

**Table S3** Drifts in the energies, temperature and velocity of proton in structure **E1-[1]** in the  $S_1$  state obtained from NVT-BOMD simulations at 250 K. Energies and velocity are in atomic unit (au) and temperature is in K.

<b>Property A</b>	$\delta_A$	$\langle A \rangle$	$\sigma_A$
$E^{\text{Tot}}$	0.0566	-207.9748	0.0040
$E^{\text{Pot}}$	0.0639	-207.9819	0.0030
$E^{\text{Kin}}$	0.0130	0.0071	0.0030
$v^{\text{H}^+}$	-0.5205	0.0012	0.0005
T	0.0130	248.4	104.00

$\delta_A$  = drift in property A;  $\langle A \rangle$  = average of property A;  $\sigma_A$  = SD of property A;  $E^{\text{tot}}$  = total energy;  $E^{\text{pot}}$  = potential energy;  $E^{\text{kin}}$  = kinetic energy;  $v^{\text{H}^+}$  = velocity of proton in H-bond; T = temperature.