Pristane isomerization ratio: Novel maturity index for highly mature and overmature oils

YINGQIN WU [1,2], YONGLI WANG [1]*, TIANZHU LEI [1], SUPING MA[1], YOUXIAO WANG [1], YUAN GAO[1] AND YANQING XIA [1]*

[1]Key Laboratory of Petroleum Resources Research, Institute of Geology and Geophysics, Chinese Academy of Science, Lanzhou 730000, China (wuyingqin001@163.com) (*correspondence: yqxia@lzb.ac.cn,wyll6800@163.com)

[2] Graduate School of the Chinese Academy of Sciences, Beijing 100049, China

Thermal maturity is an important parameter in assessing petroleum evolution in sedimentary basins. However, the maturity parameters based on biomarkers cannot be applied to highly mature oils (Ro > 1.5%), especially to overmature oils (Ro > 2.0%) (e.g. the sterane and terpane isomerization ratios, methyl phenanthrene index and methyl diamantane index). The reason is that these ratios reach their equilibrium values before or at the onset of the “oil window”. Therefore, the peak hydrocarbon generation stage cannot be assessed using these parameters, particularly for highly mature and overmature crude oils.

In this experiment, pristane isomers were identified in extracts from the coal samples of Junggar Basin, China. From brown coal to subbituminous coal, corresponding to Ro 0.36-2.99 %, the PIR [pristane isomerization ratio = { [6(R)10(R) + 6(S)10(S)] /6(R)10(S)] ranges from 42 to 97% for the coal extracts. The value of PIR, a molecular maturity parameter, is evaluated by analyzing a series of samples from the Junggar Basin with known values of the molecular maturity parameter based on the sterane and hopane isomerization and methyl phenanthrene index. Changes in the PIR in these highly mature Ai-13 (Ro>1.5%) and overmature Ha-01 and Ha-02 (Ro>2.0%) are still obvious and with linear correlation between PIR and Ro. As a result, our results suggest that the PIR is an appropriate indicator of maturity for the highly mature and overmature oils and sediments.

It is clear that the PIR increases with the increasing of Ro, which possibly suggests an isomerization of RS isomer into the RR and/or SS isomer.

In summary, the PIR may be potential interest as it can efficiently be used in measuring the maturity of highly mature oils, sediments and may work throughout the “oil window”. However, the same case may be expected to take place in other molecular parameters, but the current work does not observe the dependence of the PIR on the kerogen type. It is necessary to make further investigation and collect data of the PIR from other samples (elsewhere) in order to attain better results of the present study.

Supported by grants No. XDB03020405, 2012CB214701, NSFC No. 41272147,41172169, 40672123 and TPR-2012-18.

Elasticity of ferropericlase at lower mantle conditions

ZHONGQING WU[1,2], JOÃO F. JUSTO,[1,3] AND RENATA M. WENTZCOVITCH[1]

[1]Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455

[2]Laboratory of Seismology and Physics of Earth's Interior, School of Earth and Space Sciences, University of Science and Technology of China, Hefei, Anhui 230026, China

[3]Escola Politécnica, Universidade de São Paulo, CP 61548, CEP 05424-970, São Paulo, SP, Brazil

Clarification of the effect of the iron spin state change on properties of Fp is important to address the relative abundance of Fp in the lower mantle. However, recent works addressing this question have reached different conclusions. The calculated density of a pyrolite aggregate with spin crossover-related change in iron partitioning compared well with the density in PREM up to 45 GPa [1]. In contrast, Murakami *et al*’s analysis of V_S in aggregates with variable amounts of Fp concluded that the lower mantle is more perovskitic than pyrolitic [2].

We investigated the thermoelasticity of Fp by first principles using the DFT+U functional. The calculated thermoelastic coefficients are consistent with available experimental data on samples with various iron concentrations. Results help us to understand some discrepancies among different experimental data sets regarding the shear modulus softening [3,4]. We predict velocities of Fp at lower mantle conditions and suggest that pyrolite is a reasonable compositional model for the lower mantle. Our results show the importance of constraining the elastic properties of minerals without extrapolations for analyses of the thermochemical state of this region.

[1] Irifune *et al*. *Science* **327**, 193 (2010). [2] Murakami *et al*. *Nature* **485**, 90 (2012). [3] Crowhurst *et al*. *Science* **319**, 451 (2008). [4] Marquardt *et al*. *Science* **324**, 224 (2009).

DOI:10.1180/minmag.2013.077.5.23