Supporting Information

Theoretical study of the dissociative photodetachment dynamics of the hydrated superoxide anion cluster

Yu Hashimoto, Kohei Saito, Toshiyuki Takayanagi[*]

Department of Chemistry, Saitama University, Shimo-Okubo 255, Saitama City, Saitama 338-8570, Japan

Hiroto Tachikawa

Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido 060-8628, Japan
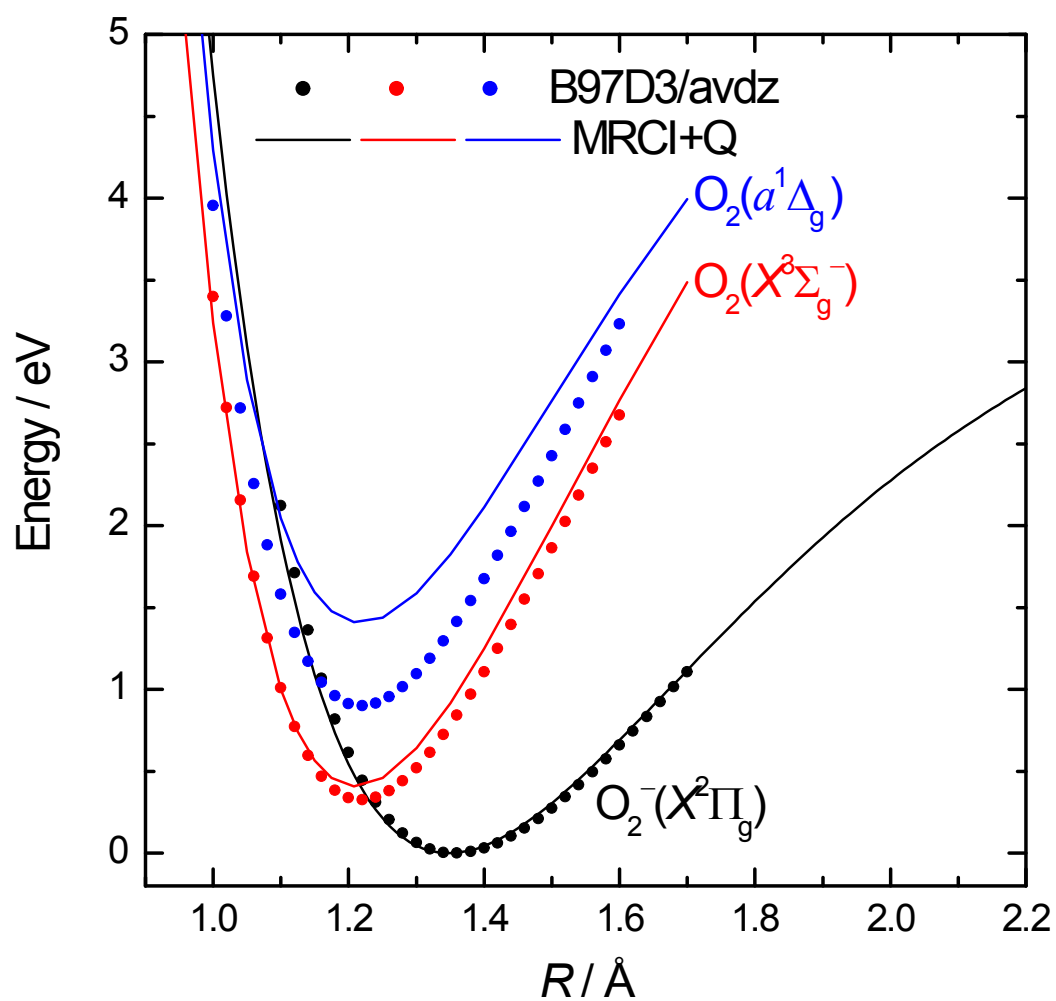
Fig. S1 Comparison of O_2/O_2^- potential energy curves calculated at the B97D3/aug-cc-pVDZ DFT level and MRCI+Q level (taken from the paper by Bytautas et al., *J. Chem. Phys.*, 2010, **132**, 074307).
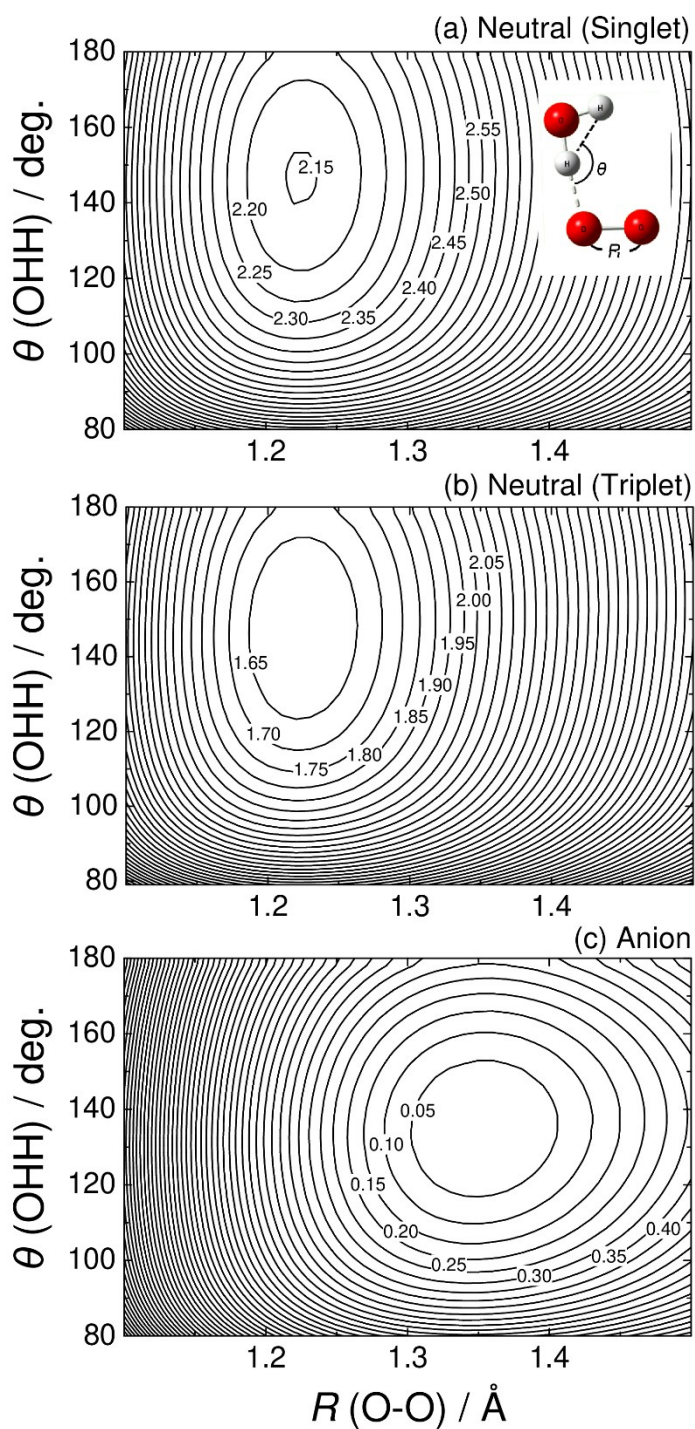
Fig. S2 Two-dimensional contour plots of the (a) neutral singlet, (b) neutral triplet, and (c) anionic states as a function of the OO distance and HHO angle, which are defined in panel (a). The contour increment was set to 0.05 eV and the energy is measured from the energy level of the most stable structure of $O_2^- \cdot H_2O$.
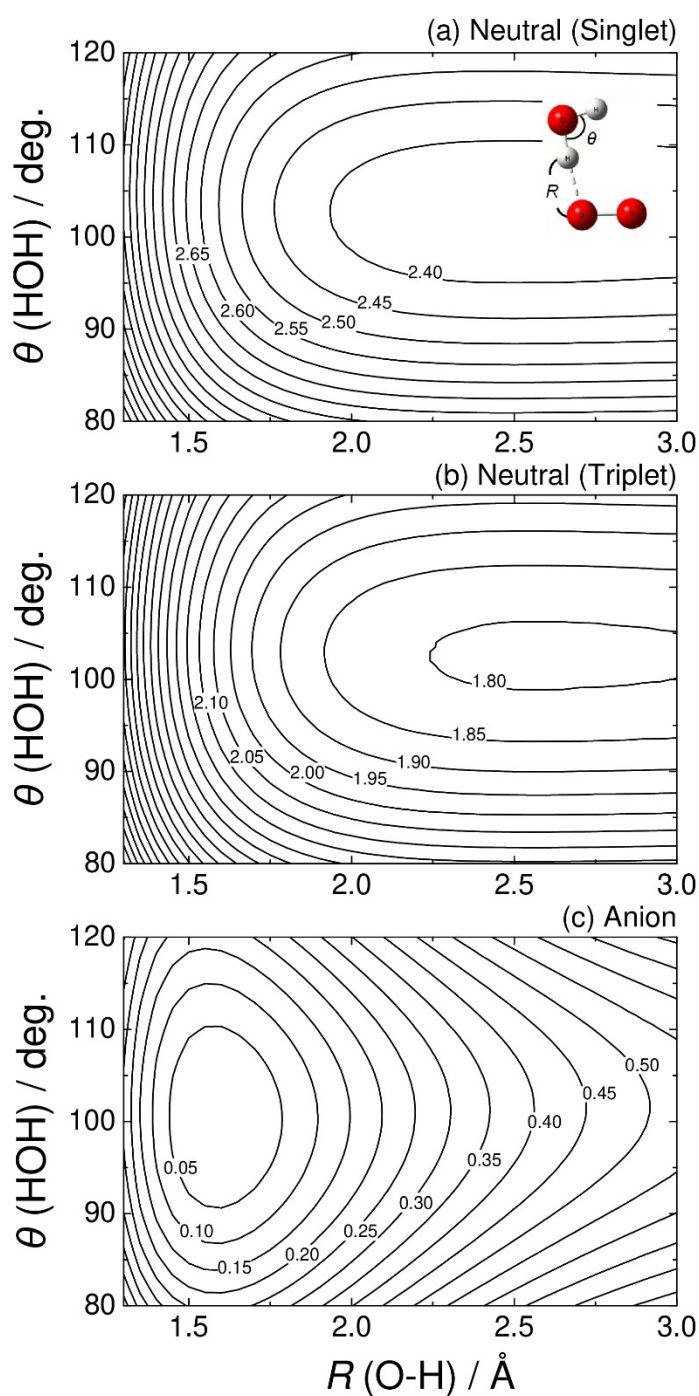
Fig. S3 Two-dimensional contour plots of the (a) neutral singlet, (b) neutral triplet, and (c) anionic states as a function of the OH distance and HOH angle, which are defined in panel (a). The contour increment was set to 0.05 eV and the energy is measured from the energy level of the most stable structure of $O_2^- \cdot H_2O$.
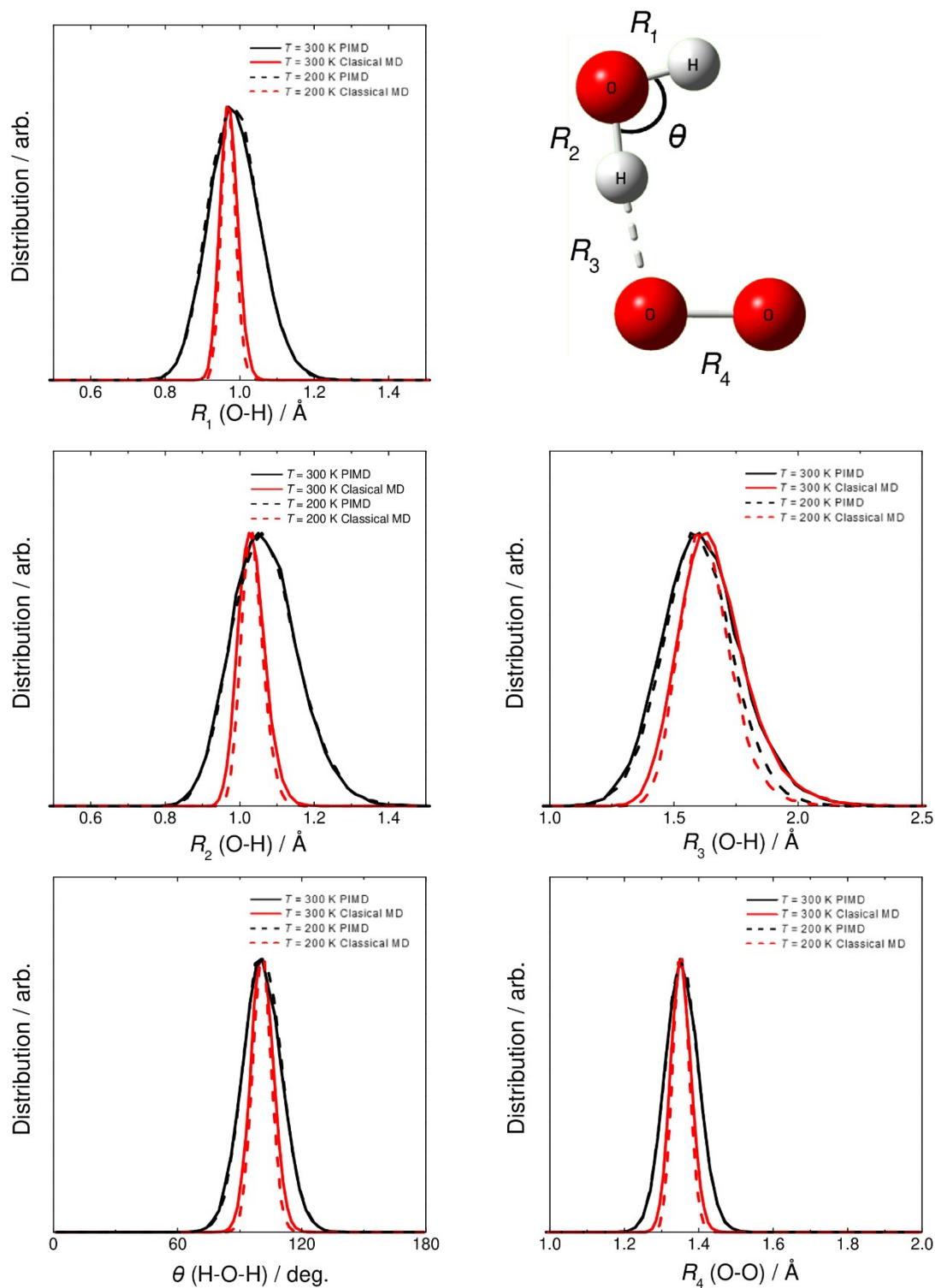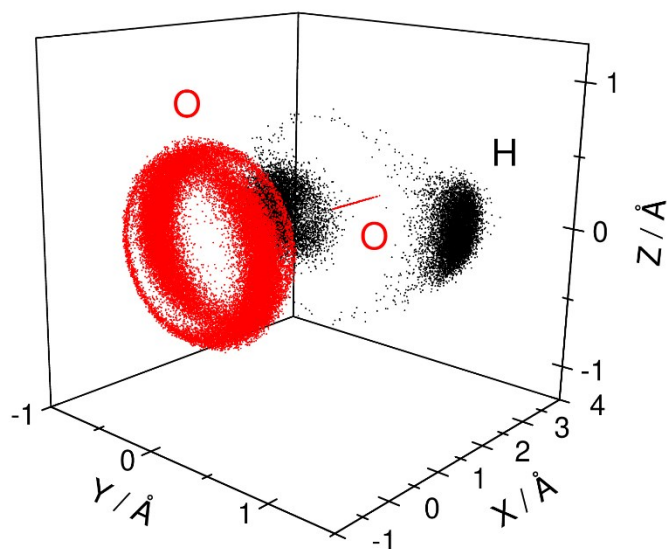
Fig. S4 Atom-atom distance distribution functions calculated using the PIMD and classical MD simulations at $T = 200$ K and 300 K.
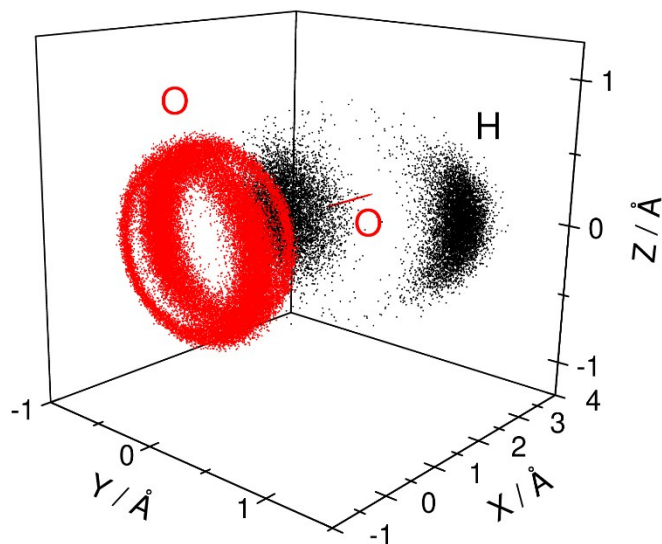
Fig. S5 Three-dimensional perspective plot of the nuclear probability distributions calculated using the (a) PIMD and (b) classical MD simulations at $T = 200$ K. In this plot, the center of mass of O_2 is fixed to the coordinate origin and the oxygen atom in H_2O is always located on the X-axis. In addition, the center of mass of the two hydrogen atoms in H_2O is always located at $Z = 0$.