Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Vibrational Spectral Simulation Connects Theoretical Cluster Structure Identification and Vibrational Spectral Evidence

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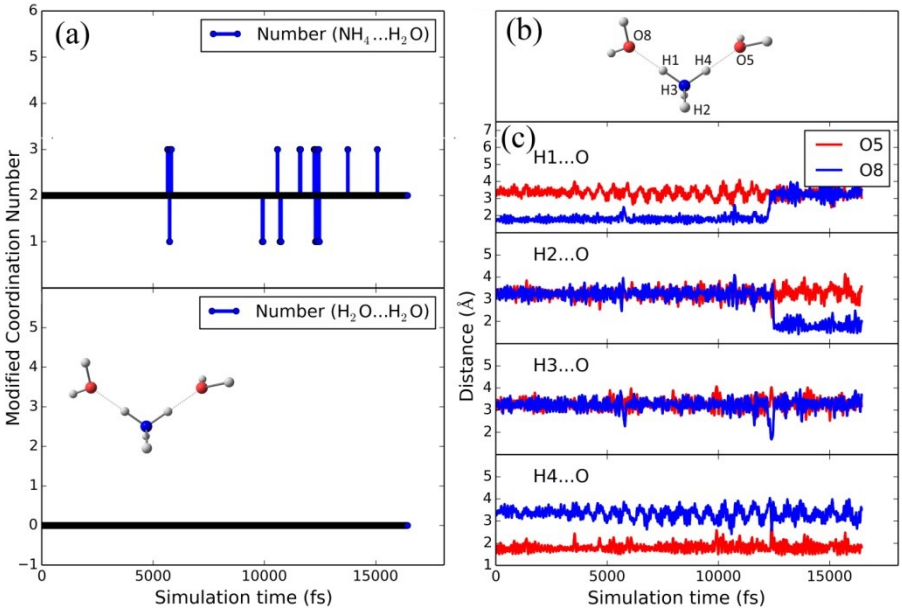

Figure S1. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 2a of $NH_4^+(H_2O)_2$; (b) the configuration of isomer 2a; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 2a.

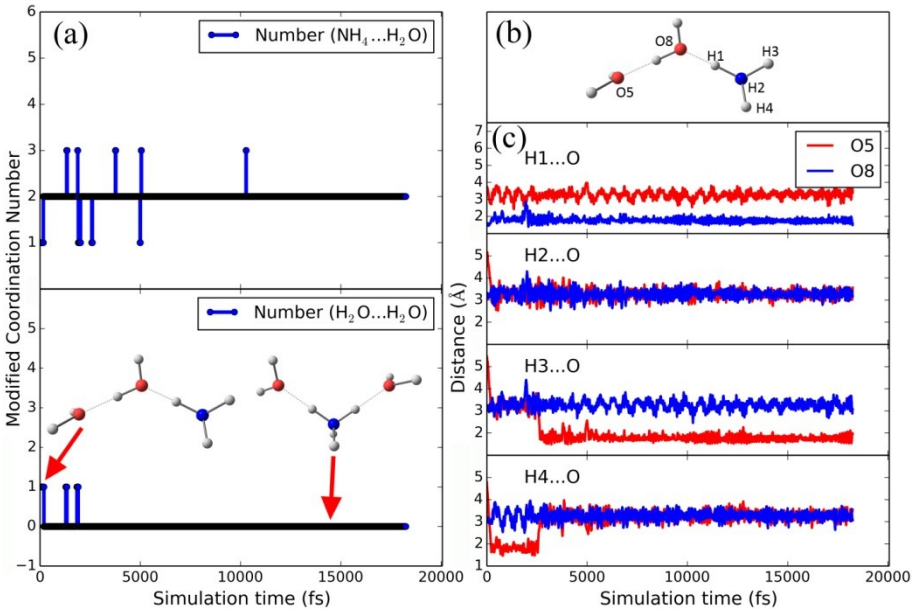

Figure S2. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 2b of $NH_4^+(H_2O)_2$; (b) the configuration of isomer 2b; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 2b.

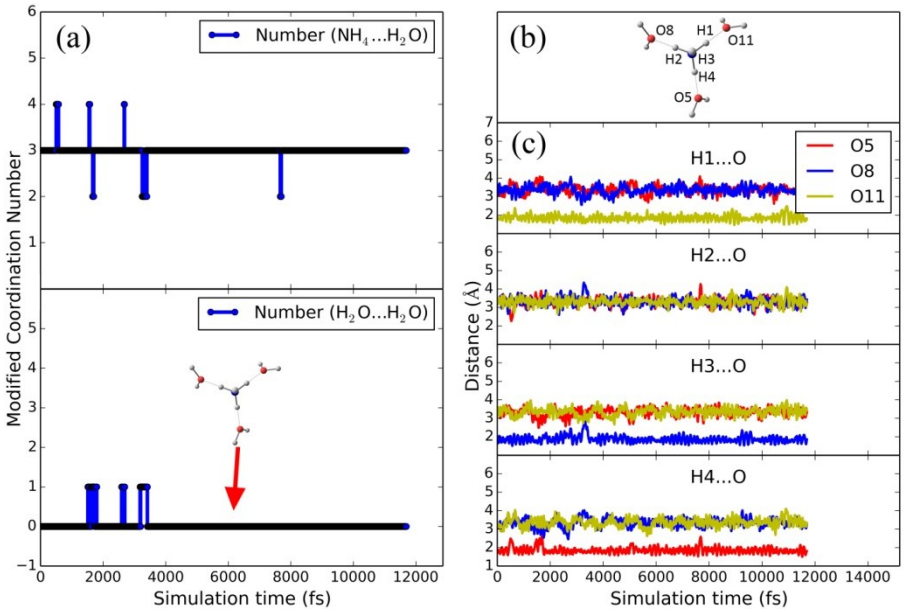

Figure S3. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 3a of $NH_4^+(H_2O)_3$; (b) the configuration of isomer 3a; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 3a.

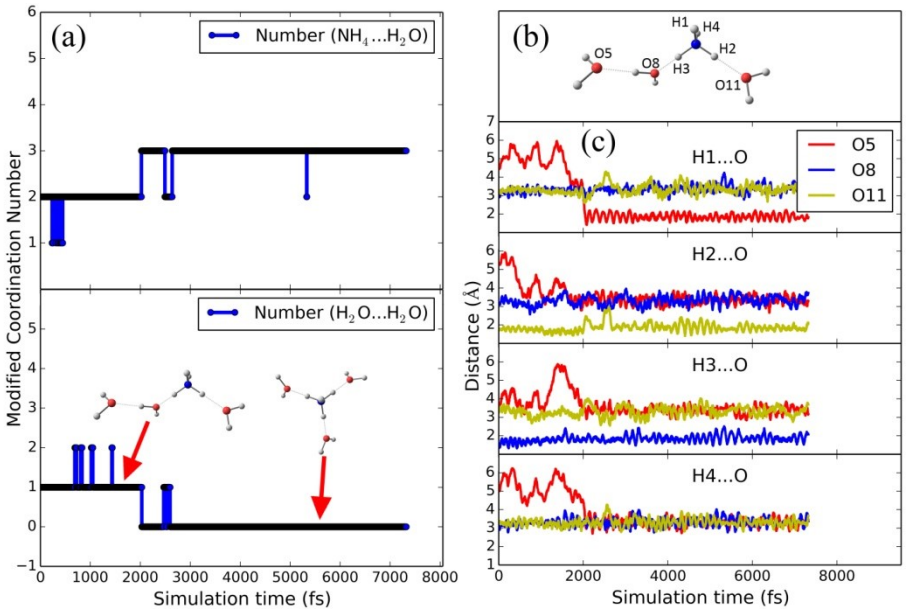

Figure S4. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 3b of $NH_4^+(H_2O)_3$; (b) the configuration of isomer 3b; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 3b.

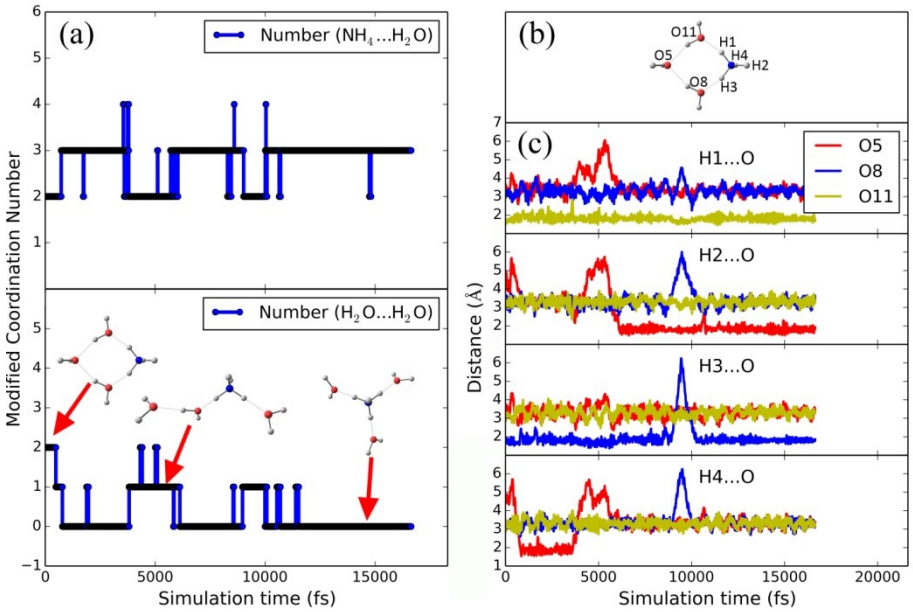

Figure S5. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 3c of $NH_4^+(H_2O)_3$; (b) the configuration of isomer 3c; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 3c.

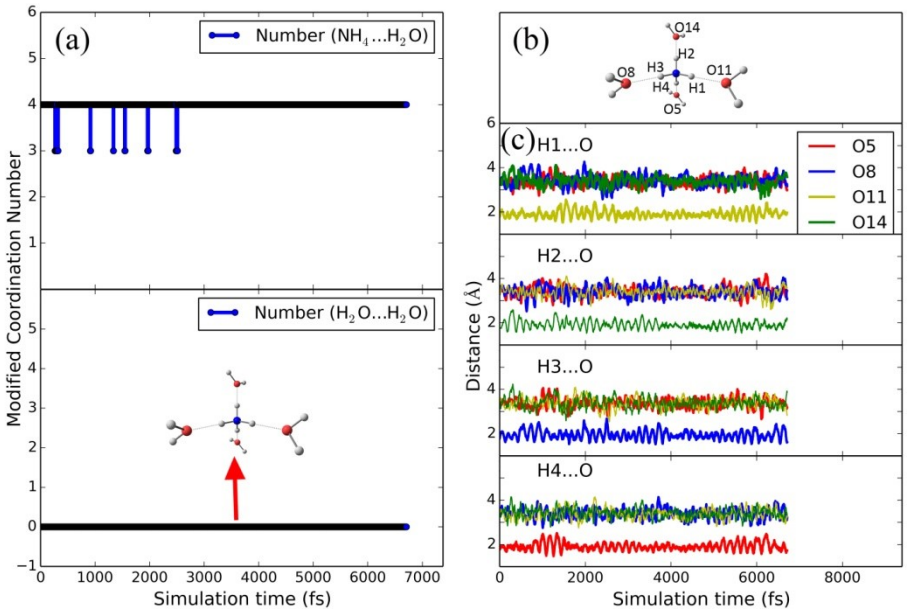

Figure S6. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 4a of $NH_4^+(H_2O)_4$; (b) the configuration of isomer 4a; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 4a.

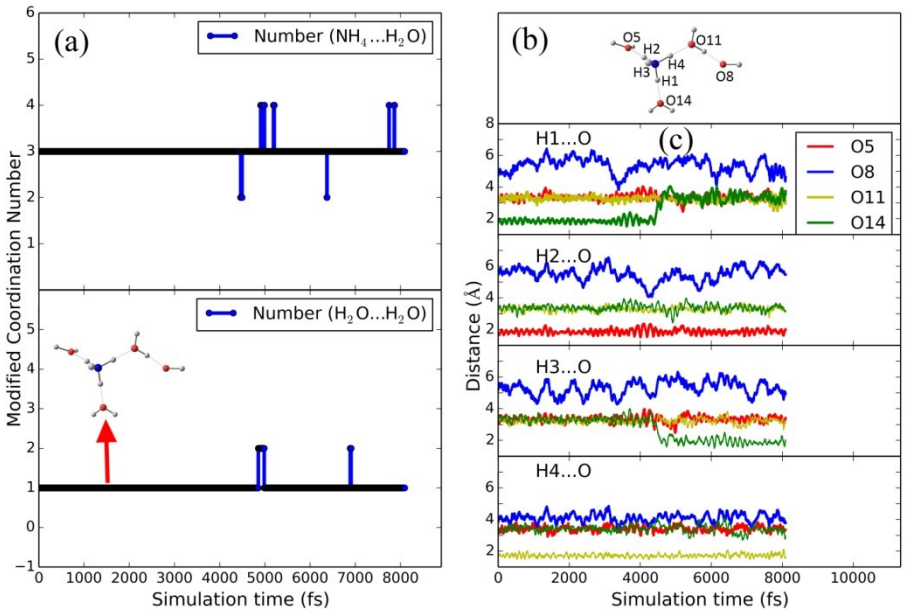

Figure S7. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 4b of $NH_4^+(H_2O)_4$; (b) the configuration of isomer 4b; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 4b.

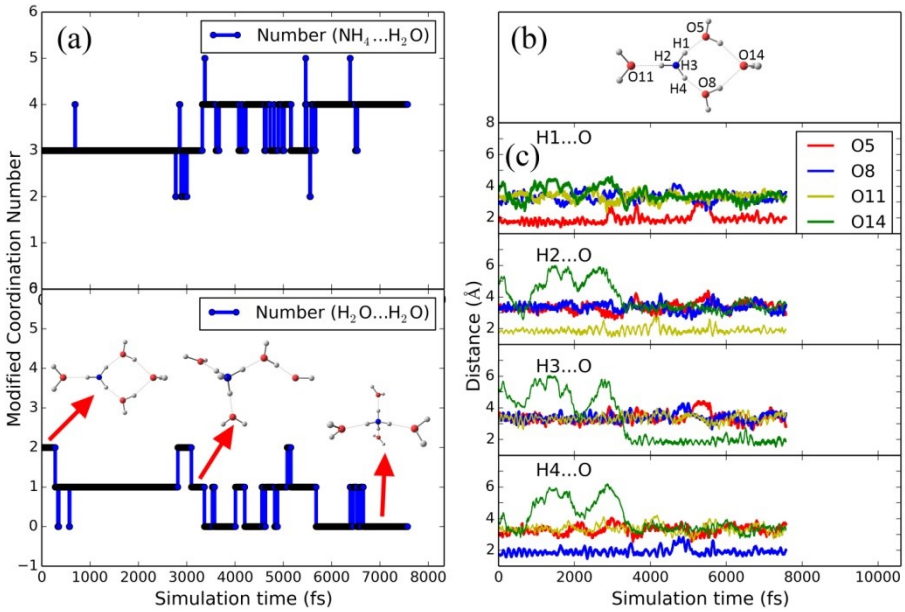

Figure S8. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 4c of $NH_4^+(H_2O)_4$; (b) the configuration of isomer 4c; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 4c.

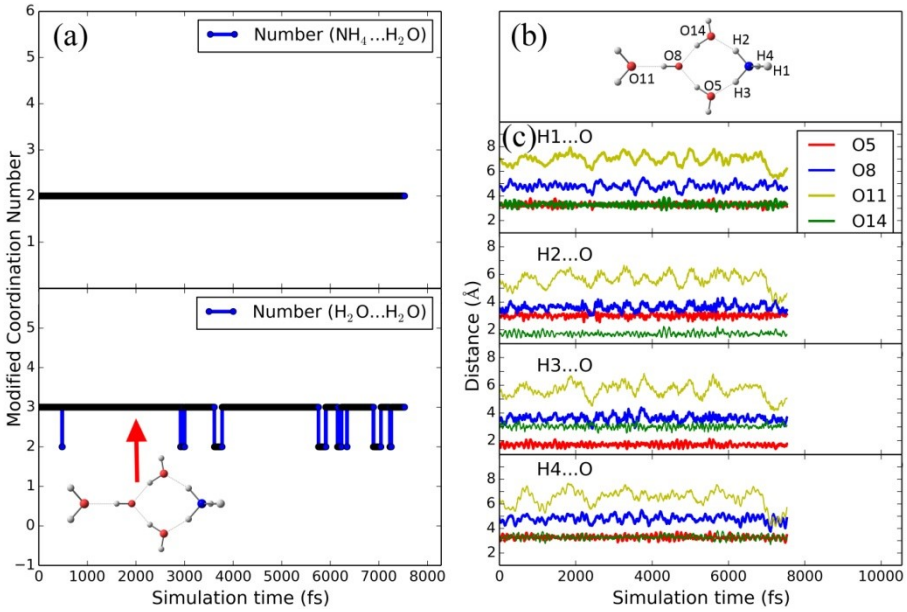

Figure S9. (a) The number of hydrogen bonding (NH…O and OH…OH) as a function of the simulation time in structural clustering for isomer 4d of $NH_4^+(H_2O)_4$; (b) the configuration of isomer 4d; and (c) the distance between atom H in $NH_4^+$and O in H_2O in as a function of the simulation time for isomer 4d.