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TITLE Example 1.--Add uranium and speciate seawater.
SOLUTION 1  SEAWATER FROM NORDSTROM AND OTHERS (1979)
        units   ppm
        pH      8.22
        pe      8.451
        density 1.023
        temp    25.0
        redox   O(0)/O(-2)
        Ca              412.3
        Mg              1291.8
        Na              10768.0
        K               399.1
        Fe              0.002
        Mn              0.0002  pe
        Si              4.28
        Cl              19353.0
        Alkalinity      141.682 as HCO3
        S(6)            2712.0
        N(5)            0.29    gfw   62.0
        N(-3)           0.03    as    NH4
        U               3.3     ppb   N(5)/N(-3)
        O(0)            1.0     O2(g) -0.7
SOLUTION_MASTER_SPECIES
        U       U+4     0.0     238.0290     238.0290
        U(4)    U+4     0.0     238.0290
        U(5)    UO2+    0.0     238.0290
        U(6)    UO2+2   0.0     238.0290
SOLUTION_SPECIES
        #primary master species for U
        #is also secondary master species for U(4)
        U+4 = U+4
                log_k           0.0
        U+4 + 4 H2O = U(OH)4 + 4 H+
                log_k           -8.538
                delta_h         24.760 kcal
        U+4 + 5 H2O = U(OH)5- + 5 H+
                log_k           -13.147
                delta_h         27.580 kcal
        #secondary master species for U(5)
        U+4 + 2 H2O = UO2+ + 4 H+ + e-
                log_k           -6.432
                delta_h         31.130 kcal
        #secondary master species for U(6)
        U+4 + 2 H2O = UO2+2 + 4 H+ + 2 e-
                log_k           -9.217
                delta_h         34.430 kcal
        UO2+2 + H2O = UO2OH+ + H+
                log_k           -5.782
                delta_h         11.015 kcal
        2UO2+2 + 2H2O = (UO2)2(OH)2+2 + 2H+
                log_k           -5.626
                delta_h         -36.04 kcal
        3UO2+2 + 5H2O = (UO2)3(OH)5+ + 5H+
                log_k           -15.641
                delta_h         -44.27 kcal
        UO2+2 + CO3-2 = UO2CO3
                log_k           10.064
                delta_h         0.84 kcal
        UO2+2 + 2CO3-2 = UO2(CO3)2-2
                log_k           16.977
                delta_h         3.48 kcal
        UO2+2 + 3CO3-2 = UO2(CO3)3-4
                log_k           21.397
                delta_h         -8.78 kcal
PHASES
        Uraninite
        UO2 + 4 H+ = U+4 + 2 H2O
        log_k           -3.490
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        delta_h         -18.630 kcal
END
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