

Water content and OH speciation in natural Fe-bearing pyroxenes

K. BEGAUDEAU¹, Y. MORIZET² AND J-C.C. MERCIER¹

¹LIENSs, University of La Rochelle, La Rochelle, France

²LPGN, University of Nantes, Nantes, France

(*correspondence: yann.morizet@univ-nantes.fr)

H in NAMs plays a crucial role on the physical and chemical properties of the Earth's mantle [1]. FTIR and NMR analyses were used to measure H contents and constrain OH dissolution mechanisms for natural Fe-bearing pyroxenes of 40 mantle xenoliths brought up by alkaline basalts magmas. Crystal chemistry was analyzed by EMPA. Equilibrium P-T conditions were determined by a new geothermobarometer developed yielding $T^{\circ}\text{C}=644\text{-}1151$ and $P(\text{GPa})=0.85\text{-}2.7$. Polarized FTIR spectra display the main absorption bands in OH species region. H_2O estimates [2] range between 38-450 ppm H_2O for cpx and 19-184 ppm H_2O for opx. Cpx/Opx partitioning coefficients range to 0.6-3.7. H_2O variations seem correlated to $f\text{O}_2$, P, T and crystals chemistry allowing us development of geohygrometers.

¹H, ²⁷Al, ²⁹Si MAS NMR were also carried out with different magnetic fields. ¹H spectra are not exploitable because of paramagnetic components [3]. Their influences on the change of NMR spectral features are tested with mixtures of kaolinite + magnetite. ²⁹Si and ²⁷Al spectra are slightly affected. Tests on pyroxenes show an Al species distinction. Additional data reveals H proximity around Al species confirming relationships described by FTIR [4]. Thus, the use of both spectroscopic methods opens new perspectives for mineralogy and geochemistry of mantle's peridotites.

[1] Bell & Rossman (1992) *Science* **255**, 1391-1397 [2] Libowitzky & Rossman (1997) *Am.Min* **82**, 1111-1115 [3] Stebbing *et al* (2009) *Am. Min* **94**, 626-629 [4] Stalder (2004) *Eur. Journal of Min* **16**, 703-711.

Decarboxylation of fatty acids during petrogenesis: Qualitative and quantitative analyses of bitumen NSOs by FTICR-MS

F. BEHAR¹, E. SALMON², A.W. KAMGA² AND P.G. HATCHER^{2*}

¹IFP Energies Nouvelles, 1-4 avenue de Bois Préau, Rueil-Malmaison 92500, France.

(Francoise.BEHAR@ifpenergiesnouvelles.fr)

²Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529. (esalmon@odu.edu, akamga@odu.edu, *correspondence: phatcher@odu.edu)

The NSO compounds generated during the artificial maturation of kerogen from Green River Formation were collected by successive *n*-pentane and dichloromethane (DCM) extractions and analyzed using electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI-FTICR-MS). Compounds containing only CHO elements in their make-up are dominant in each spectrum and are comprised mostly of the series $\text{C}_n\text{H}_{2n}\text{O}_2$, $\text{C}_n\text{H}_{2n-2}\text{O}_2$, $\text{C}_n\text{H}_{2n-2}\text{O}_4$, and $\text{C}_n\text{H}_{2n-10}\text{O}_2$ which all correspond to carboxylic acid-containing compounds. By calibrating the FTICR-MS with internal standard, it was possible to assign a response factor for the carboxylic acids and consequently get better quantification of the total carboxylic acids content. This response factor is invariant in the carbon number range of C_{20} to C_{40} . Also, after calibration, the carboxylic acid yield remains dominant among the other peaks detected by FTICR-MS. The same quantitative strategy was used for determining the response factor of the alcohols and dicarboxylic acids in order to determine the quantitative proportions of these functional groups in the NSOs.

Results clearly demonstrate that hydrocarbon generation from kerogen is mainly attributed to decarboxylation of the NSOs compounds. Moreover, there is a strong qualitative and quantitative relationship between the hydrocarbon distributions and the fatty acid distributions. For example, the carbon preference index for hydrocarbons matches exactly that observed for the fatty acids.