

Abstract Submitted
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Temperature dependence of the Oxygen-Oxygen separations in water from high energy x-ray diffraction LAWRIE SKINNER, Stony Brook Univ. & Argonne Nat. Lab., CHRIS BENMORE, Argonne National Laboratory, JOHN PARISE, Stony Brook University — We have used state of the art, high energy x-ray diffraction to obtain detailed measurements of the Oxygen-Oxygen (O-O) pair distribution function ($g(r)$) of liquid water between -20 and 92 degrees Celsius. These measurements show ordinary linear behavior of the first O-O distance, over the full temperature range, even through the density maximum. Conversely we do see interesting, non-linear behavior in the O-O distribution at higher separations distances, particularly around the 4.5Å peak. Another interesting feature of these measurements is the presence of a temperature-independent crossover point in the running O-O coordination number at the location of the first minimum in $r^2[g(r)-1]$, which defines the end of the first shell. At this 3.4(1)Å distance the O-O coordination number is 4.5(2) at all the temperatures studied. We believe this work offers important insight into some of the unusual physical properties of water, and provides a valuable validation point for the many Molecular dynamics models of liquid water.

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