Poster Presentation

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Structure of methane and ethane at high pressure

A. Goncharov[1], E. Stavrou[1, 2], S. Lobanov[1, 3], A. Oganov[4], V. Roisen[4], A. Chanyshev[3], K. Litasov[3], Z. Konopkova[5], K. Zhuravlev[6], V. Prakapenka[6]

[1]Geophysical Laboratory, Carnegie Insitution of Washington, Washington DC, USA, [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece, [3]V.S. Sobolev Institute of Geology and Mineralogy SB RAS , Novosibirsk, Russian Federation, [4]Department of Geosciences, State University of New York, Stony Brook, NY, United States, [5]Petra III, P02.2, DESY, Hamburg, Germany, [6]Center for Advanced Radiation Sources, University of Chicago, Chicago, IL, United States

Methane is one of the most abundant hydrocarbon molecules in the universe and is expected to be a significant part of the icy giant planets (Uranus and Neptune) and their satellites. Ethane is one of the most predictable products of chemical reactivity of methane at extreme pressures and temperatures. In spite of numerous experimental and theoretical studies, the structure and relative stability of these materials even at room temperature remains controversial. We have performed a combined experimental and theoretical study of both methane and ethane up at high pressures up to 120 GPa at 300 K using x-ray diffraction and Raman spectroscopy and the ab-initio evolutionary algorithm, respectively. In the case of methane we have successfully solved the structure of phase B by determining the space group and the positional parameters of carbon atoms, and by completing these results for the hydrogen positions using the theoretical calculations. The general structural behavior under pressure and the relation between phase B and phases A and pre-B will be also discussed. For ethane we have determined the crystallization point, for room temperature, at 1.7 GPa and also the low pressure crystal structure (Phase A). This crystal structure is orientationally disordered (plastic phase) and deviates from the known crystal structures for ethane at low temperatures. Moreover, a pressure induced phase transition has been indentified, for the first time, at 18 GPa to a monoclinic phase III, the structure of which is solved based on a good agreement of the experimental results and theoretical predictions. We have determined the equations of state of methane and ethane, which provides a solid basis for the discussion of their relative stability at high pressures.

Keywords: high pressure, hydrocarbons, crystal structure