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Order parameter defining liquid-liquid transition in water[1] J. RAUL GRIGERA, OSVALDO CHARA, ANDRES MCCARTHY, IFLYSIB (UNLP-CONICET), c.c. 565, La Plata, Argentina — Water presents both open tetrahedral and compact hexagonal structures. Although several order parameters have been proposed to quantify this, all of them are only applicable to data produced by simulation. We present an order parameter (P_r) that is calculated from the radial distribution function $g(r)$, also available from experiment. We hereby extract the tetrahedral and hexagonal components from the $g(r)$, each one reconstructed as the sum of a Freundlich distribution for the first peak, two subsequent Gaussian distributions, and a sigmoidal to account for the rest. The order parameter can be calculated from the relative contribution of tetrahedral over hexagonal contribution. We obtained the P_r for SPC/E water model from molecular dynamics simulations of water at different pressures and temperatures. At 300K, the pressure in which both, tetrahedral and hexagonal contributions become equal (P_r= 0), a structural crossover is found in the vicinity of 2kbar, close to the pressure at which the ''anomalous" behavior manifests. Having computed P_r for this wide range of pressure and temperature we then calculate the HDL spinodal, the coexistence line, the second critical point, and the Widom line.

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