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Handbook of chemistry and physics density of water

CRC Handbook of Chemistry and Physics 101st Edition Editor-in-Chief: John R. Rumble The 101st Edition of the Handbook of Chemistry and Physics print version is available for purchase here. We have calculated the model's water potential density—using the potential of effective pairwise additives (RER) and the potential of ab initio-derived many-body including polarizabilities (NEMO)—as a function of temperature at constant pressure. It was found that the model could not quantitatively reproduce the density of liquid water between 250 and 373 K. More disturbingly, there is no potential to indicate maximum density. Modifying the effective potential to provide the correct density at different temperatures reveals subtle changes in the importance of different water configurations. This configuration change is indicated as a possible cause of liquid water anomaly density behavior.¹ W. Blokzijl and J.B. F. N. Engberts, *Angew. Chem. Int. Ed. Engl.* 32, 1545 (1993). Google ScholarCrossref². 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