The volatile abundance pattern of the mantle-atmosphere: Clues to origin and reservoir fluxes

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I present a volatile (water, C, N, S, noble gases) budget for the different mantle reservoirs - the depleted mantle source of N-MORBs, the enriched mantle source of E-MORBs, and the mantle source of plumes - and for the atmosphere. The N- and E- mantle abundances are estimated from MORB data after correction for fractional degassing and partial melting. The plume source abundance is estimated from both measurements of plume-related material and a K-Ar mass balance for bulk Earth. Normalized to Chondritic, the resulting patterns are consistent with an asteroidal source for major volatiles. Independently, stable isotope (H and N) systematics of the Sun (now documented for N thanks to the Genesis mission [1]), meteorites, giant planets and comets suggest that volatile elements of Earth were mainly supplied by a cosmochemical reservoir which vestiges are found now in chondrites. The CI-normalized volatile abundance pattern indicates extensive exchange between the mantle and the Earth surface for water and carbon. In contrast, nitrogen is depleted by one order of magnitude in the mantle-crust-atmosphere, suggesting either trapping in a hidden reservoir (the core?) or retention in a N-rich mantle phase not yet identified. Neon, argon and krypton are enriched relative to Chondritic, as a result of the addition of cometary material during the late heavy bombardment 3.8 Gr ago. We shall discuss elsewhere in this conference the well-known xenon depletion (and heavy isotope enrichment) known as the 'xenon paradox'.

[1] Marty, Zimmermann & Burnard *et al*. (2010) *GCA* **74**, 340.

Ab initio molecular dynamics studies of aqueous solutions: Solvation of salts and amino acids

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The structure and dynamics of salts and amino acids in liquid water are studied using ab initio molecular dynamics. We show by comparison to neutron scattering data that the ab initio yields a more accurate description of these systems than the empirical models commonly to describe them used today. New structural motifs are observed in the ab initio simulations that are not favored by the empirical models and novel dynamical pathways are found. In particular, in the salt solution, a new type of water solvation structure around the ions is discovered with quite interesting exchange pathways with the bulk.