Appendix G Calculation of fO_2 based on composition of the AuPd capsule using model 2 from Barr and Grove (2010)

The Fe and Ni contents of the AuPd (75:25) capsule material in PC experimental run products were measured with an electron microprobe (Cameca SX-100 at the University of Michigan). Pure Au, Pd, Fe and Ni metals were used as standards for the microprobe analyses. The activity of Fe in each capsule ($aFe^{capsule}$) was calculated using the spreadsheet provided by Barr and Grove (2010). The mole fraction of Fe in the liquid (XFe^{liq}) was calculated with an initial estimate of fO_2 using the model from Kress and Carmichael (1991). The equilibrium coefficient K was calculated using the AuPdFe solution model 2 from Barr and Grove (2010; shown in Fig. 2b). Subsequently, Equation 3 from Barr and Grove (2010) was used, with iteration, to calculate the fO_2 of the capsule, based on $aFe^{capsule}$, XFe^{liq}, and lnK. Results are shown in the table below for the calculated fO_2 of capsule for each experiment based on the average capsule composition. ΔNNO is calculated from logfO_2 (below) and temperature of each experiment (see Table 2 of main paper).

Expt #	Au (mol%)	Pd (mol%)	Fe (mol%)	Ni (mol%)	$aFe^{capsule}$	XFe^{liq}	logfO_2	ΔNNO
PC10	62.9%	37.1%	0.05%	0.00%	5.61E-05	4.13E-02	-6.7	1.9
PC12	62.7%	37.1%	0.19%	0.01%	2.54E-04	5.06E-02	-7.9	0.8
PC13	62.4%	37.4%	0.21%	0.01%	2.79E-04	5.11E-02	-8.0	0.7
PC14	62.7%	36.9%	0.32%	0.03%	4.27E-04	5.40E-02	-8.3	0.4
PC17	62.6%	37.3%	0.12%	0.01%	1.99E-04	4.87E-02	-8.1	1.0
PC36	62.8%	37.0%	0.12%	0.00%	1.50E-04	3.84E-02	-6.7	2.4
PC37	62.7%	37.0%	0.29%	0.01%	3.57E-04	4.36E-02	-6.7	2.3
PC33	62.7%	36.8%	0.52%	0.02%	4.38E-04	6.00E-02	-7.5	0.5
PC35	62.8%	37.0%	0.27%	0.01%	3.32E-04	5.43E-02	-7.3	0.6

References

Barr, J.A. and Grove, T.L. (2010) AuPdFe ternary solution model and applications to understanding the fO2 of hydrous, high-pressure experiments. Contributions to Mineralogy and Petrology, 160, 631-643.