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Archean Atmospheres Modeled with the KROME Chemistry Package

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Sulfur isotopic fractionation has been used as a tool to understand the composition of reducing atmospheres. Our previous work (Danielache et al., 2008 and 2012) have shown that UV-light triggers a large Sulfur Mass-Independent Fractionation (S-MIF) on the SO_2 photodissociation products. However photodissociation of unshielded UV-light alone cannot reproduce the S-MIF signals reported for the Archean and Early Proterozoic (>2300 Ma) nor its large variability mainly at 2600 Ma (D33S = +11 ‰) (Johnston, 2011). In order to study a planetary-like chemical network capable of accounting for a sulfur cycle in reducing conditions we have introduced a high-order solver (DLSODES) administrated by the KROME (Grassi et al.,) chemistry package. The package automatically generates a set of FORTRAN subroutines with build-in rate equations and solves them with accuracy and e?ciency for sparse networks. This technique allows us to couple a detailed 4 sulfur isotopes chemistry to a 1D transport model capable of calculating the opacities influencing photochemistry and the temperature structure of an Archean atmosphere. We present preliminary results showing the ability of the code to deal with small isotopic fractionations and compare with already existing model studies of the Archean atmosphere.

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Grassi T., et al., (2014), KROME - a package to embed chemistry in astrophysical simulations, Monthly Notices of the Royal Astronomical Society., DOI: 10.1093/mnras/stu114 (arXiv:1311.1070 [astro-ph.GA]).

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