**Supplementary Material**

**Greigite formation in aqueous environments: critical constraints from thermodynamic modelling.**

**Jack Turney**, Dominik Weiss, Adrian Muxworthy, Al Fraser

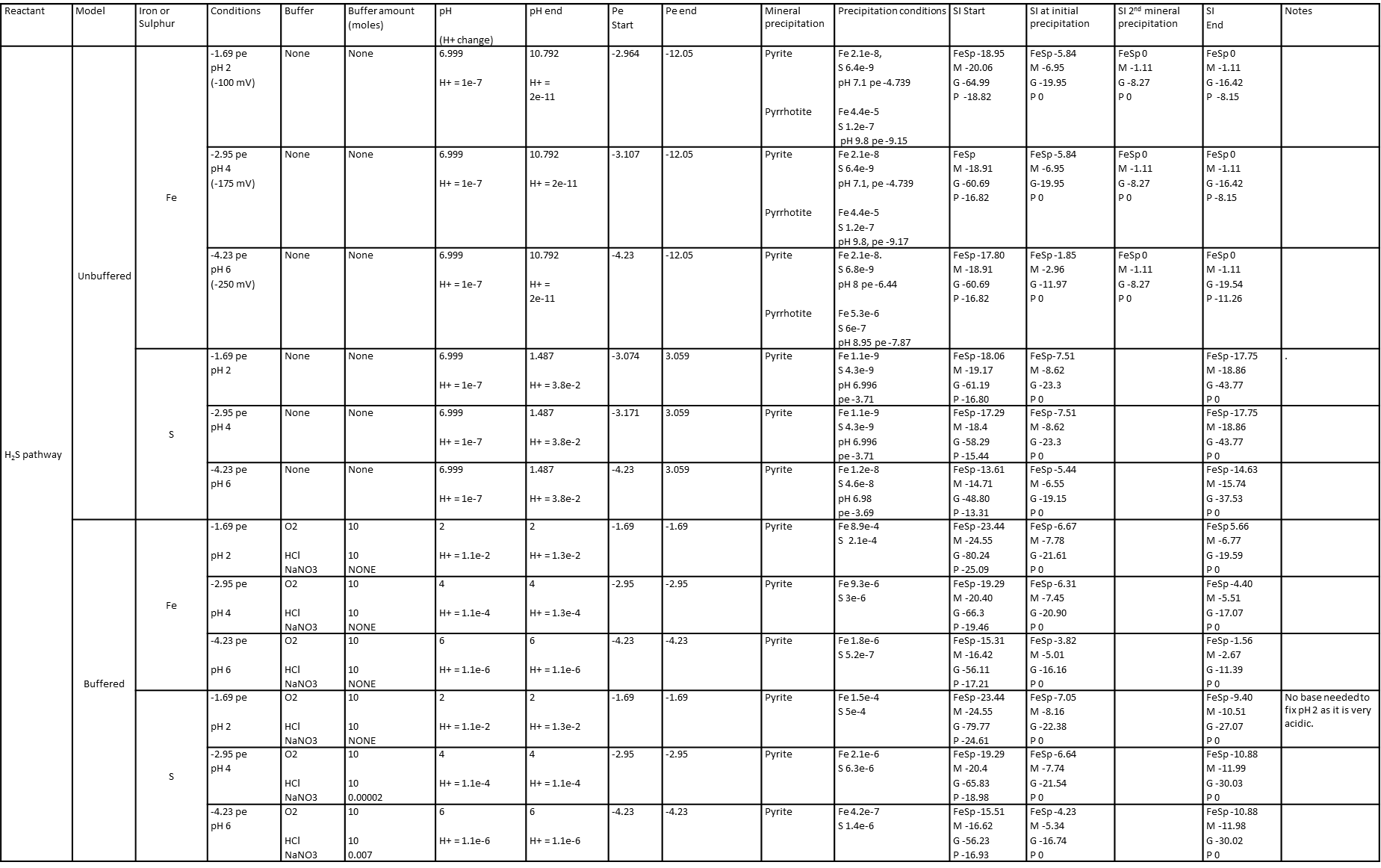


Table S1. Full experimental results for the H2S reaction pathway showing unbuffered and buffered solutions.

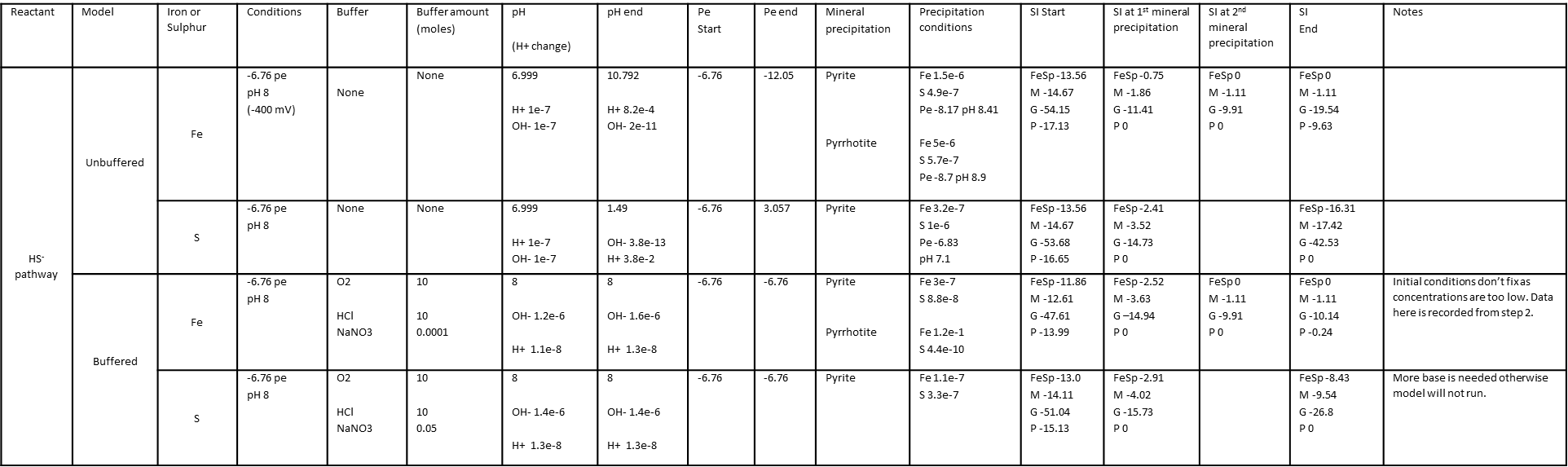


Table S2. Full experimental results for the HS- reaction pathway showing unbuffered and buffered solutions.

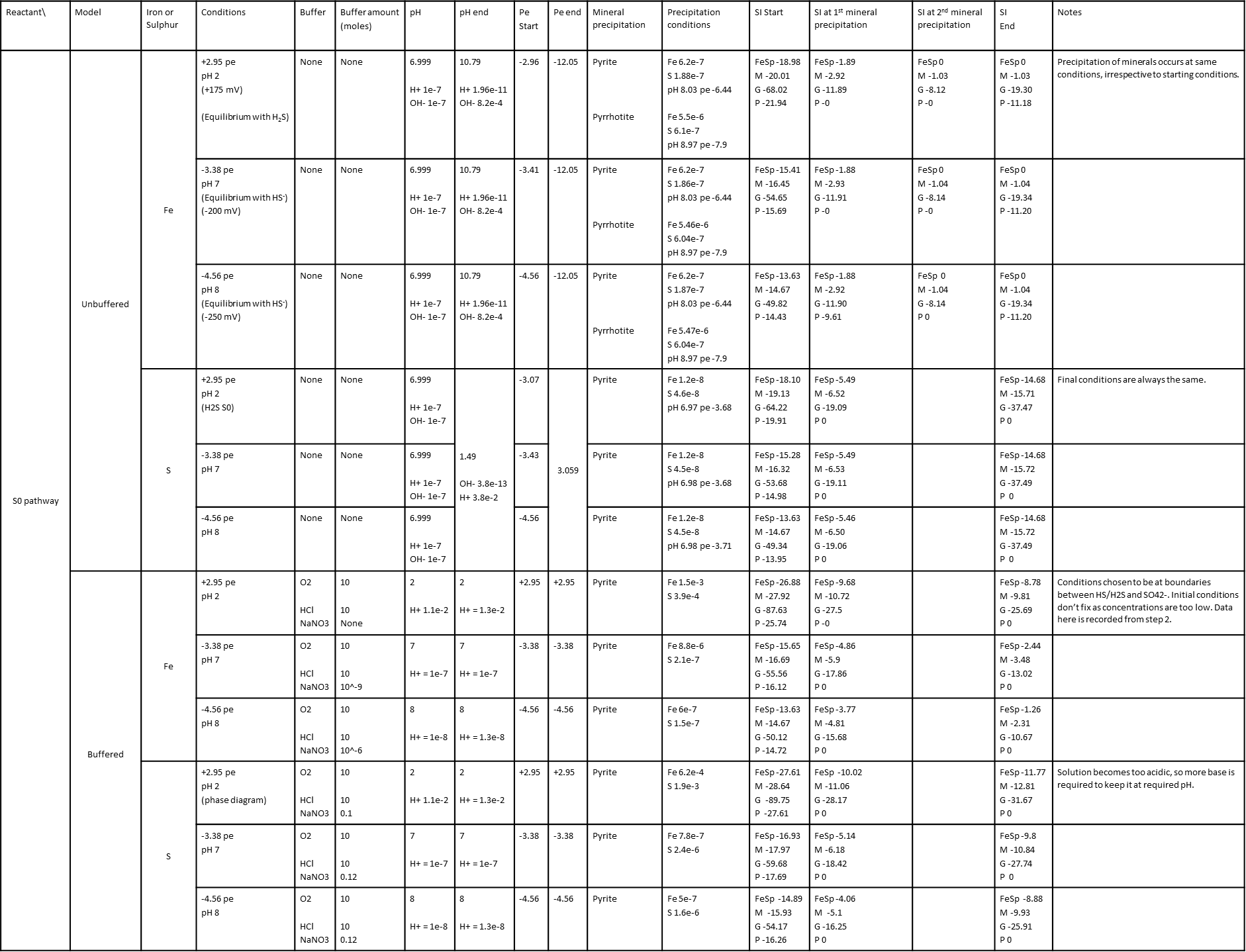


Table S3. Full experimental results for the S0 reaction pathway showing unbuffered and buffered solutions.

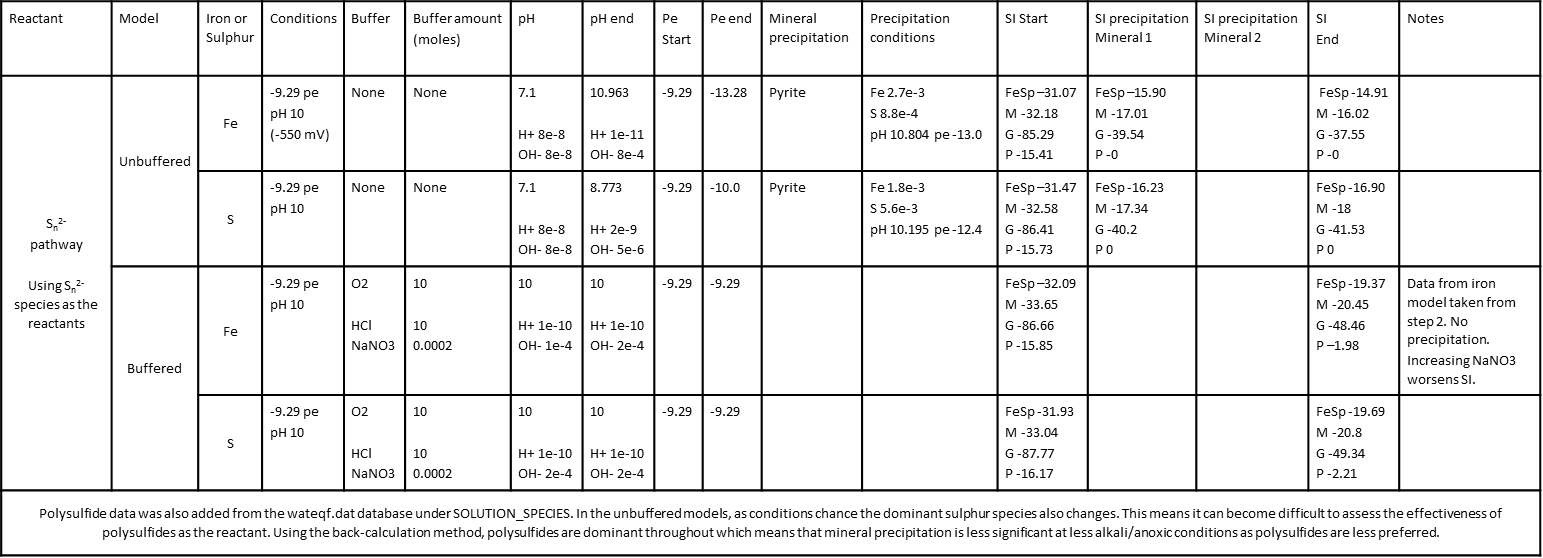
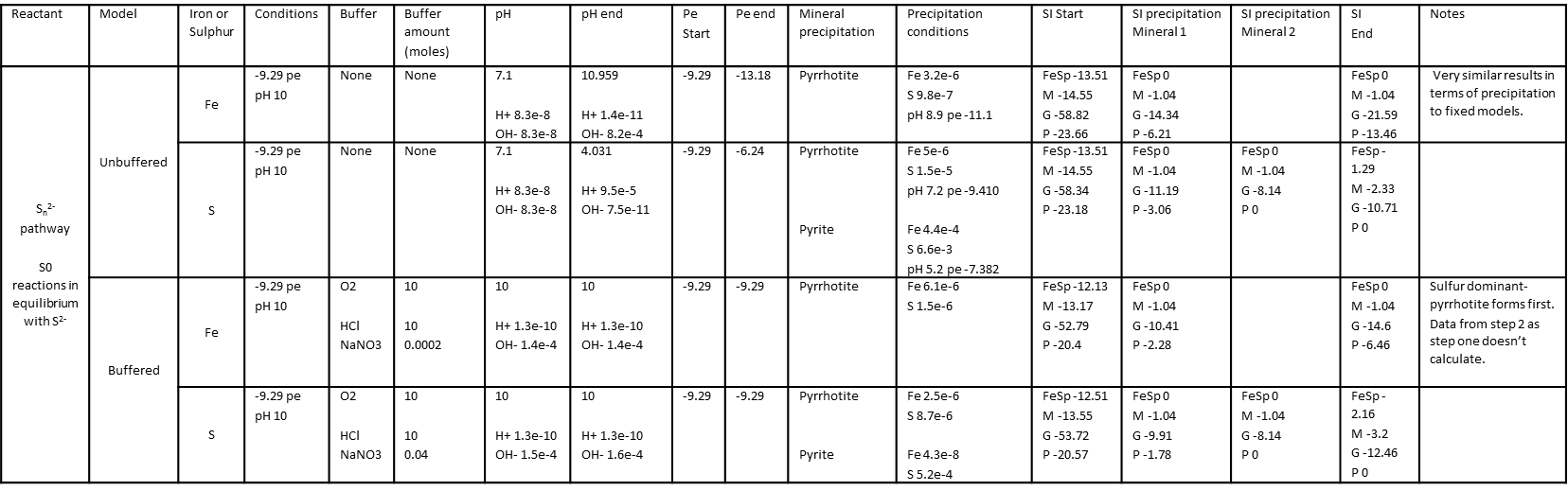


Table S5. Full experimental results for the polysulfide reaction pathway showing unbuffered and buffered solutions. Reactions use S0 which is in equilibrium with Sn2- and PHEREQC calculates the polysulfides species present under the specified conditions.

Table S4. Full experimental results for the polysulfide reaction pathway showing unbuffered and buffered solutions. Reactions use individual polysulfide species.

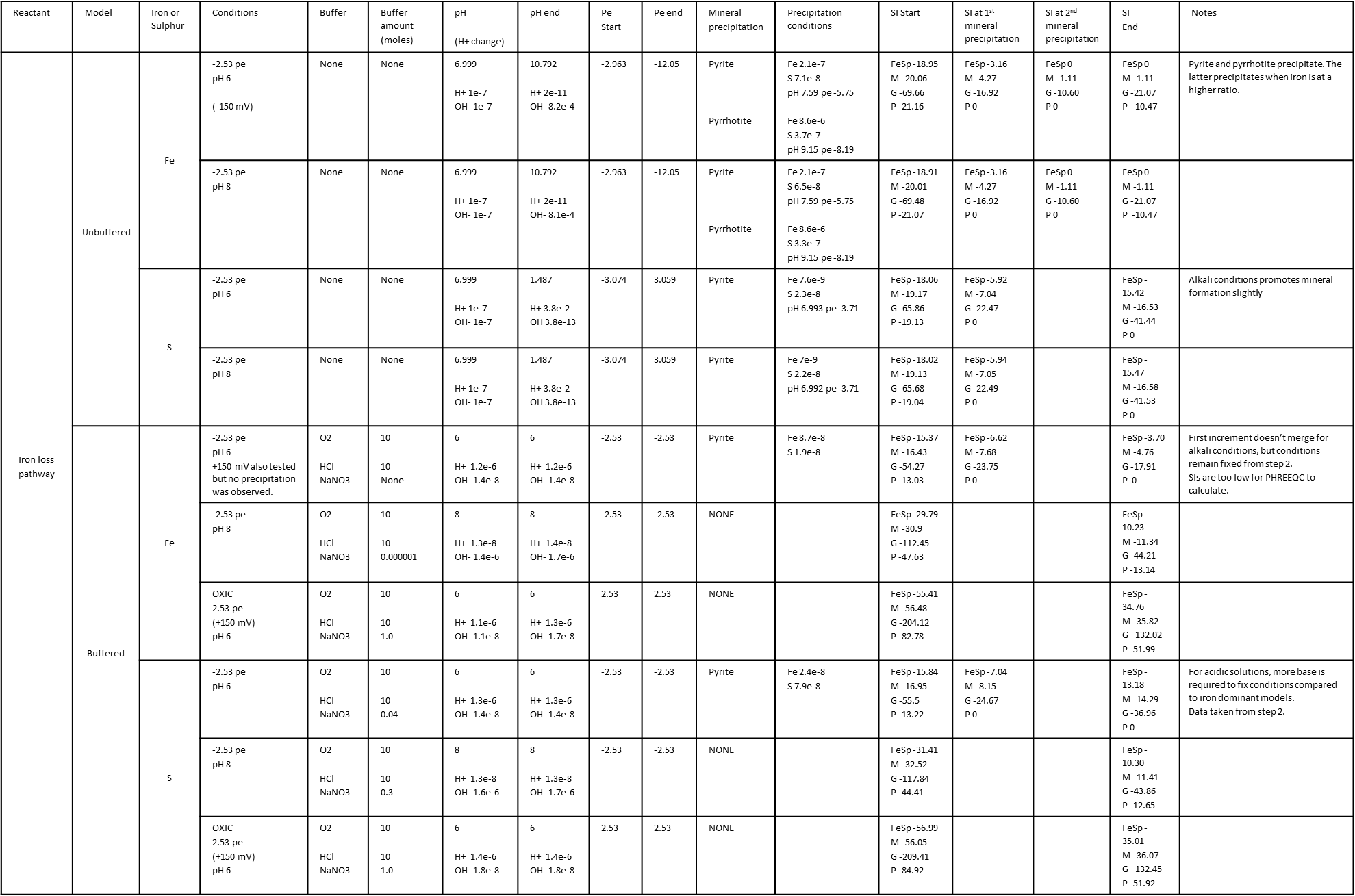


Table S6. Full experimental results for the iron loss reaction pathway showing unbuffered and buffered solutions.

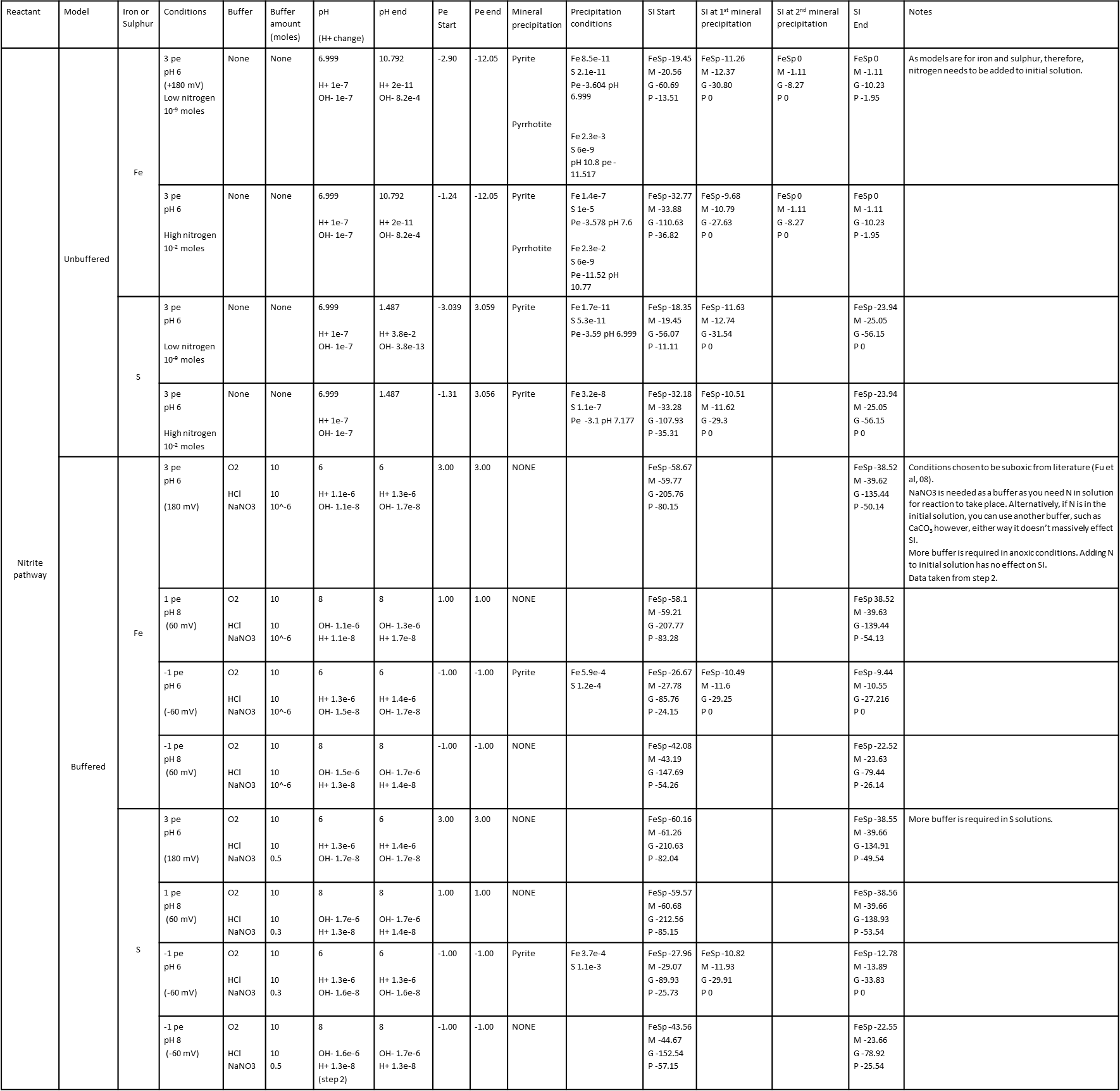


Table S7. Full experimental results for the nitrite pathway showing unbuffered and buffered solutions. Initial solutions have low (10-9 m) and high (10-2 m) nitrogen concentrations.

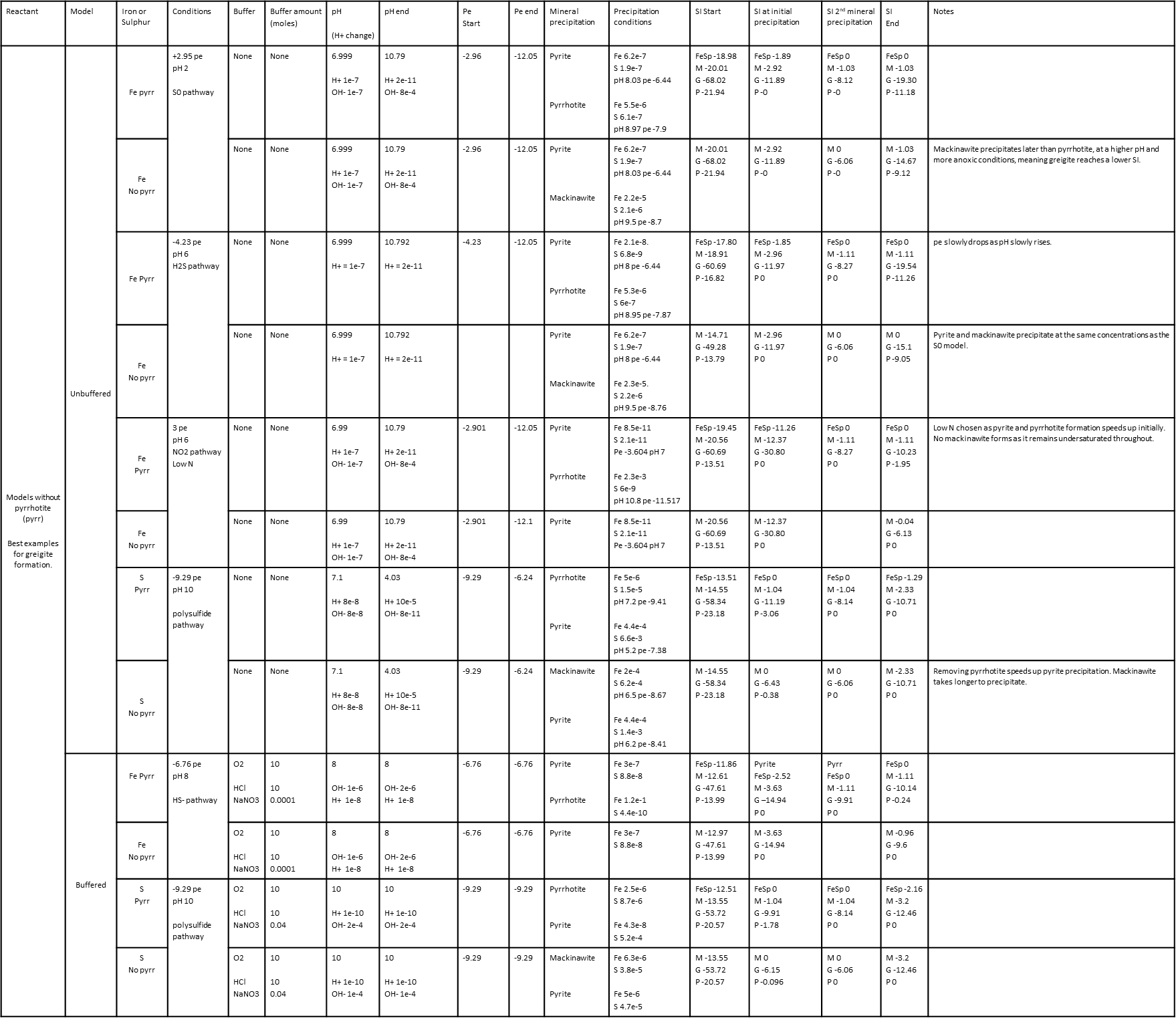


Table S8. Full experimental results showing comparisons between models with and without pyrrhotite. Models chosen produced greigite SIs that were closest to saturation with all minerals being at equilibrium.

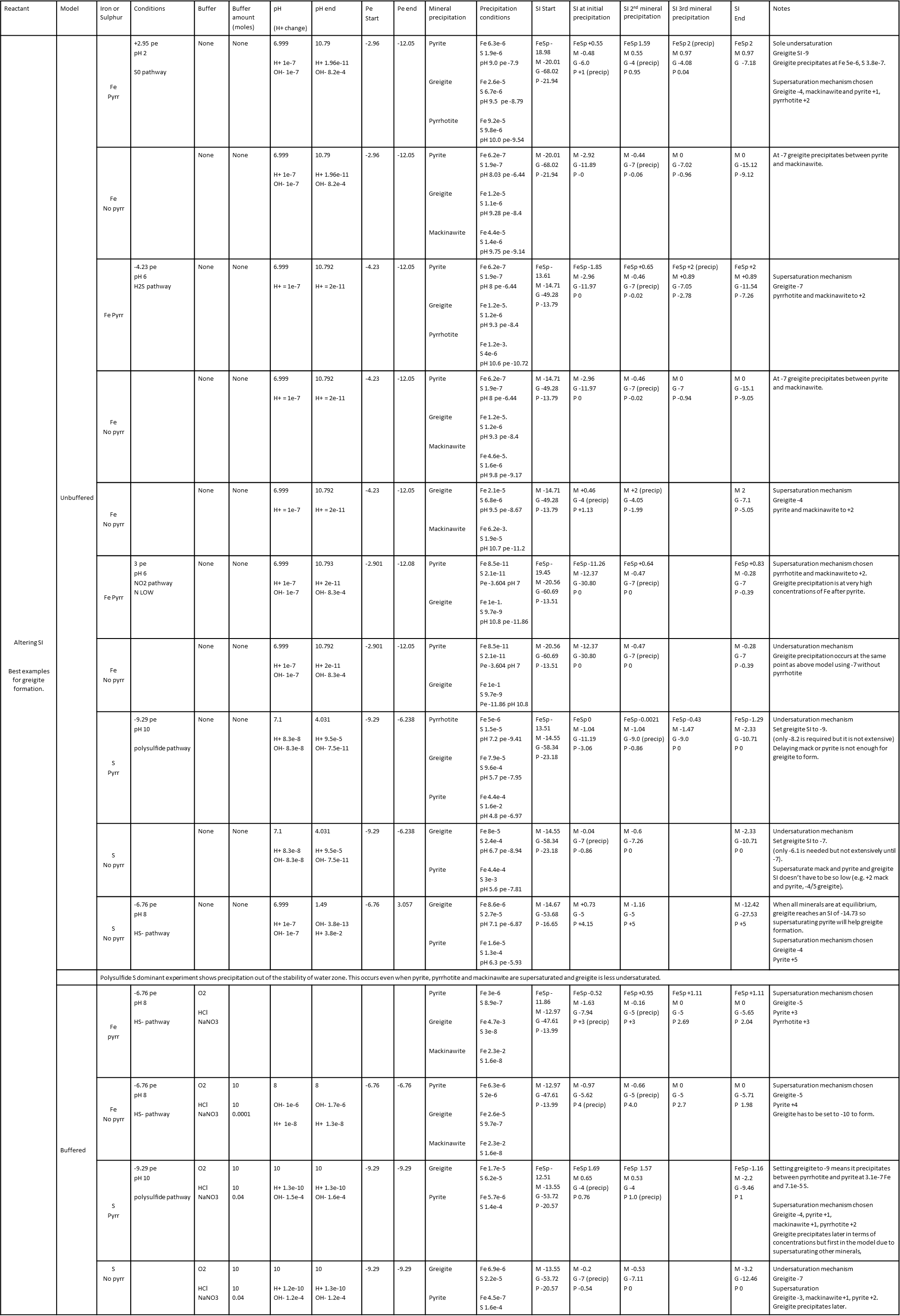


Table S9. Full experimental results for greigite forming models by the alteration of SIs. Models chosen produced greigite SIs that were closest to saturation with all minerals being at equilibrium.

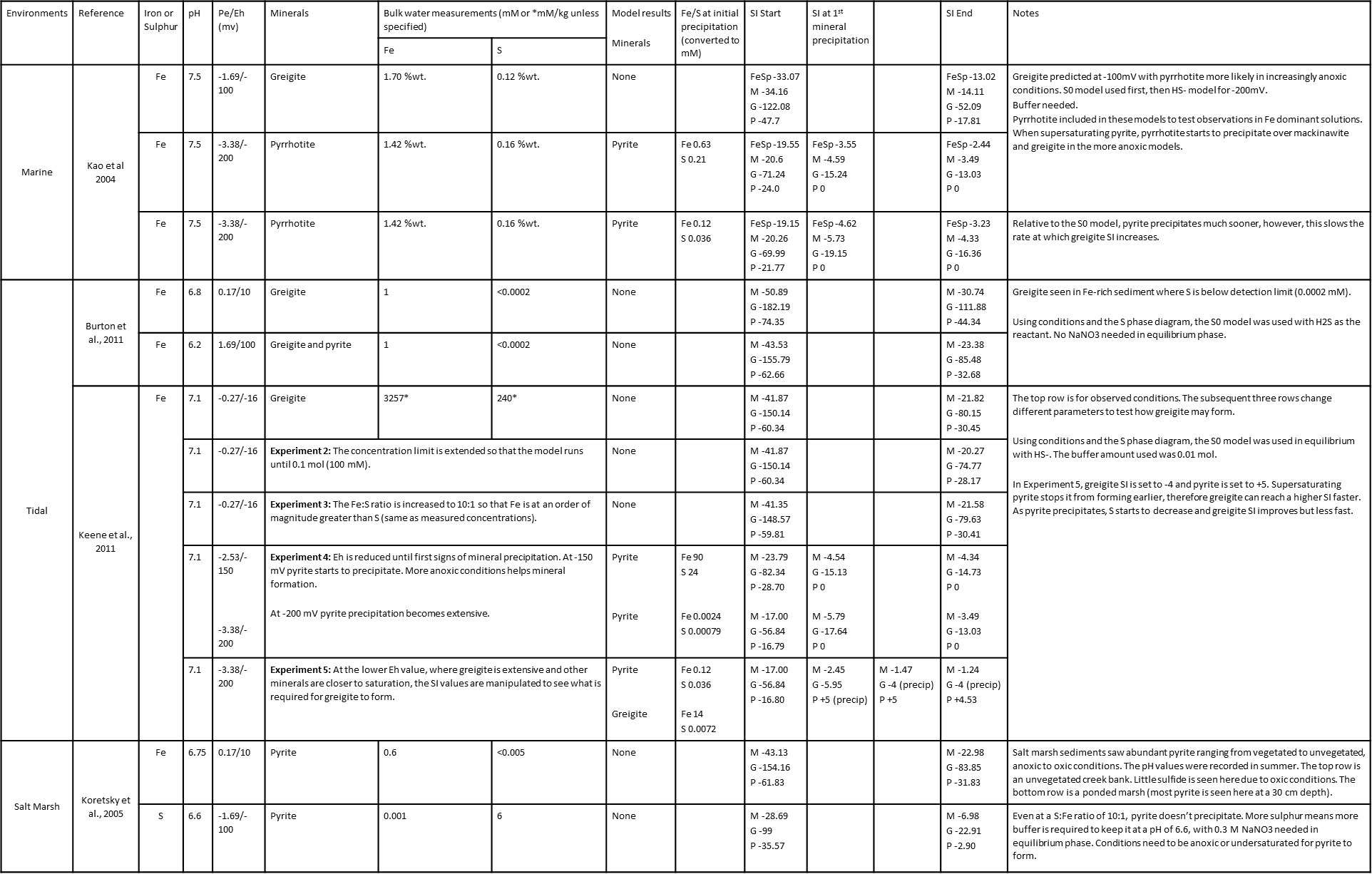


Table S10. Summary table of experiments when tested against literature observations. Using geochemical data from the literature, experiments were conducted then altered to promote the precipitation of iron sulphides.

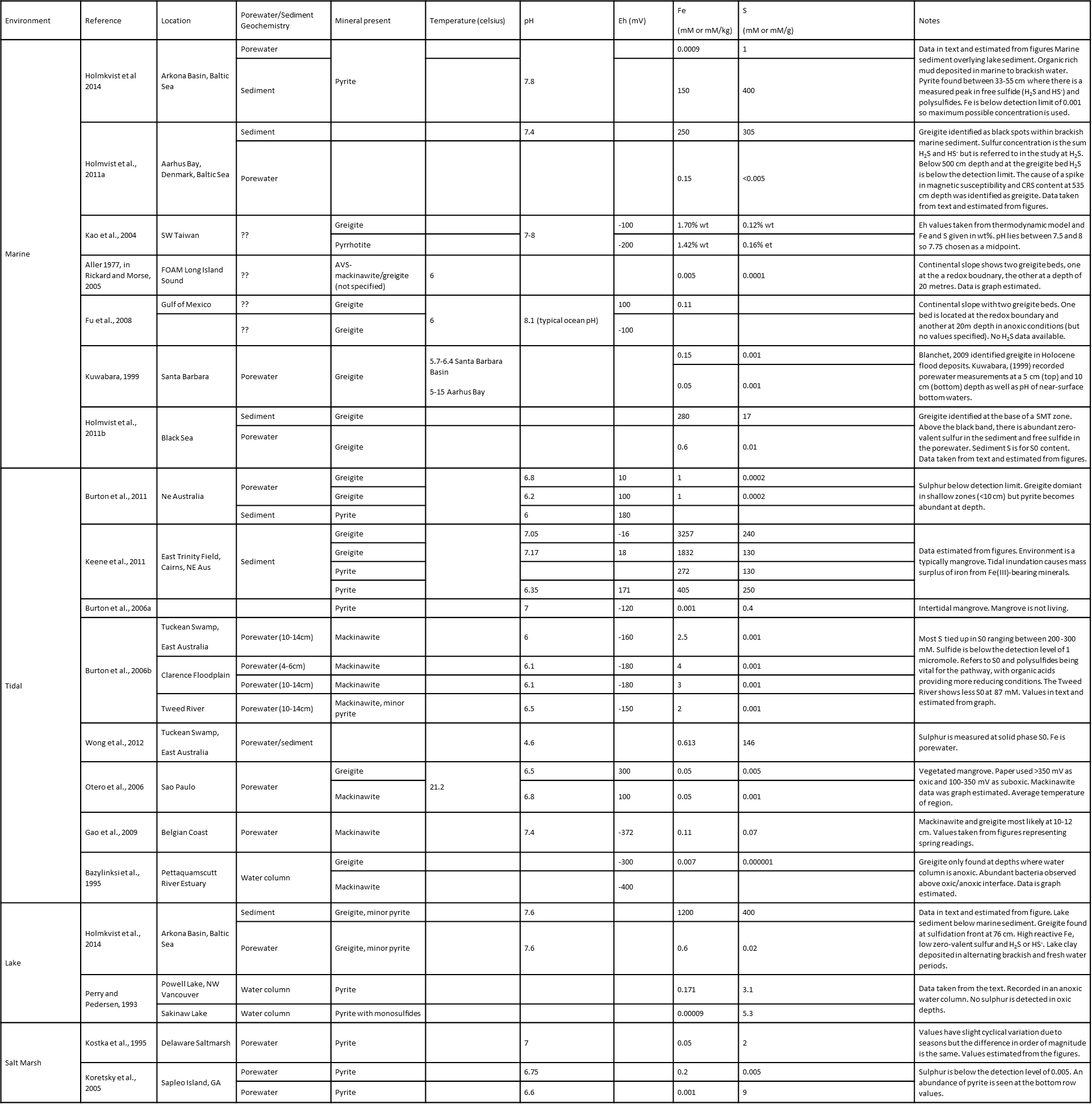


Table S11. Summary tables of geochemical data for iron sulphide-hosted natural sediments, taken from the literature. Values were estimated from the figures, taken from raw data or the text. Key observations have also been noted

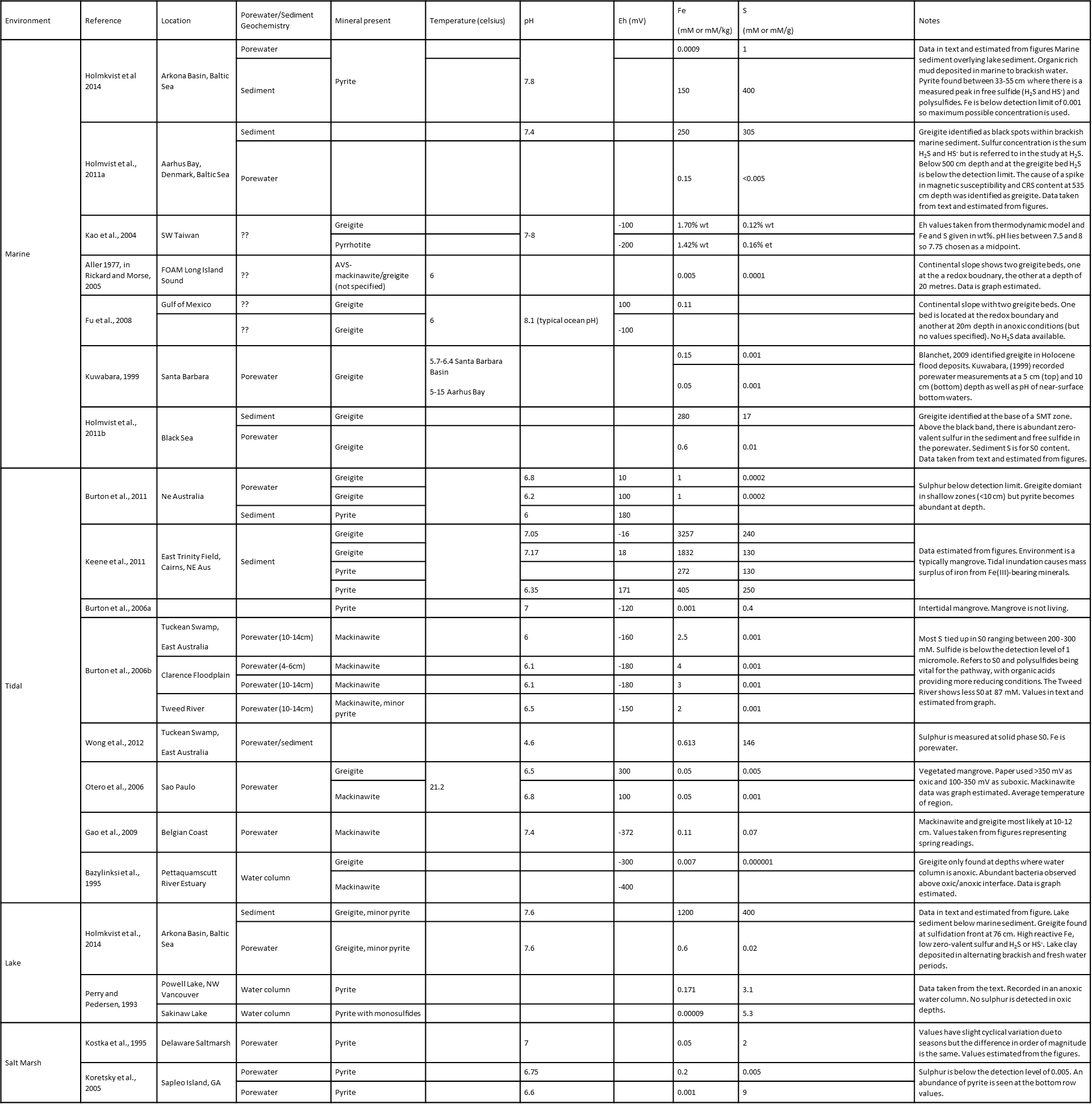
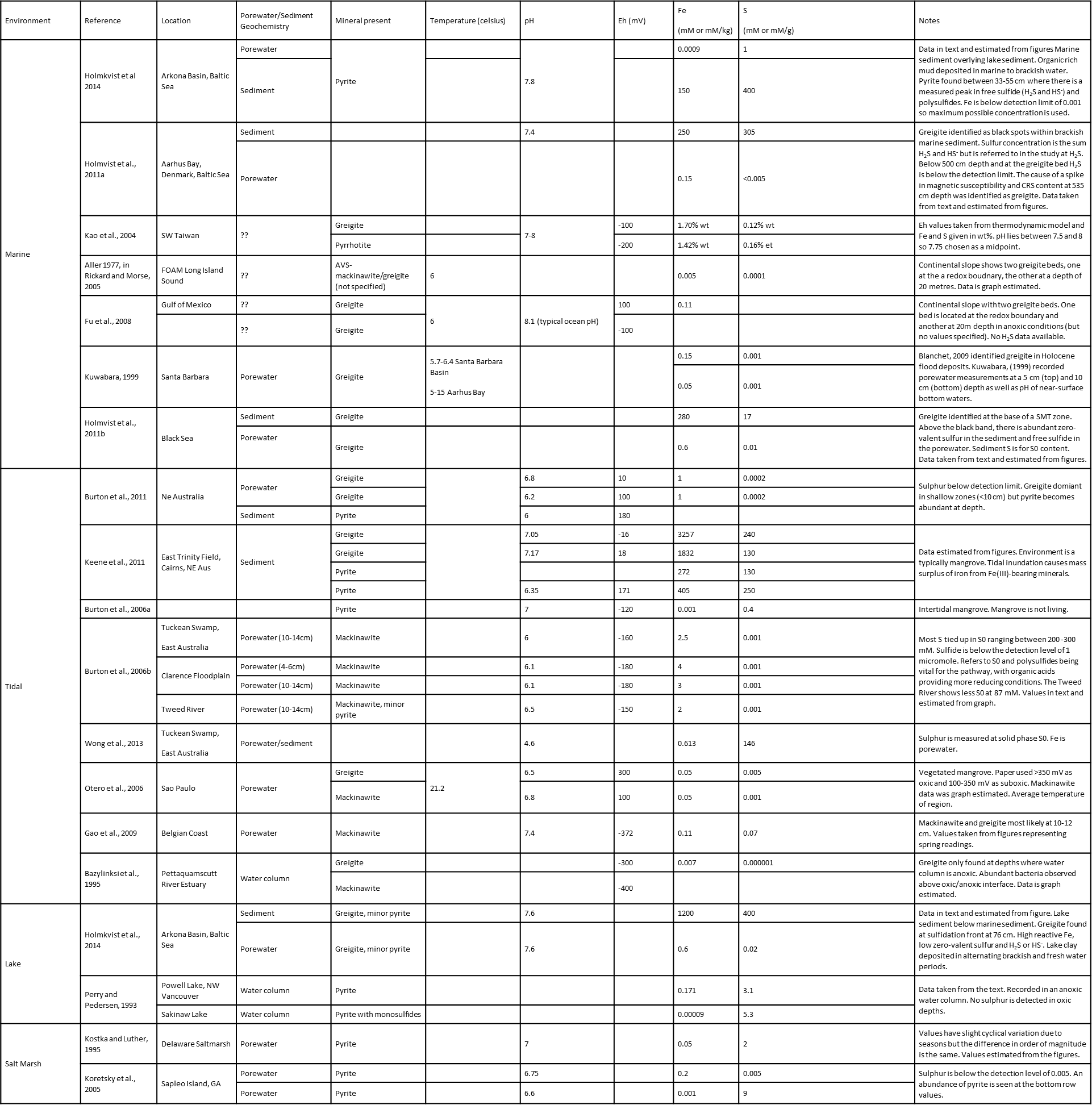


Table S11 continued.



**References cited**

Aller, R.C., (1977). The influence of macrobenthos on chemical diagenesis of marine sediments. PhD dissertation Thesis, Yale, New Haven, CT. 600 pp.

Bazylinski, D.A., Frankel, R.B., Heywood, B.R., Mann, S., King, J.W., Donaghay, P.L. et al., (1995). Controlled biomineralization of magnetite (Fe3O4) and greigite (Fe3S4) in a magnetotactic bacterium. *Applied and Environmental Microbiology* 61, 3232-3239.

Burton, E. D., Bush, R. T. and Sullivan, L. A., (2006a). Fractionation and extractability of sulfur, iron and trace elements in sulfidic sediments. *Chemosphere* 64, 1421–1428.

Burton, E. D., Bush, R. T. and Sullivan, L. A., (2006b). Sedimentary iron geochemistry in acidic waterways associated with coastal lowland acid sulfate soils. *Geochimica et Cosmochimica Acta* 70(22), 5455-5468.

Gao, Y., Lesven, L., Gillan, D., Sabbe, K., Billon, G., De Galan, S., Elskens, M., Baeyens, W., & Leermakers, M., (2009). Geochemical behaviour of trace elements in sub-tidal marine sediments of the Belgian coast. *Marine Chemistry* 117(1-4), 88-96.

Kostka, J.E., Luther, G.W., (1995). Seasonal cycling of Fe in saltmarsh sediments. *Biogeochemistry* 29, 159–181.

Perry, K. A., & Pedersen, T. F., (1993). Sulphur speciation and pyrite formation in meromictic ex-fjords. *Geochimica et Cosmochimica Acta* 57(18), 4405-4418.

Otero, X., Ferreira, T., Vidal-Torrado, P., & Macías, F., (2006). Spatial variation in pore water geochemistry in a mangrove system (Pai Matos island, Cananeia-Brazil). *Applied Geochemistry* 21(12), 2171-2186.

Wong, V. N., Johnston, S. G., Burton, E. D., Bush, R. T., Sullivan, L. A., & Slavich, P. G., (2013). Seawater-induced mobilization of trace metals from mackinawite-rich estuarine sediments. *Water Research* 47(2), 821-832.