 050 2
5650 042 x
5651 109 RCL MEM
5652 049 1
5653 053 5
5654 041)
5655 041)

Print alkalinity Ac, stow m01

5696 119 print
5697 107 STO MEM
5698 048 0
5699 049 1

Compute and print Ac+Ab

Get B(OH)4-
5780 040 (
5781 109 RCL MEM
5782 056 8
5783 055 7
5784 107 STO MEM
5785 056 8
5786 054 6
5787 040 (
5788 049 1
5789 043 +
5790 040 (
5791 040 (
5792 109 RCL MEM
5793 049 1
5794 057 9
5795 045 -
5796 109 RCL MEM
5797 048 0
5798 051 3
5799 041)
5800 064 Inverse
5801 108 LOG 10
5802 041)
5803 041)
5804 114 1/x
5805 042 x
5806 109 RCL MEM
5807 056 8
5808 056 8
5809 041)
Print B(OH)4-, stow 87
5850 119 print
5851 107 STO MEM
5852 056 8
5853 055 7
5854 041)
5855 040 (
5856 109 RCL MEM
5857 056 8
5858 055 7
5859 045 -
5860 109 RCL MEM
5861 056 8
5862 054 6
5863 041)
5864 117 SUM MEM
5865 056 8
5866 053 5
5867 109 RCL MEM
5868 056 8
5869 053 5
Print extra acid needed
5910 119 print
Get Ab
5951 040 (
5952 109 RCL MEM
5953 048 0
5954 049 1
5955 043 +
5956 109 RCL MEM
5957 056 8
5958 055 7
5959 041)
5960 119 print
Get [Ca2+][CO32-] product
6001 040 (
6002 049 1
6003 046 .

6004	057	9	6156	109	RCL MEM
6005	056	8	6157	054	6
6006	101	EE	6158	051	3
6007	051	3	6159	043	+
6008	111	+/-	6160	109	RCL MEM
6009	042	x	6161	048	0
6010	109	RCL MEM	6162	049	1
6011	049	1	6163	041)
6012	053	5	6164	107	STD MEM
6013	042	x	6165	048	0
6014	049	1	6166	049	1
6015	101	EE	6167	109	RCL MEM
6016	051	3	6168	048	0
6017	111	+/-	6169	049	1
6018	041)	6170	119	print
Print product, stow m96			Get new C and print, stow m08		
6059	119	print	6211	040	(
6060	107	STD MEM	6212	109	RCL MEM
6061	057	9	6213	048	0
6062	054	6	6214	056	8
6063	040	(6215	043	+
6064	109	RCL MEM	6216	109	RCL MEM
6065	057	9	6217	054	6
6066	054	6	6218	051	3
6067	047	/	6219	041)
6068	109	RCL MEM	6220	119	print
6069	049	1	6221	107	STD MEM
6070	055	7	6222	048	0
6071	041)	6223	056	8
Print Omega solubility			6224	109	RCL MEM
6112	119	print	6225	048	0
Dissolve calcite following acid pulse			6226	048	0
6153	040	(6227	039	Dec JPNZ
6154	050	2	6228	104	Hyperbol
6155	042	x	6229	002	HALT

Oct 10 2020 TITRATE HNO3 or CO2
 Revised Jun20 2023 KPSZ inputs
 CO2TIT4:2
 Models Mauna Loa ti titration
 Inputs pH, pCO2 K to compute C,A Flg1
 Computes pCO2 ex A, PH, K Flg2
 Varies H,K1,K2,Kw,Kc with T & salt S
 $C=[CO_2+HCO_3^-+CO_3^{2-}]$ total C mmoles/kg
 $A=[HCO_3^-+2CO_3^{2-}+OH^-+H^++B(OH_4)^-]$
 Alkalinity label
 167 moles CO2/m² dCO2=1=0.4175 m/m²
 Number increments A or pCO2
 To limit CO2, use Khx0.75 at 1353
 Omit M,T for dA; use U for dA

0560	096	LABEL
0561	073	I
0562	107	STD MEM
0563	048	0
0564	048	0
0565	119	print
0566	002	HALT

Margin, say 0.000001 for d(pCO2)

0607	096	LABEL
0608	077	M
0609	107	STD MEM
0610	057	9
0611	057	9
0612	119	print
0613	002	HALT

Input pCO2 trend 0.0000001 1 ppm

0654	096	LABEL
0655	084	T
0656	107	STD MEM
0657	055	7
0658	056	8
0659	119	print
0660	002	HALT

Add strong acid mmoles/kg -0.001

0701	096	LABEL
0702	085	U
0703	107	STD MEM
0704	056	8
0705	057	9
0706	119	print
0707	002	HALT

Alkalinity= $[HCO_3^-]+2[CO_3^{2-}]+B(OH+OH^-)$

0748	096	LABEL
0749	065	A
0750	107	STD MEM
0751	048	0
0752	049	1
0753	119	print
0754	002	HALT

Label $C[CO_2+HCO_3^-+CO_3^{2-}]$ mmol/kg

0795	096	LABEL
0796	067	C
0797	107	STD MEM
0798	048	0
0799	056	8
0800	119	print

0801	002	HALT
------	-----	------

Input pH value

0842	096	LABEL
0843	080	P
0844	107	STD MEM
0845	048	0
0846	051	3
0847	119	print
0848	002	HALT

Label pK1o

0889	096	LABEL
0890	078	N
0891	107	STD MEM
0892	048	0
0893	052	4
0894	119	print
0895	002	HALT

Label pK2o

0936	096	LABEL
0937	079	D
0938	107	STD MEM
0939	048	0
0940	053	5
0941	119	print
0942	002	HALT

Label Henry's constant Ho

0983	096	LABEL
0984	072	H
0985	107	STD MEM
0986	048	0
0987	054	6
0988	119	print
0989	002	HALT

Input temperature K

1030	096	LABEL
1031	075	K
1032	107	STD MEM
1033	053	5
1034	055	7
1035	119	print
1036	002	HALT

Input salinity S ‰ g/kg

1077	096	LABEL
1078	083	S
1079	107	STD MEM
1080	048	0
1081	057	9
1082	119	print
1083	002	HALT

Input pCO2 atmospheres

1124	096	LABEL
1125	090	Z
1126	107	STD MEM
1127	049	1
1128	056	8
1129	119	print
1130	002	HALT

Execute

1171	096	LABEL
1172	088	X

1173	040	(1311	101	EE
1174	109	RCL MEM	1312	050	2
1175	053	5	1313	111	+/-
1176	055	7	1314	041)
1177	107	STD MEM	1315	110	LOG e
1178	048	0	1316	042	x
1179	055	7	1317	050	2
Get Bt =total borates			1318	051	3
1220	040	(1319	046	.
1221	048	0	1320	051	3
1222	046	.	1321	053	5
1223	052	4	1322	056	8
1224	049	1	1323	053	5
1225	054	6	1324	041)
1226	042	x	1325	043	+
1227	040	(1326	040	(
1228	109	RCL MEM	1327	109	RCL MEM
1229	048	0	1328	048	0
1230	057	9	1329	057	9
1231	047	/	1330	042	x
1232	051	3	1331	040	(
1233	053	5	1332	048	0
1234	041)	1333	046	.
1235	041)	1334	048	0
1236	119	print	1335	050	2
1237	107	STD MEM	1336	051	3
1238	056	8	1337	053	5
1239	056	8	1338	049	1
Get pKo Henry's coefficient repCO2			1339	055	7
1280	040	(1340	045	-
1281	048	0	1341	040	(
1282	045	-	1342	049	1
1283	054	6	1343	101	EE
1284	048	0	1344	050	2
1285	046	.	1345	111	+/-
1286	050	2	1346	042	x
1287	052	4	1347	109	RCL MEM
1288	048	0	1348	048	0
1289	057	9	1349	055	7
1290	043	+	1350	041)
1291	040	(1351	042	x
1292	057	9	1352	048	0
1293	051	3	1353	046	.
1294	052	4	1354	048	0
1295	053	5	1355	050	2
1296	046	.	1356	051	3
1297	049	1	1357	054	6
1298	055	7	1358	053	5
1299	047	/	1359	054	6
1300	109	RCL MEM	1360	043	+
1301	048	0	1361	040	(
1302	055	7	1362	049	1
1303	041)	1363	101	EE
1304	043	+	1364	050	2
1305	040	(1365	111	+/-
1306	109	RCL MEM	1366	042	x
1307	048	0	1367	109	RCL MEM
1308	055	7	1368	048	0
1309	042	x	1369	055	7
1310	049	1	1370	041)

1371	113	Square	1548	057	9
1372	042	x	1549	046	.
1373	048	0	1550	055	7
1374	046	.	1551	057	9
1375	048	0	1552	052	4
1376	048	0	1553	052	4
1377	052	4	1554	041)
1378	055	7	1555	045	-
1379	048	0	1556	040	(
1380	051	3	1557	048	0
1381	054	6	1558	046	.
1382	041)	1559	048	0
1383	041)	1560	049	1
1384	041)	1561	049	1
Print lnK'o function;give rate factor			1562	056	8
1425	119	print	1563	042	x
1426	064	Inverse	1564	109	RCL MEM
1427	110	LOG e	1565	048	0
1428	042	x	1566	057	9
1429	049	1	1567	041)
1430	101	EE	1568	043	+
1431	051	3	1569	040	(
1432	042	x	1570	109	RCL MEM
1433	049	1	1571	048	0
1434	046	.	1572	057	9
1435	048	0	1573	113	Square
1436	048	0	1574	042	x
Print Ho' mM			1575	048	0
1477	061	=	1576	046	.
1478	119	print	1577	048	0
1479	107	STD MEM	1578	048	0
1480	048	0	1579	048	0
1481	054	6	1580	049	1
Get pk1'			1581	049	1
1522	040	(1582	054	6
1523	040	(1583	041)
1524	051	3	1584	041)
1525	054	6	Print pk1'		
1526	055	7	1625	119	print
1527	048	0	1626	107	STD MEM
1528	046	.	1627	048	0
1529	055	7	1628	052	4
1530	047	/	Get pk2'		
1531	109	RCL MEM	1669	040	(
1532	048	0	1670	040	(
1533	055	7	1671	049	1
1534	045	-	1672	051	3
1535	054	6	1673	057	9
1536	050	2	1674	052	4
1537	046	.	1675	046	.
1538	048	0	1676	055	7
1539	048	0	1677	047	/
1540	056	8	1678	109	RCL MEM
1541	043	+	1679	048	0
1542	040	(1680	055	7
1543	109	RCL MEM	1681	041)
1544	048	0	1682	043	+
1545	055	7	1683	052	4
1546	110	LOG e	1684	046	.
1547	042	x	1685	055	7

1884	045	-	2061	047	/
1885	048	0	2062	109	RCL MEM
1886	046	.	2063	048	0
1887	048	0	2064	055	7
1888	049	1	2065	041)
1889	054	6	2066	045	-
1890	049	1	2067	040	(
1891	053	5	2068	109	RCL MEM
1892	042	x	2069	048	0
1893	109	RCL MEM	2070	055	7
1894	048	0	2071	108	LOG 10
1895	057	9	2072	042	x
1896	041)	2073	055	7
Print ln Kw			2074	049	1
1937	119	print	2075	046	.
1938	107	STD MEM	2076	053	5
1939	048	0	2077	057	9
1940	050	2	2078	053	5
1941	064	Inverse	2079	041)
1942	110	LOG e	2080	043	+
Print Kw			2081	040	(
1983	119	print	2082	048	0
1984	107	STD MEM	2083	046	.
1985	054	6	2084	055	7
1986	049	1	2085	055	7
Get calcite pKs for solubility product			2086	055	7
2027	040	(2087	049	1
2028	049	1	2088	050	2
2029	055	7	2089	045	-
2030	049	1	2090	040	(
2031	046	.	2091	048	0
2032	057	9	2092	046	.
2033	048	0	2093	048	0
2034	054	6	2094	048	0
2035	053	5	2095	050	2
2036	043	+	2096	056	8
2037	040	(2097	052	4
2038	048	0	2098	050	2
2039	046	.	2099	054	6
2040	048	0	2100	042	x
2041	055	7	2101	109	RCL MEM
2042	055	7	2102	048	0
2043	057	9	2103	055	7
2044	057	9	2104	041)
2045	051	3	2105	045	-
2046	042	x	2106	040	(
2047	109	RCL MEM	2107	049	1
2048	048	0	2108	055	7
2049	055	7	2109	056	8
2050	041)	2110	046	.
2051	045	-	2111	051	3
2052	040	(2112	052	4
2053	050	2	2113	047	/
2054	056	8	2114	109	RCL MEM
2055	051	3	2115	048	0
2056	057	9	2116	055	7
2057	046	.	2117	041)
2058	051	3	2118	041)
2059	049	1	2119	042	x
2060	057	9	2120	040	(

2121	109	RCL MEM	2298	048	0
2122	048	0	2299	045	-
2123	057	9	2300	056	8
2124	064	Inverse	2301	057	9
2125	113	Square	2302	054	6
2126	041)	2303	054	6
2127	041)	2304	046	.
2128	043	+	2305	057	9
2129	040	(2306	048	0
2130	048	0	2307	045	-
2131	046	.	2308	109	RCL MEM
2132	048	0	2309	048	0
2133	055	7	2310	057	9
2134	055	7	2311	064	Inverse
2135	049	1	2312	113	Square
2136	049	1	2313	042	x
2137	042	x	2314	050	2
2138	109	RCL MEM	2315	056	8
2139	048	0	2316	057	9
2140	057	9	2317	048	0
2141	041)	2318	046	.
2142	045	-	2319	053	5
2143	040	(2320	051	3
2144	048	0	2321	045	-
2145	046	.	2322	109	RCL MEM
2146	048	0	2323	048	0
2147	048	0	2324	057	9
2148	052	4	2325	042	x
2149	049	1	2326	055	7
2150	050	2	2327	055	7
2151	052	4	2328	046	.
2152	057	9	2329	057	9
2153	042	x	2330	052	4
2154	040	(2331	050	2
2155	109	RCL MEM	2332	043	+
2156	048	0	2333	109	RCL MEM
2157	057	9	2334	048	0
2158	091	Exponent	2335	057	9
2159	049	1	2336	091	Exponent
2160	046	.	2337	049	1
2161	053	5	2338	046	.
2162	041)	2339	053	5
2163	041)	2340	042	x
2164	041)	2341	049	1
Print pKs calcite			2342	046	.
2205	119	print	2343	055	7
2206	107	STO MEM	2344	050	2
2207	049	1	2345	056	8
2208	054	6	2346	045	-
2209	111	+/-	2347	109	RCL MEM
2210	064	Inverse	2348	048	0
2211	108	LOG 10	2349	057	9
Print Ks calcite solubility product			2350	113	Square
2252	119	print	2351	042	x
2253	107	STO MEM	2352	048	0
2254	049	1	2353	046	.
2255	055	7	2354	048	0
Get lnKb boric acid			2355	057	9
2296	040	(2356	057	9
2297	040	(2357	054	6

2358	041)	2418	048	0
2359	047	/	2419	056	8
2360	109	RCL MEM	2420	053	5
2361	048	0	2421	043	+
2362	055	7	2422	109	RCL MEM
2363	043	+	2423	048	0
2364	049	1	2424	057	9
2365	052	4	2425	042	x
2366	056	8	2426	048	0
2367	046	.	2427	046	.
2368	048	0	2428	050	2
2369	050	2	2429	052	4
2370	052	4	2430	055	7
2371	056	8	2431	052	4
2372	043	+	2432	041)
2373	109	RCL MEM	2433	042	x
2374	048	0	2434	040	(
2375	057	9	2435	109	RCL MEM
2376	064	Inverse	2436	048	0
2377	113	Square	2437	055	7
2378	042	x	2438	110	LOG e
2379	049	1	2439	041)
2380	051	3	2440	043	+
2381	055	7	2441	109	RCL MEM
2382	046	.	2442	048	0
2383	049	1	2443	055	7
2384	057	9	2444	042	x
2385	052	4	2445	109	RCL MEM
2386	050	2	2446	048	0
2387	043	+	2447	057	9
2388	109	RCL MEM	2448	064	Inverse
2389	048	0	2449	113	Square
2390	057	9	2450	042	x
2391	042	x	2451	048	0
2392	049	1	2452	046	.
2393	046	.	2453	048	0
2394	054	6	2454	053	5
2395	050	2	2455	051	3
2396	049	1	2456	049	1
2397	052	4	2457	048	0
2398	050	2	2458	053	5
2399	045	-	2459	041)
2400	040	(Print lnkb		
2401	050	2	2500	119	print
2402	052	4	2501	047	/
2403	046	.	2502	049	1
2404	052	4	2503	048	0
2405	051	3	2504	110	LOG e
2406	052	4	2505	041)
2407	052	4	2506	111	+/-
2408	043	+	Print pKb		
2409	109	RCL MEM	2547	119	print
2410	048	0	2548	107	STO MEM
2411	057	9	2549	049	1
2412	064	Inverse	2550	057	9
2413	113	Square	Get R= [HCO3-]/[CO2] lnlg (pH-pK1)		
2414	042	x	2591	040	(
2415	050	2	2592	109	RCL MEM
2416	053	5	2593	048	0
2417	046	.	2594	051	3

2595	045	-	Get [C02]=a = m18xm06
2596	109	RCL MEM	2851 040 (
2597	048	0	2852 109 RCL MEM
2598	052	4	2853 049 1
2599	041)	2854 056 8
2600	119	print	2855 042 x
2601	064	Inverse	2856 109 RCL MEM
2602	108	LOG 10	2857 048 0
2603	119	print	2858 054 6
2604	107	STD MEM	2859 041)
2605	049	1	Print a
2606	049	1	2900 119 print
Get [C032-]/HC03-]=S			2901 107 STD MEM
2647	040	(2902 052 4
2648	109	RCL MEM	2903 048 0
2649	048	0	Get [HC03-]=b=Rxa=m11xm40
2650	051	3	2944 040 (
2651	045	-	2945 109 RCL MEM
2652	109	RCL MEM	2946 049 1
2653	048	0	2947 049 1
2654	053	5	2948 042 x
2655	041)	2949 109 RCL MEM
2656	119	print	2950 052 4
2657	064	Inverse	2951 048 0
2658	108	LOG 10	2952 041)
Print S			Print b stow m41
2699	119	print	2993 119 print
2700	107	STD MEM	2994 107 STD MEM
2701	049	1	2995 052 4
2702	050	2	2996 049 1
Get B(OH)4-			Get c=bxS=m41xm12
2743	040	(3037 040 (
2744	040	(3038 109 RCL MEM
2745	049	1	3039 052 4
2746	043	+	3040 049 1
2747	040	(3041 042 x
2748	040	(3042 109 RCL MEM
2749	109	RCL MEM	3043 049 1
2750	049	1	3044 050 2
2751	057	9	3045 041)
2752	045	-	Print c stow m42
2753	109	RCL MEM	3086 119 print
2754	048	0	3087 107 STD MEM
2755	051	3	3088 052 4
2756	041)	3089 050 2
2757	064	Inverse	Get a+b+c=C
2758	108	LOG 10	3130 040 (
2759	041)	3131 109 RCL MEM
2760	041)	3132 052 4
2761	114	1/x	3133 048 0
2762	042	x	3134 043 +
2763	109	RCL MEM	3135 109 RCL MEM
2764	056	8	3136 052 4
2765	056	8	3137 049 1
2766	041)	3138 043 +
Print B(OH)4-			3139 109 RCL MEM
2807	119	print	3140 052 4
2808	107	STD MEM	3141 050 2
2809	056	8	3142 041)
2810	055	7	Print C stow m08

```

3142 041 )
Print C stow m08
3183 119 print
3184 107 STO MEM
3185 048 0
3186 056 8
Get A=b+2c
3227 040 (
3228 109 RCL MEM
3229 052 4
3230 049 1
3231 043 +
3232 109 RCL MEM
3233 052 4
3234 050 2
3235 043 +
3236 109 RCL MEM
3237 052 4
3238 050 2
3239 041 )

```

```

Print A stow m01
3280 119 print
3281 107 STO MEM
3282 048 0
3283 049 1
Get b/c
3324 040 (
3325 109 RCL MEM
3326 052 4
3327 049 1
3328 047 /
3329 109 RCL MEM
3330 052 4
3331 050 2
3332 041 )
3333 119 print
3334 107 STO MEM
3335 052 4
3336 053 5
3337 002 HALT

```

Table S6

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Appendix 4.2 equations were employed in CO2TIT1, CO2TIT3, CO2Tit4 to establish various constants for different temperature and salt concentrations.

$$K_{p,3} = \frac{[\text{PO}_4^{3-}] \times [\text{H}^+]}{[\text{HPO}_4^{2-}]} \quad (4A1.6)$$

$$K_w = [\text{OH}^-] [\text{H}^+] \quad (4A1.7)$$

4A1.2

The following Matlab function program finds the root of the cubic equation for $[\text{H}^+]$ in terms of $A_{\text{C\&B}}$ and DIC resulting from the combination of the equations in 4A1.1 (a) and (b) above (Zeebe and Wolf-Gladrow, 2000). Input values are temperature, salinity, depth, $A_{\text{C\&B}}$ and DIC and the outputs are f_{CO_2} , pH, $[\text{CO}_2]$, $[\text{HCO}_3^-]$ and $[\text{CO}_3^{2-}]$. Units and equilibrium constants used are indicated in the comment statements, which are preceded by a % sign.

```
function [fco2, pH, co2, hco3, co3] = co3eq(temp, s, z, alk, dic)
% Function to calculate fCO2, HCO3, and CO3 from ALK and DIC as a
% f(temp,sal,Z)
% temp = temp(deg C),
% sal = salinity(ppt), depth = z(m), alk = ALK(microeq/kg),
% dic = DIC(micromol kg-1)
% HCO3, CO3, and CO2 are returned in mol kg-1, fCO2 in atm
% This program uses the equations in Zeebe and Wolf-Gladrow (2000) and
% Matlab's root finding routine
% checked for fCO2 against Luecker et al. (2000), May 2002;
% Depth dependence has not been checked
t = temp + 273.15;
Pr = z/10;
alk = alk * .000001;
dic = dic * .000001;
R = 83.131;
% Calculate total borate (tbor) from chlorinity
tbor = .000416 * s / 35.0;
% Calculate Henry's Law coeff, KH (Weiss, 1974)
U1 = -60.2409 + 93.4517 * (100/t) + 23.3585 * log(t/100);
U2 = s * (.023517 - .023656 * (t/100) + .0047036 * (t/100) ^ 2);
KH = exp(U1 + U2);
% Calculate KB from temp & sal (Dickson, 1990)
KB = exp((-8966.9 - 2890.53 * s ^ 0.5 - 77.942 * s + 1.728 * s ^ 1.5
- 0.0996 * s ^ 2)/t ... + 148.0248 + 137.1942 * s ^ 0.5 + 1.62142 * s
- (24.4344 + 25.085 * s ^ 0.5 + ... 0.2474 * s) * log(t) + 0.053105 * s ^ 0.5 * t);
% Calculate K1 and K2 (Luecker et al., 2000)
K1 = 10^(-(3633.86/t - 61.2172 + 9.67770 *
log(t) - 0.011555 * s + 0.0001152 * s ^ 2));
K2 = 10^(-(471.78/t + 25.9290 - 3.16967 *
log(t) - 0.01781 * s + 0.0001122 * s ^ 2));
% Pressure variation of K1, K2, and KB (Millero, 1995)
dvB = -29.48 + 0.1622 * temp - .002608 * (temp)^2;
dv1 = -25.50 + 0.1271 * temp;
dv2 = -15.82 - 0.0219 * temp;
dkB = -.00284;
dk1 = -.00308 + 0.0000877 * temp;
```

```

dk2 = +.00113 -.0001475 * temp;
KB = (exp(- (dvB/(R*t))*Pr + (0.5 * dkB/(R*t))*Pr^2)) * KB;
K1 = (exp(- (dv1/(R*t))*Pr + (0.5 * dk1/(R*t))*Pr^2)) * K1;
K2 = (exp(- (dv2/(R*t))*Pr + (0.5 * dk2/(R*t))*Pr^2)) * K2;
% temperature dependence of Kw (DoE, 1994)
KW1 = 148.96502-13847.26/t-23.65218*log(t);
KW2 = (118.67/t-5.977 + 1.0495*log(t))*s ^ .5-0.01615*s;
KW = exp(KW1 + KW2);
% solve for H ion (Zeebe and Wolf-Gladrow, 2000)
a1 = 1;
a2 = (alk + KB + K1);
a3 = (alk*KB - KB*tbor - KW + alk*K1 + K1*KB + K1*K2 - dic*K1);
a4 = (-KW*KB + alk*KB*K1 - KB*tbor*K1 - KW*K1 + alk*K1*K2
      + KB*K1*K2 - dic*KB*K1 - 2*dic*K1*K2);
a5 = (-KW*KB*K1 + alk*KB*K1*K2 - KW*K1*K2 - KB*tbor*K1*K2 - 2*dic*KB
      K1*K2);
a6 = -KB*KW*K1*K2;
p = [a1 a2 a3 a4 a5 a6];
r = roots(p);
h = max(real(r));
% calculate the HCO3, CO3 and CO2aq using DIC, Alk and H +
format short g;
hco3 = dic/(1 + h/K1 + K2/h);
co3 = dic/(1 + h/K2 + h*h/(K1*K2));
co2 = dic/(1 + K1/h + K1*K2/(h*h));
fco2 = co2 / KH;
pH = -log10(h);
% calculate B(OH)4- and OH
BOH4 = KB*tbor/(h + KB); OH = KW/h;
% recalculate DIC and Alk to check calculations
Ct = (hco3 + co3 + co2)*1e6;
At = (hco3 + 2*co3 + BOH4 + OH-h)*1e6;

```

Appendix 4.2 Equations for calculating the equilibrium constants of the carbonate and borate buffer system

Constants are based on the "total" pH scale, pH_T (Dickson, 1984, 1993). Values are first presented at 1 atm pressure and then equations are given for calculating the pressure effect on K . T is temperature in either degrees Kelvin (T), or degrees centigrade (T_C). Salinities are on the practical salinity scale. Equilibrium constants for the equilibria other than K_H , K'_1 , K'_2 , K'_B , and K'_W given in Appendix 4A1.1(c) can be found in DoE (1994) and in Zeebe and Wolf-Gladrow (2000).

4A2.1. Values at 1 atmosphere

(a) The Henry's Law constant for CO_2 in seawater ($\text{mol kg}^{-1}\text{atm}^{-1}$), Eq. (4.14)

Source: From Weiss (1974) as reported in DoE (1994).

$$\begin{aligned} \ln K_H &= \frac{9345.17}{T} - 60.2409 + 23.3585 \ln \left(\frac{T}{100} \right) \\ &+ S \left[0.023517 - 0.00023656T + 0.0047036 \left(\frac{T}{100} \right)^2 \right] \\ &= -3.5617 \quad (T_C = 25 \text{ (} T = 298.15 \text{), } S = 35). \end{aligned} \quad (4A2.1)$$

(b) The first (Eq. (4.11)) and second (Eq. (4.9)) dissociation constants for carbonic acid in seawater (mol kg⁻¹)

Mehrbach's constants are given on the total pH scale (Luecker *et al.*, 2000).

$$\begin{aligned} \text{p}K_1' &= \frac{3633.86}{T} - 61.2172 + 9.6777 \ln(T) - 0.011555S + 0.0001152S^2 \\ &= 5.847 \quad (T_C = 25, S = 35) \end{aligned} \quad (4A2.2)$$

$$\begin{aligned} \text{p}K_2' &= \frac{471.78}{T} + 25.9290 - 3.16967 \ln(T) - 0.01781S + 0.0001122S^2 \\ &= 8.966 \quad (T_C = 25, S = 35). \end{aligned} \quad (4A2.3)$$

(c) Boric acid in seawater, mol kg⁻¹ (Eqs. (4.19 and 4.20))

Based on Dickson (1990) as reported in DoE (1994).

$$B_T = [\text{B(OH)}_3] + [\text{B(OH)}_4^-] = 4.16 \times 10^{-4} \quad (S = 35) \quad (4A2.4)$$

$$\begin{aligned} \ln K_B &= \frac{-8966.90 - 2890.53S^{1/2} - 77.942S + 1.728S^{3/2} - 0.0996S^2}{T} \\ &+ 148.0248 + 137.1942S^{1/2} + 1.62142S \\ &- \left(24.4344 + 25.085S^{1/2} + 0.2474S \right) \ln(T) + 0.053105S^{1/2}T \\ &= -19.7964 \quad (T_C = 25, S = 35). \end{aligned} \quad (4A2.5)$$

(d) The dissociation constant of water, mol² kg⁻¹

From Dickson and Riley (1979) as reported in DoE (1994).

$$\begin{aligned} \ln K_W &= 148.96502 - \frac{13847.26}{T} - 23.6521 \ln(T) \\ &+ \left(\frac{118.67}{T} - 5.977 + 1.0495 \ln(T) \right) S^{1/2} - 0.01615S \\ &= -30.434 \quad (T_C = 25, S = 35). \end{aligned} \quad (4A2.6)$$

4A2.2 The pressure dependence (from Millero, 1995)

The effect of pressure can be calculated from the molal volume, ΔV , and compressibility, $\Delta \kappa$, changes for any given reaction

$$\ln \frac{K_P}{K_0} = - \left(\frac{\Delta V}{RT} \right) P + \left(\frac{0.5 \Delta \kappa}{RT} \right) P^2, \quad (4A2.7)$$

Table 4A2.1. Parameters for calculating the effect of pressure change on carbonate buffer system reactions and values of equilibrium constants at $P=0$ and 300 bar

Constant	a_0	a_1	$a_2 \times 10^3$	$b_0 \times 10^3$	$b_1 \times 10^3$	$P=0$	$P=300$	K^{300}/K^0
pK_1'	25.50	-0.1271	0.0	3.08	-0.0877	5.847	5.726	1.32
pK_2'	15.82	0.0219	0.0	-1.13	0.1475	8.966	8.883	1.21
pK_B'	29.48	-0.1622	2.608	2.84	0.0	8.598	8.455	1.39
pK_W'	25.60	0.2324	-3.6246	5.13	0.0794	13.217	13.106	1.43

where K_p and K_0 are equilibrium constants for the reaction of interest at pressure P and at 0 bars (1 atm), respectively. P is pressure in bars, $R = 83.131 \text{ (cm}^3 \text{ bar mol}^{-1} \text{ K}^{-1}\text{)}$ and T is in degrees Kelvin. The molar volume ($\text{cm}^3 \text{ mol}$) and compressibility can be fit to equations of the form ($S=35$)

$$-\Delta V = a_0 + a_1 T_C + a_2 T_C^2; \quad (4A2.8)$$

$$-\Delta \kappa = b_0 + b_1 T_C, \quad (4A2.9)$$

where T_C is now temperature in degrees C. Values for the coefficients a and b are presented in Table 4A2.1 along with calculated differences in pK' and K' at two different pressures ($T_C = 25^\circ \text{C}$, $S = 35$).

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