

Phase diagram calculations and internally consistent databases: John Holloway's insights

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I was looking for a job in 1980 and John Holloway (who had a NASA grant) suggested that I come to Tempe and work on trying to calculate phase relationships for plausible compositions of the martian mantle. This would require putting together an internally-consistent data base for the system $\text{Na}_2\text{O}-\text{CaO}-\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2-\text{FeO}$ (end-members and solid-solutions) and development of an efficient free energy minimisation program. The latter was essential because although I would have a TERAC (PDP-11) computer dedicated to the project it had only 32K of memory. So began a fruitful and entertaining year working with JRH.

Our efforts led to one paper about Mars [1] and one about the CMAS system [2] but I only published the complete set of calculations in Reviews in Mineralogy [3]. Much more important for me was the path John set me on towards thinking about other complex phase equilibria such as those of the 410 discontinuity and transition zone, the Earth's multicomponent core and condensation during the early history of the solar system. It also enabled me to identify potential experimental projects aimed at refining thermodynamic data for mantle phases.

Those few months working with John in Tempe had, as indicated above, a great influence on the remainder of my career. This brings me to my current work on free energy minimisation and the condensation temperatures of the elements. I find that the generally accepted condensation temperatures have considerable uncertainties and errors which will be discussed in the final part of this presentation.

[3]Wood, B.J., 1987.Reviews in Mineralogy 17, 71-95.

[1]Wood, B.J., Holloway, J.R., 1982. Journal of Geophysical Research 87, A19-A30.

[2]Wood, B.J., Holloway, J.R., 1984. Geochimica et Cosmochimica Acta 48, 159-176.