Table S4   Drifts in the energies, temperature and velocity of proton in structure **E1-[1]** in the
S_1 state obtained from NVT-BOMD simulations at 350 K. Energies and velocity
are in atomic unit (au) and temperature is in K.

Property A	δ_A	$<A>$	σ_A
E^{Tot}	0.0272	-207.9685	0.0077
E^{Pot}	-0.0280	-207.9784	0.0056
E^{Kin}	0.0766	0.0099	0.0048
v^{H+}	0.2974	0.0015	0.0007
T	0.0766	346.6	168.13

δ_A = drift in property A; $<A>$ = average of property A; σ_A = SD of
property A; E^{tot} = total energy; E^{pot} = potential energy; E^{kin} = kinetic
energy; v^{H+} = velocity of proton in H-bond; T = temperature.