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

Supporting Information:

Excited State Hydrogen or Proton Transfer Pathways in microsolvated n-cyanoindole fluorescent probes

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In this document we show additional results that support the results and conclusions in the main paper. In Section 1 potential energy surfaces of all isomers studied are shown using alternative methods to the ones in the main paper. Section 2 shows the orbitals used in the CASSCF calculations. Section 3 discusses the charge transfer analysis used to determine whether hydrogen or proton transfer occurs. Section 4 discusses additional benchmarking studies used to determine the validity of our approach. Section 5 discusses implicit solvent results, and Section 6 shows the MD simulations used to determine the frequency of hydrogen bonding in aqueous solution. Lastly, section 7 provides cartesian coordinates for all relevant geometries.

S1. Potential Energy Surfaces

S1.1. Non-cyclic QM Clusters

Indole

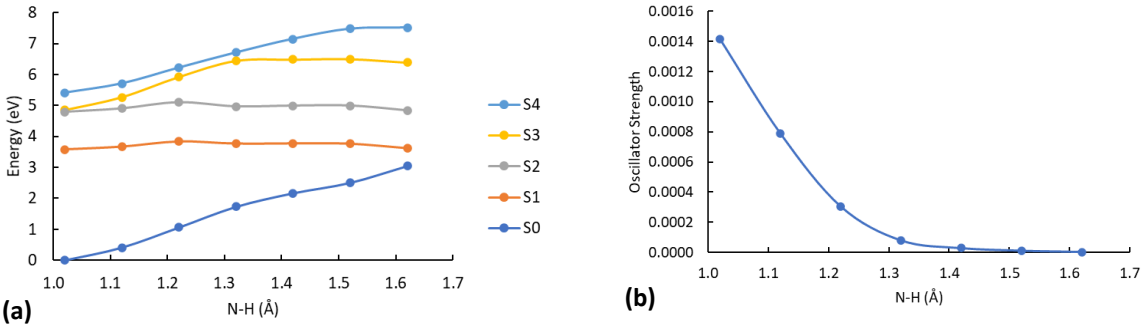


Figure S1: **(a)** PES of the S_0 and four singlet electronically excited states, S_1-S_4, of Ind-$(H_2O)_1$ computed along the N-H bond coordinate at the CASSCF(12,11)/aug-cc-pVDZ from geometries optimized using CAM-B3LYP/6-311++G(d) level of theory. **(b)** The oscillator strength corresponding to the PES of the S_1 as a function of N-H bond stretch.

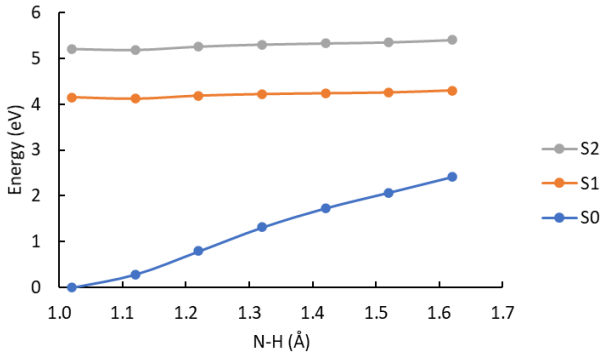


Figure S2: **(a)** PES of the electronic ground state, S_0, and first and second electronic excited states S_1 and S_2 of Ind-$(H_2O)_1$ and (b) corresponding oscillator strength of S_1 state computed along the dissociative N-H coordinate at the CASPT2/aug-cc-pVDZ level of theory using geometries optimized at the CAMB3LYP/6-311++G(d) level of theory.

3-Cyanoindole (3-CNI)

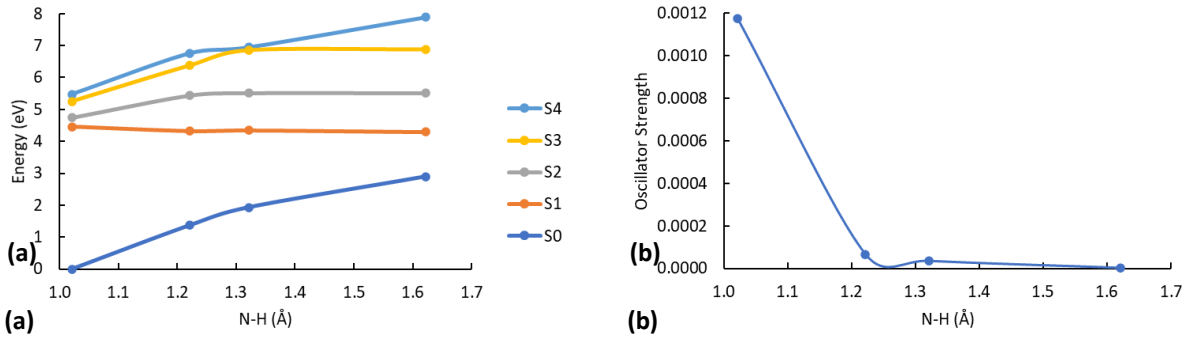


Figure S3: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 3-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASSCF (14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311++G(d) level of theory. **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

4-Cyanoindole (4-CNI)

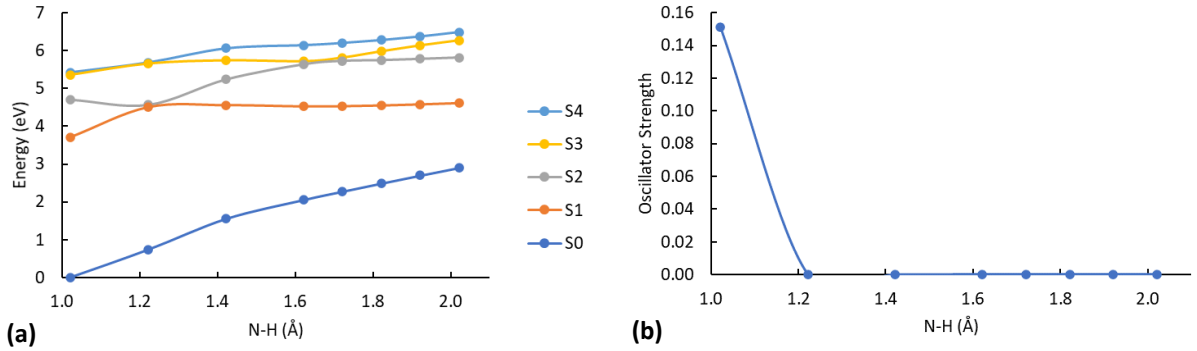


Figure S4: **(a)** PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 4-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) level of theory from geometries optimized using ADC(2)/aug-cc-pVDZ level of theory. **(b)** Oscillator strength corresponding to the PES of the S_1 as a function of N-H bond stretch.

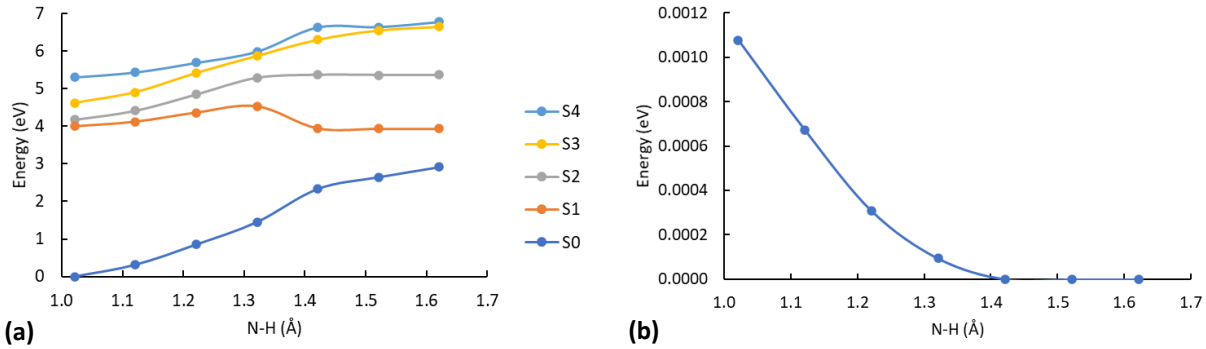


Figure S5: **(a)** PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 4-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASSCF(14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311+G(d). **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

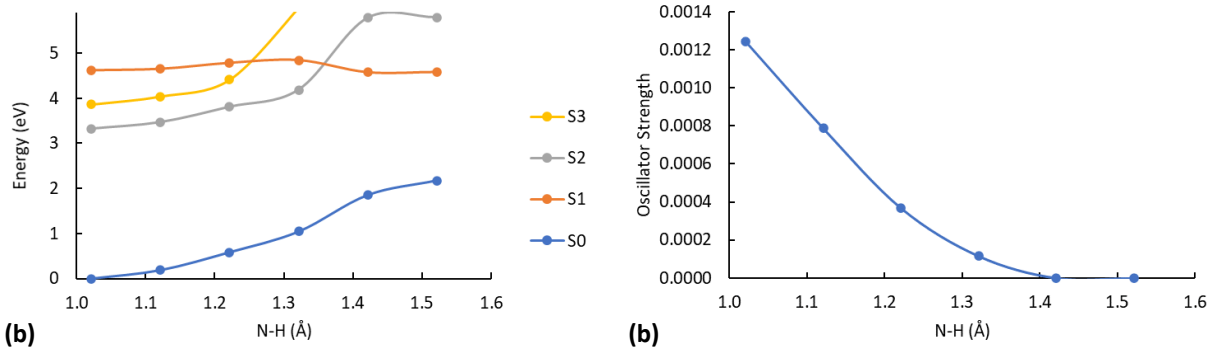


Figure S6: **(a)** PES of the S_0 and three singlet electronically excited states, S_1-S_3, of 4-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASPT2(14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311++G(d). **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch. The order of the excited states corresponds to that in CASSCF calculation in Figure S9.

5-Cyanoindole (5-CNI)

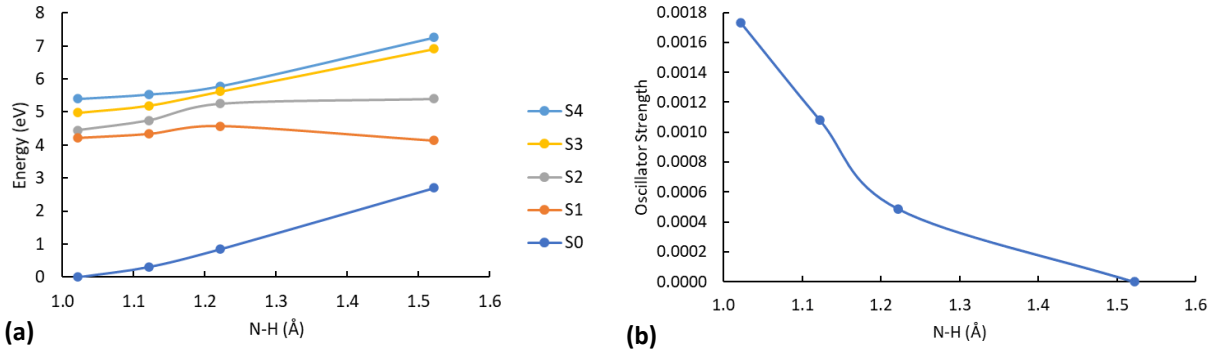


Figure S7: **(a)** PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 5-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASSCF(14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311++G(d). **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

Figure S8 shows the CASSCF PES along S1 for all non-cyclic isomers. The results are qualitatively similar to the EOM-CCSD PES shown in Figure 4 in the main paper. However, the oscillator strengths at the CASSCF level indicate that the S1 state has a small oscillator strength even initially at its minimum, indicating a πσ* character even at the S1 minimum. This probably affects the barrier height.

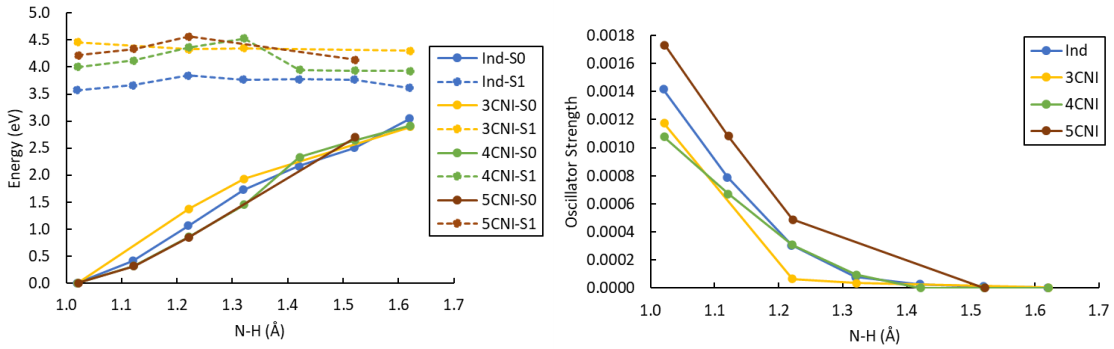


Figure S8: **(a)** PES of the S_0 and S_1 states for Ind-$(H_2O)_1$, 3-CNI-$(H_2O)_2$, 4-CNI-$(H_2O)_2$, and 5-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASSCF(14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311++G(d). **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

S1.2 CYCLIC Clusters

2-Cyanoindole (2-CNI)

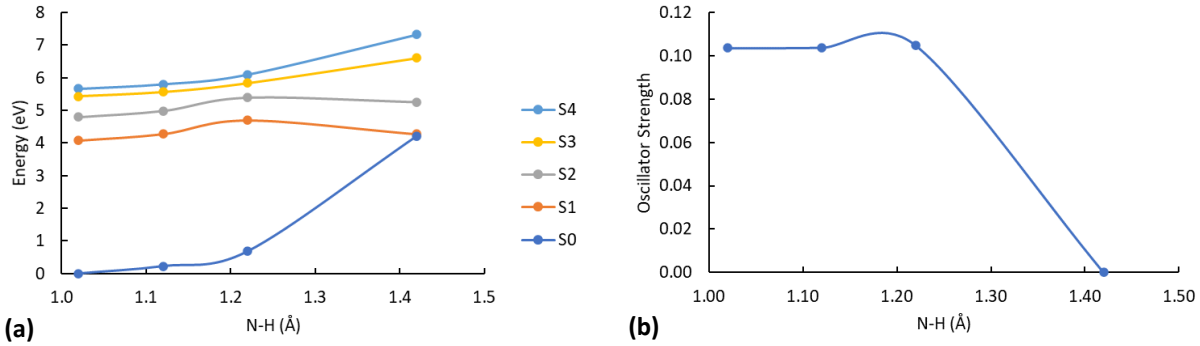


Figure S9: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 2-CNI-$(H_2O)_1$ computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) level of theory from geometries optimized using ADC(2)/ aug-cc-pVDZ level of theory. (b) Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

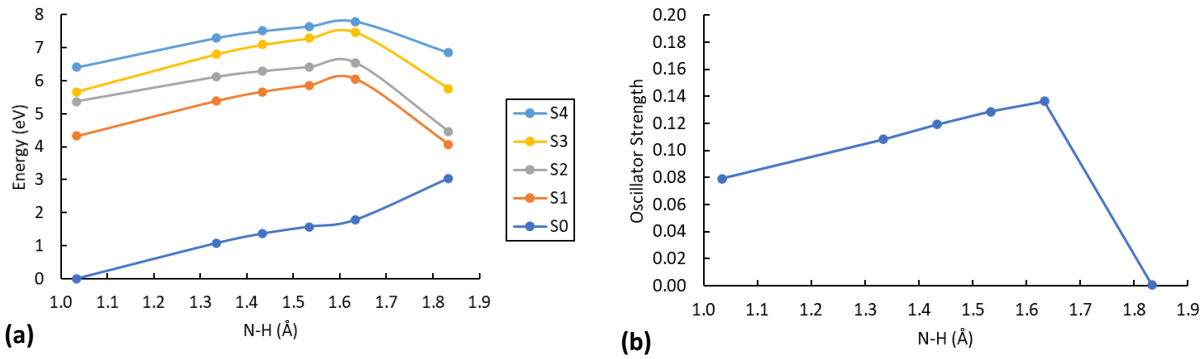


Figure S10: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 2-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASSCF(14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311++G(d) (b) Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

7-Cyanoindole (7-CNI)

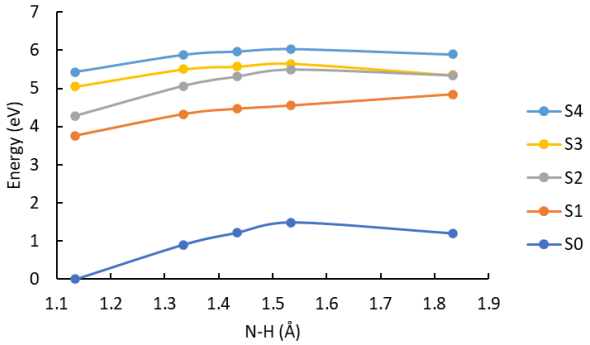


Figure S11: PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 7-CNI-$(H_2O)_1$ computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) level of theory from geometries optimized using ADC(2)/aug-cc-pVDZ level of theory.

6-Cyanoindole (6-CNI)

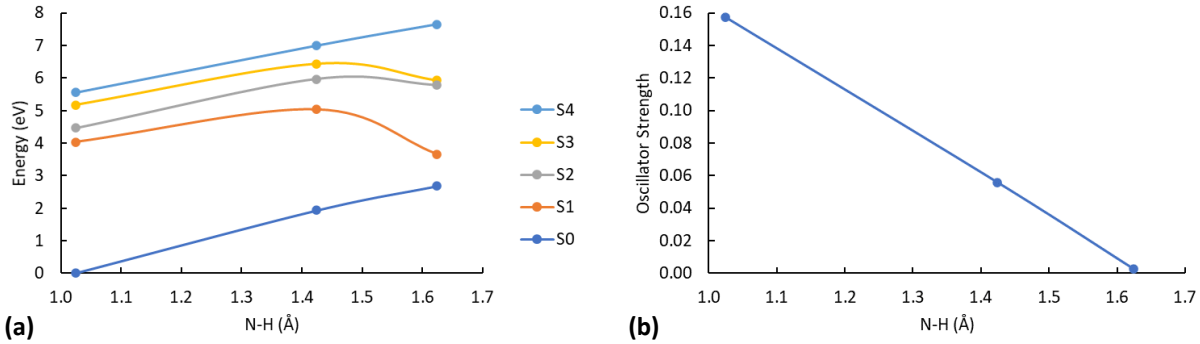


Figure S12: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 6-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) level of theory from geometries optimized using ADC(2)/aug-cc-pVDZ level of theory. **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

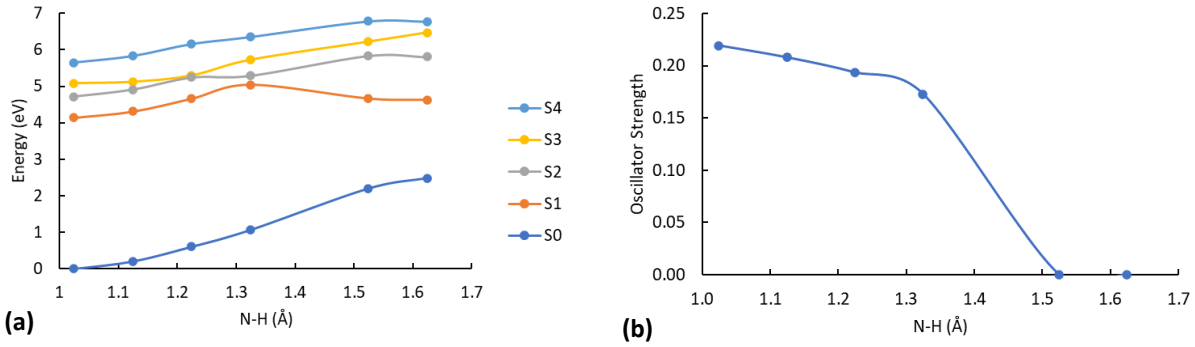


Figure S13: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 6-CNI-$(H_2O)_1$ computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) level of theory from geometries optimized using CAM-B3LYP/6-311++G(d) level of theory. **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

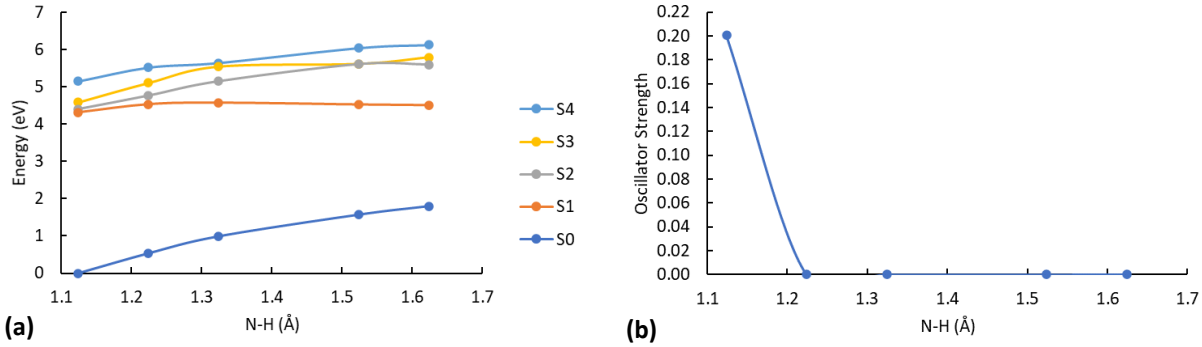


Figure S14: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 6-CNI-$(H_2O)_1$ computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) level of theory from geometries optimized using ADC(2)/aug-cc-pVDZ level of theory. **(b)** Oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

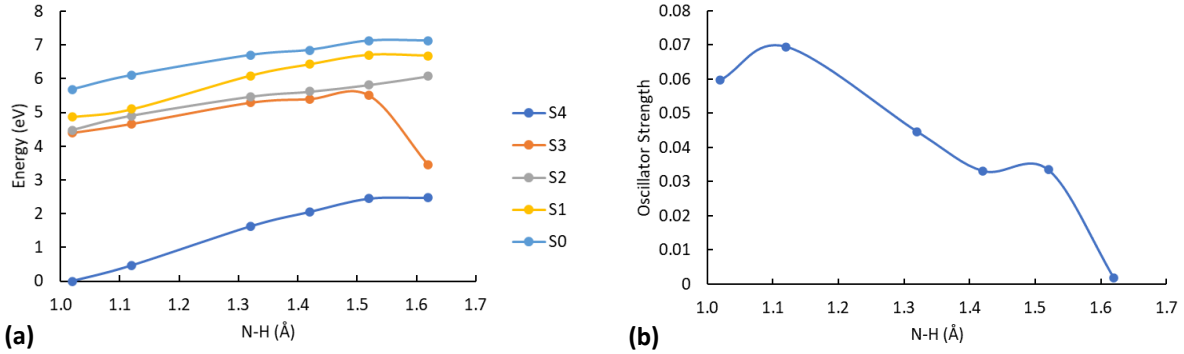


Figure S15: (a) PES of the S_0 and four singlet electronically excited states, S_1-S_4, of 6-CNI-$(H_2O)_2$ computed along the N-H bond coordinate at the CASSCF(14,13)/aug-cc-pVDZ level of theory from geometries optimized using CAM-B3LYP/6-311++G(d). **(b)** The oscillator strength corresponding to the S_1 excited state as a function of N-H bond stretch.

S1.3 One vs two water molecules

In the main text it is shown that for 5-CNI the barrier is sensitive to the number of water molecules hydrogen bonded to it. Here two examples are shown for 3CNI and 4CNI which demonstrate that the barrier is not sensitive to the number of water molecules for these systems.

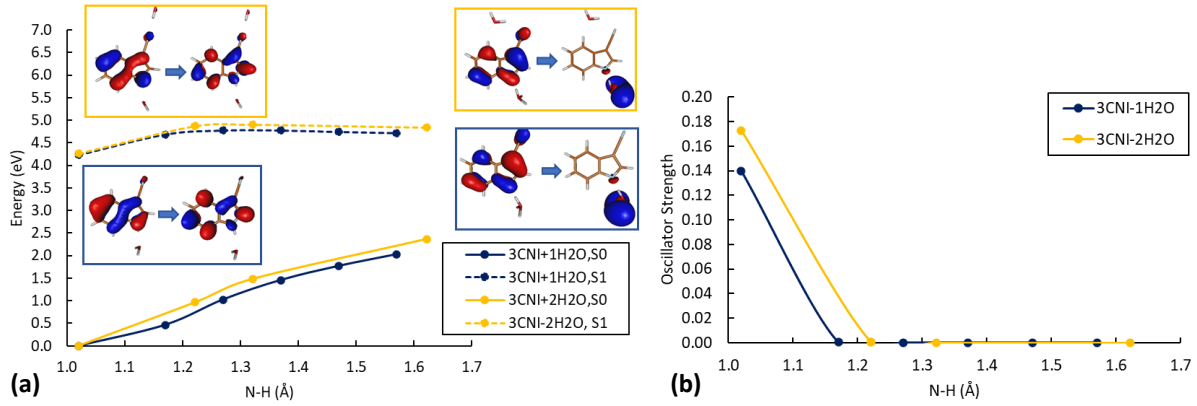


Figure S16: (a) The PES of the electronic ground state, $S_{0,}$ (solid curves) and singlet electronically excited S_1 state (dotted curves), of 3-CNI with one (blue curves) and two H_2O (yellow curve) clusters and **(b)** corresponding oscillator strength of the S_1 state computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) from geometries optimized at the CAM-B3LYP/6-311++G(d) level of theory with the exception of the S_1 minimum geometry. The $S_1(L_b)$ min geometry were optimized at the CC2/aug-cc-pVDZ level of theory. The natural transition orbitals depict the character of the S_1 minimum on the right and that of the last geometry on the left. All methods show that the character of the excited state at the last geometry of the 3-CNI-$(H_2O)_{1\text{-}2}$ clusters after ESHT takes place is a πσ* state.

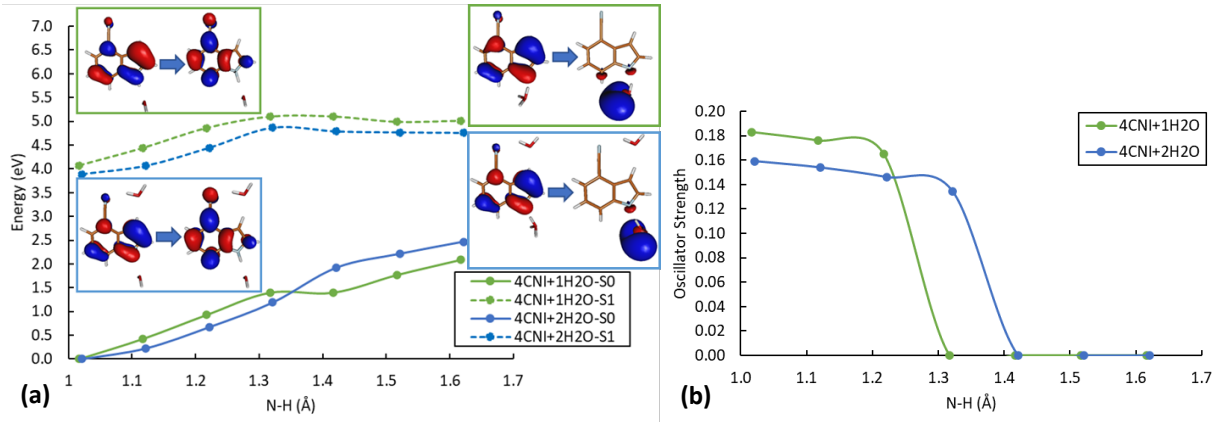


Figure S17: **(a)** PES of the electronic ground state, $S_{0,}$ (solid curves) and singlet electronically excited S_1 state (dotted curves), of 4-CNI with 1 (green curves) and 2 H_2O (blue curves) clusters and **(b)** corresponding oscillator strength of the S_1 state computed along the N-H bond coordinate at the EOMCCSD/6-311++G(d) from geometries optimized at the CAM-B3LYP/6-311++G(d) level of theory. The natural transition orbitals depicting the character of the S_1 minimum on the right and that of the last geometry on the left.

S1.4 Conical Intersections

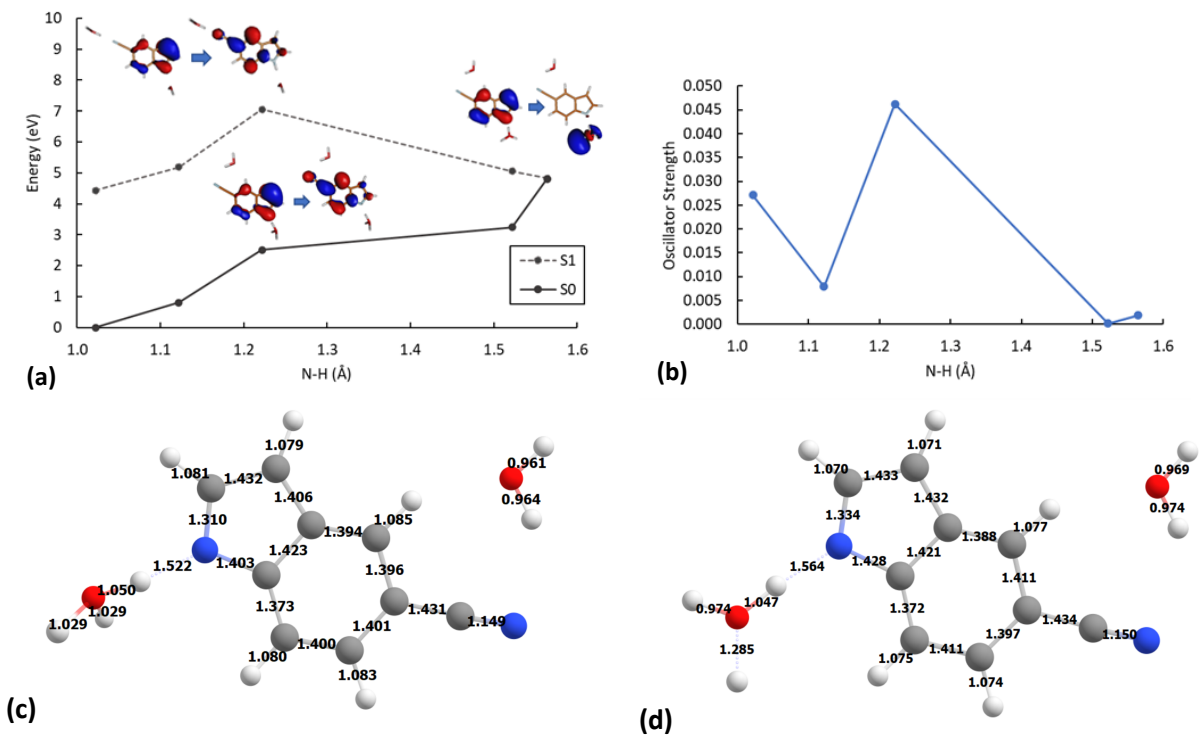
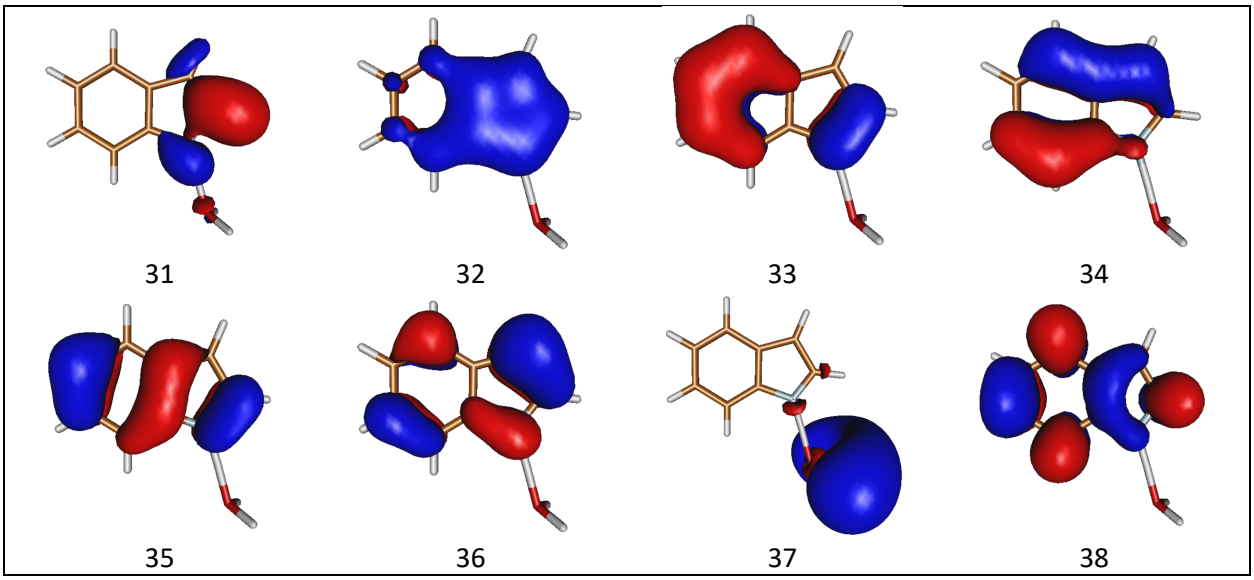


Figure S18: (a) Linear interpolation connecting the S1 minimum to the conical intersection between S1-S0 computed with CASSCF(14,13) and contracted segmented basis set aug-Seg-pc-0 for the 5-CNI-$(H_2O)_2$ cluster. The character of the excited state at the S_1 minimum (left), the energy barrier at 1.2 Å (middle), and at the conical intersection (last image on the right) is illustrated by the transition from the bonding and anti-bonding molecular orbitals involved in the active space. (b) corresponding oscillator strengths; (c) N-H 1.52 A and (d) Conical intersection geometry.

S2. Molecular Orbitals used in CASSCF active space



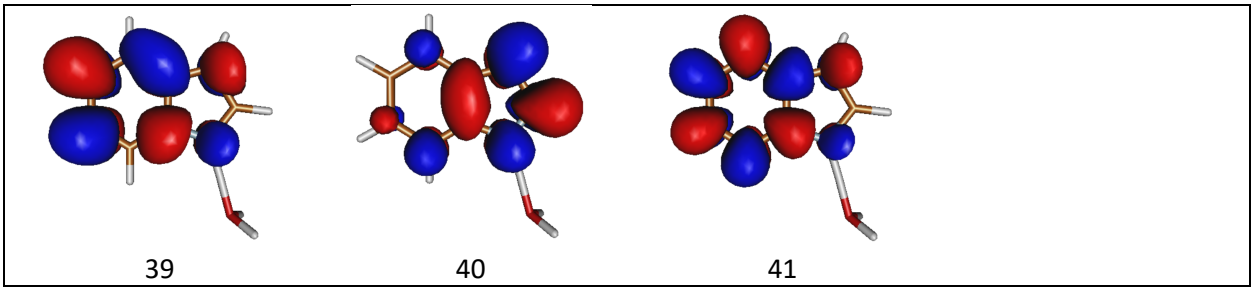
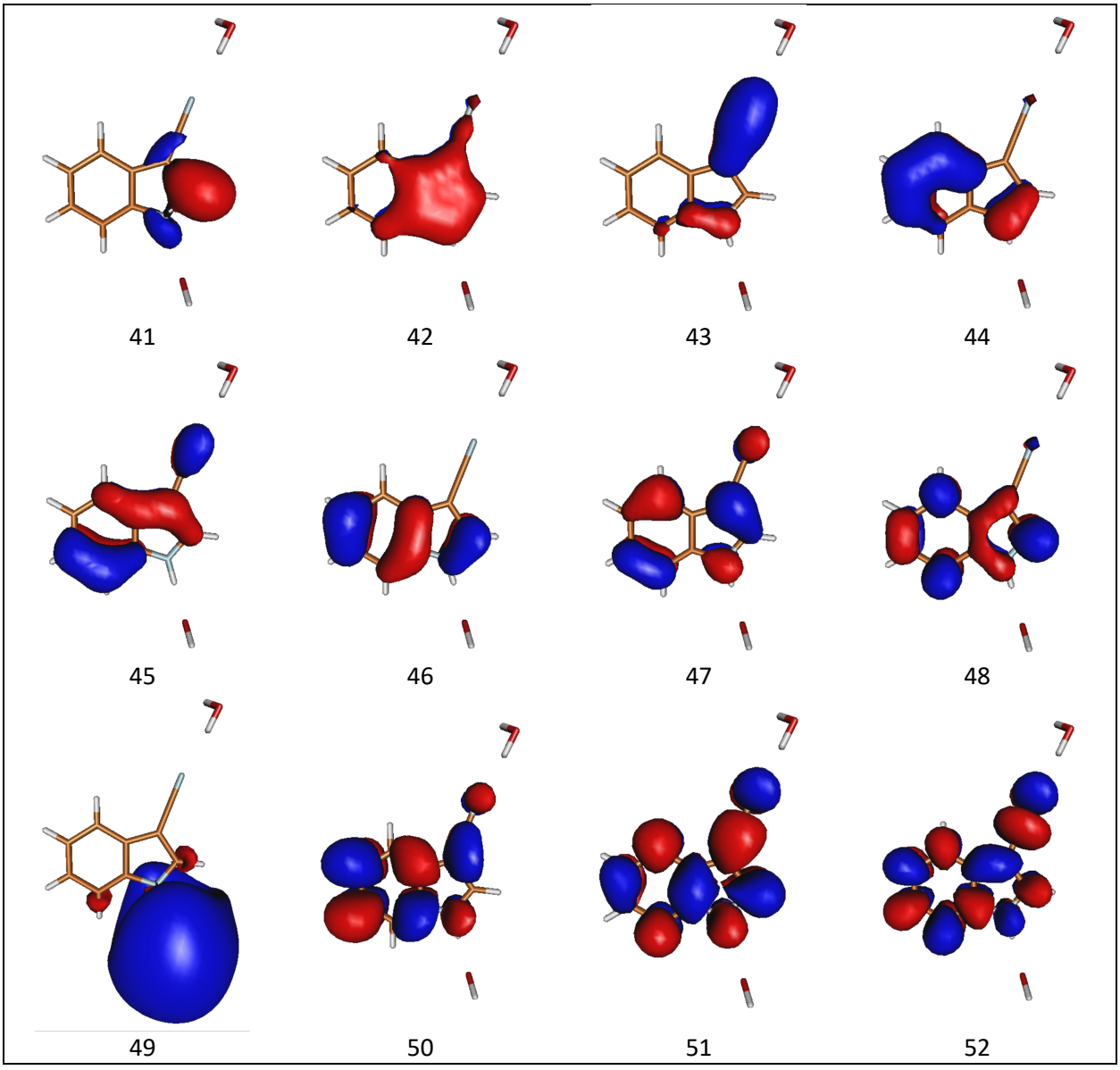


Figure S19: The molecular orbitals in the (12,11) active space of indole-$(H_2O)_1$ used to compute the PES of the electronic ground and singlet excited states at the CASSCF/aug-cc-pVDZ level of theory.



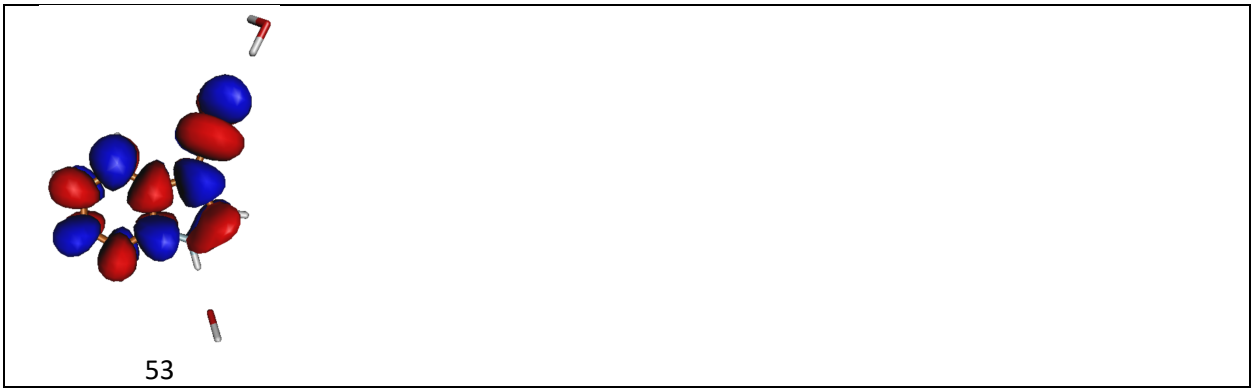
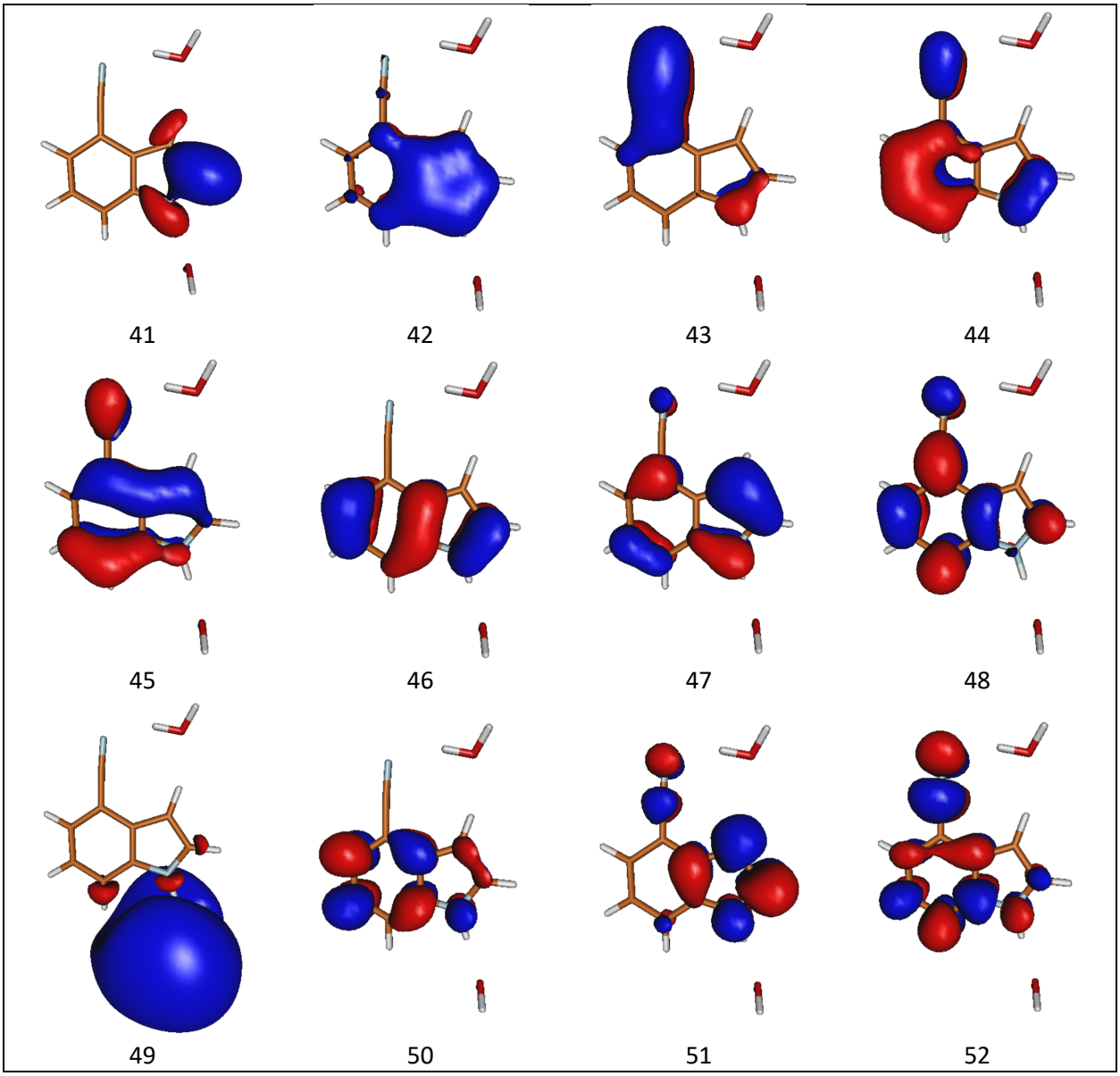


Figure S20: The molecular orbitals in the (14,13) active space of 3-CNI-$(H_2O)_2$ used to compute the PES of the electronic ground and singlet excited states at the CASSCF/aug-cc-pVDZ level of theory.



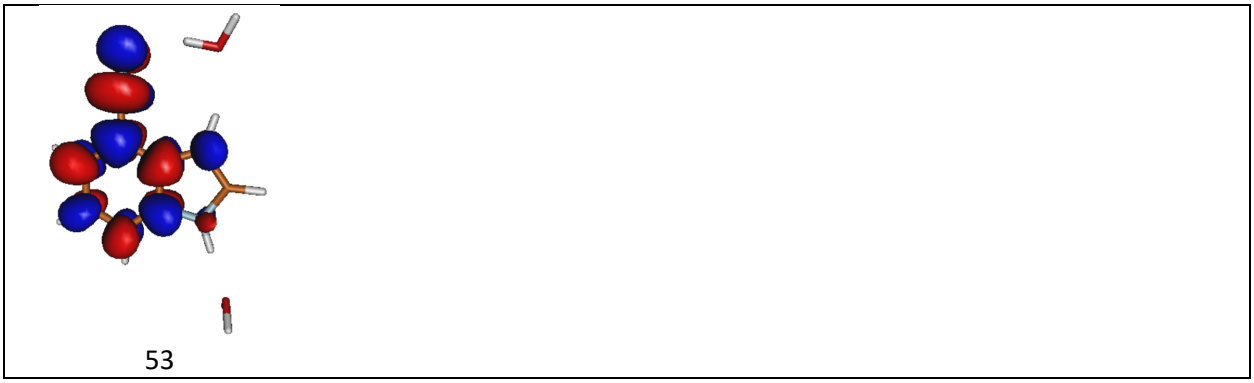


Figure S21: The molecular orbitals in the (14,13) active space of 4-CNI-$(H_2O)_2$ used to compute the PES of the electronic ground and singlet excited states at the CASSCF/aug-cc-pVDZ level of theory.

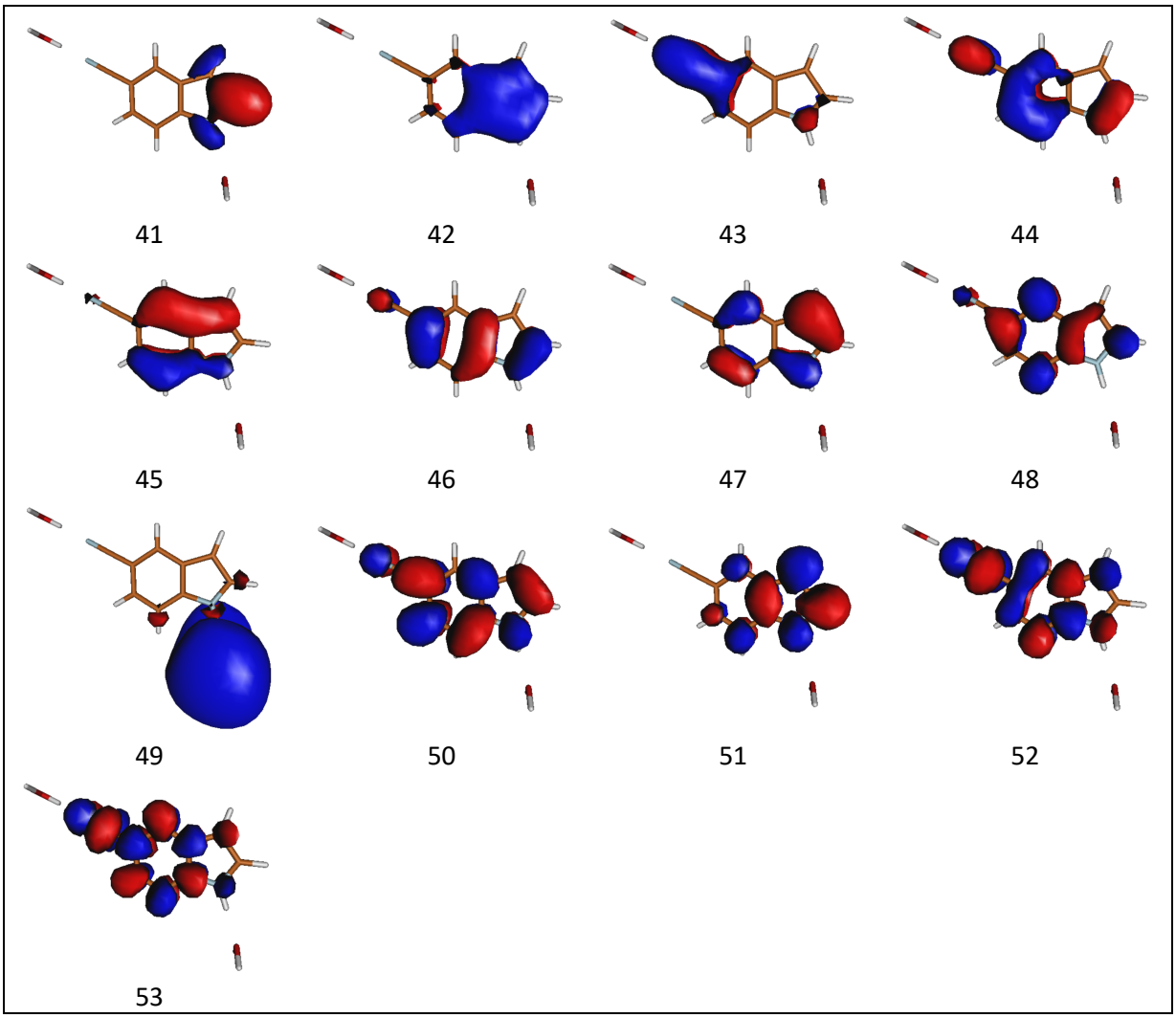


Figure S22: The molecular orbitals in the (14,13) active space of 5-CNI-$(H_2O)_2$ used to compute the PES of the electronic ground and singlet excited states at the CASSCF/aug-cc-pVDZ level of theory.

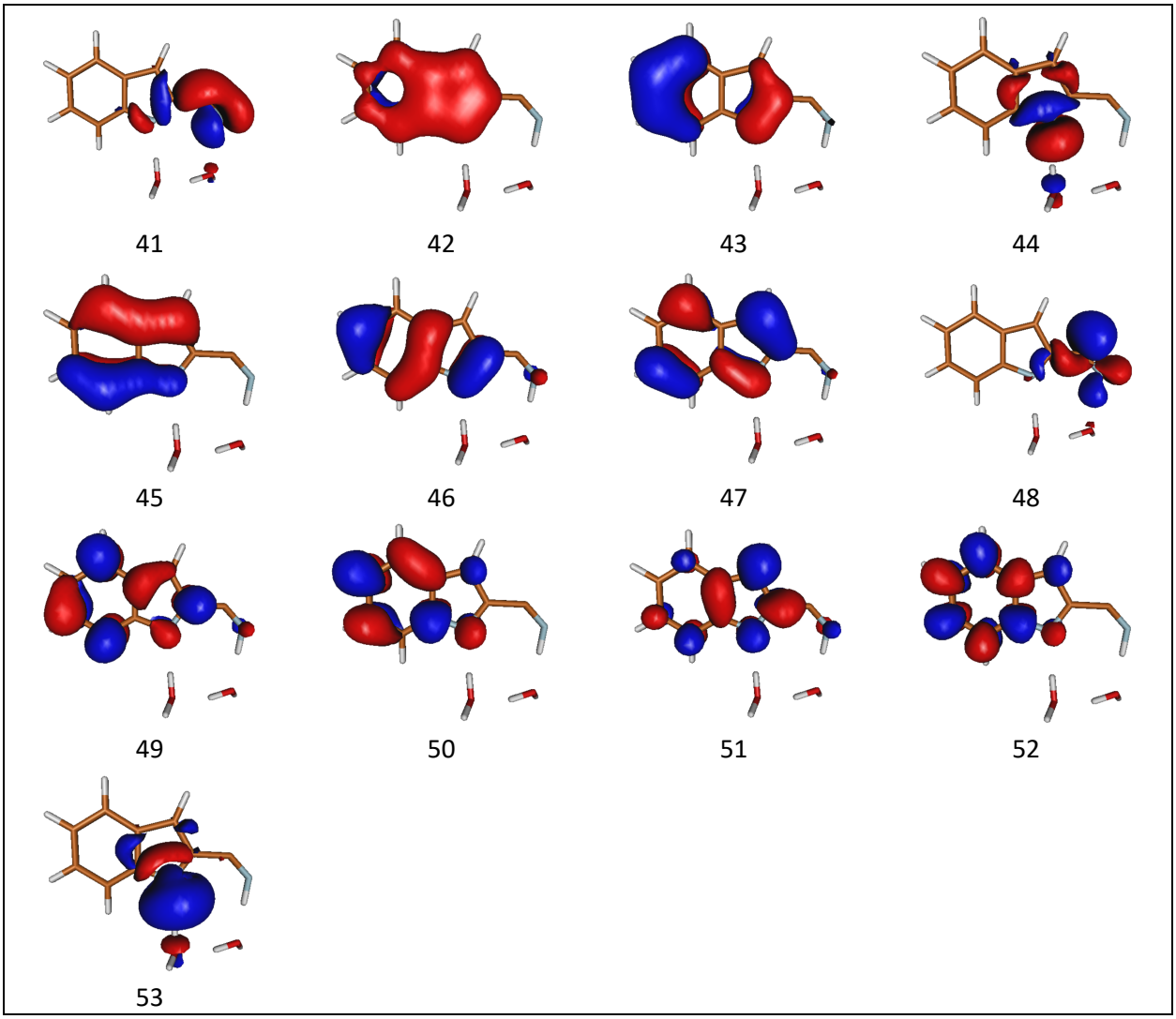
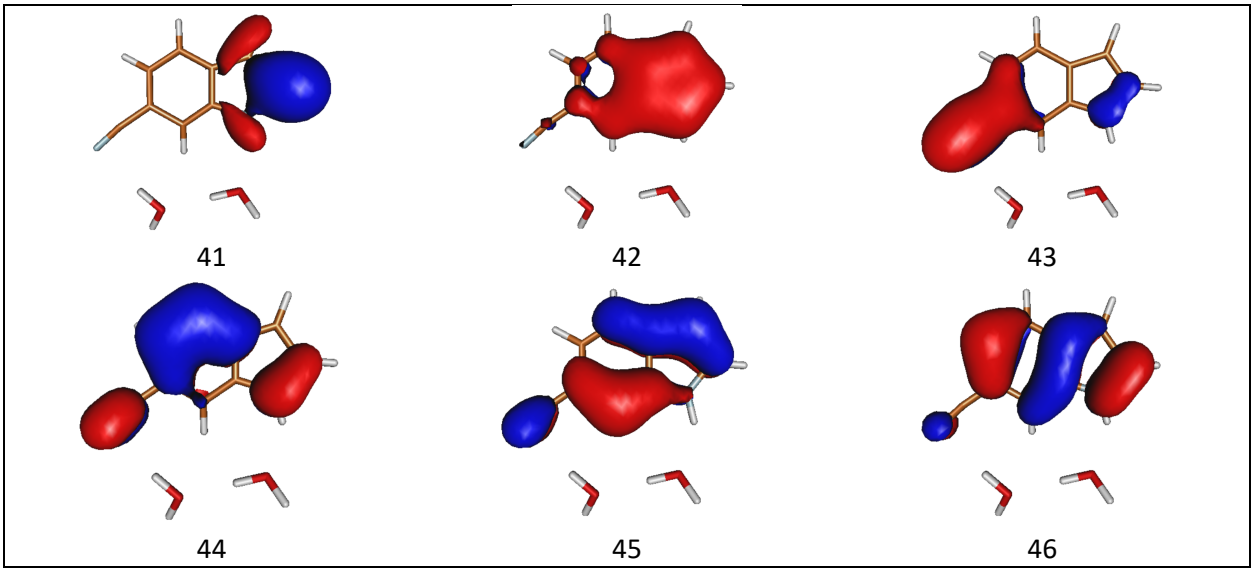


Figure S23: The molecular orbitals in the (14,13) active space of 2-CNI-$(H_2O)_2$ used to compute the PES of the electronic ground and singlet excited states at the CASSCF/aug-cc-pVDZ level of theory.



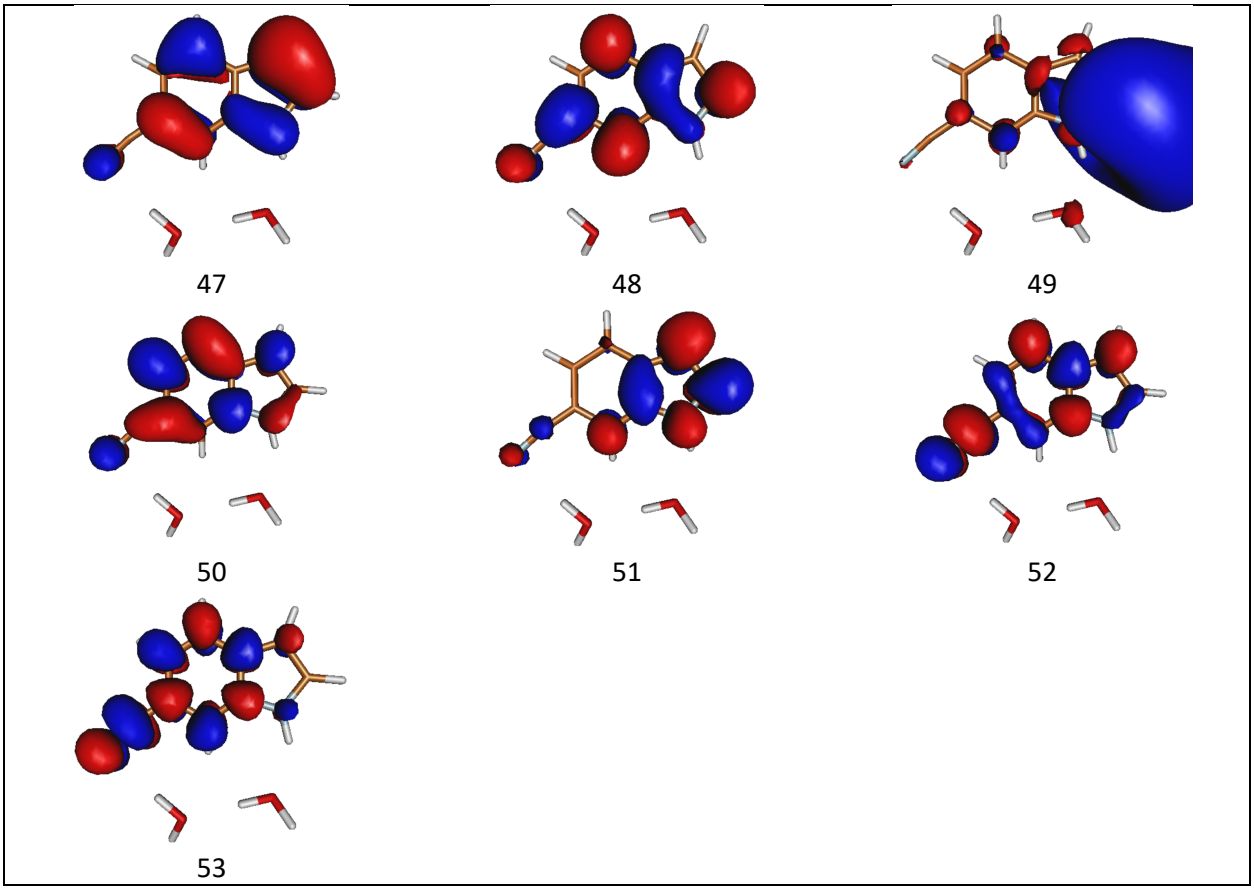


Figure S24: The molecular orbitals in the (14,13) active space of 6-CNI-$(H_2O)_2$ used to compute the PES of the electronic ground and singlet excited states at the CASSCF/aug-cc-pVDZ level of theory.

S3. Charge Transfer Analysis

This section shows the charges calculated using CHELPG at the initial and final geometries of the PES in order to determine whether hydrogen or proton transfer occurs.

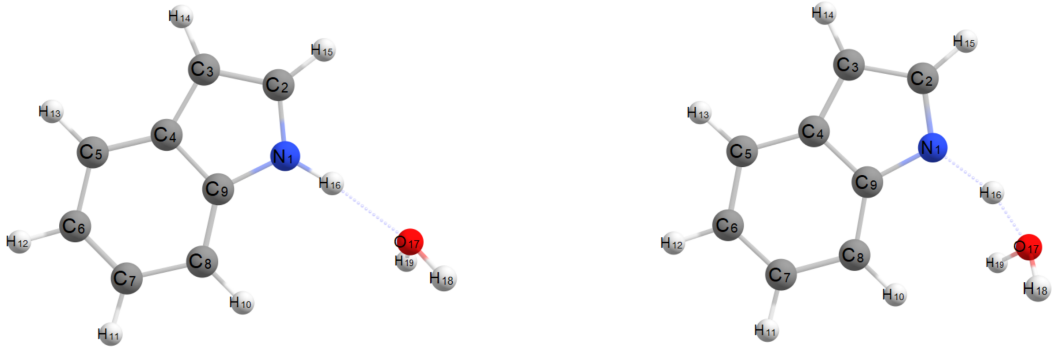
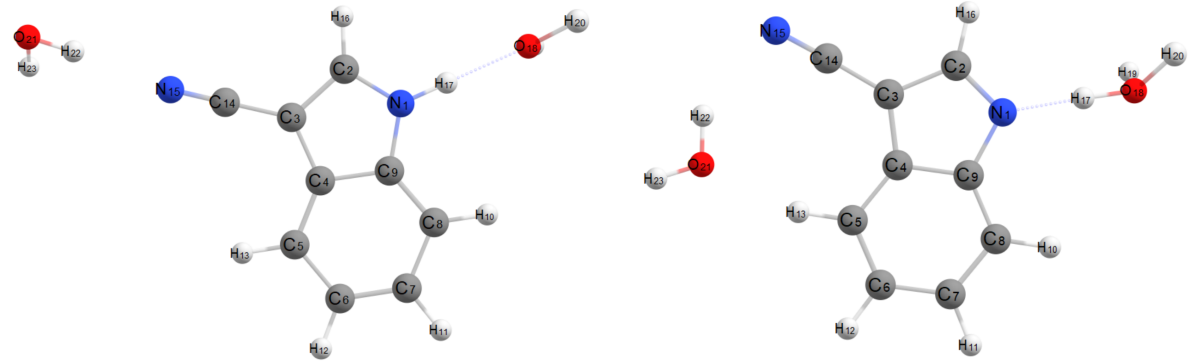


Table S1: ChelpG charges of Indole and 1 H_2O at the EOMCCSD/6-311+G(d) level of theory

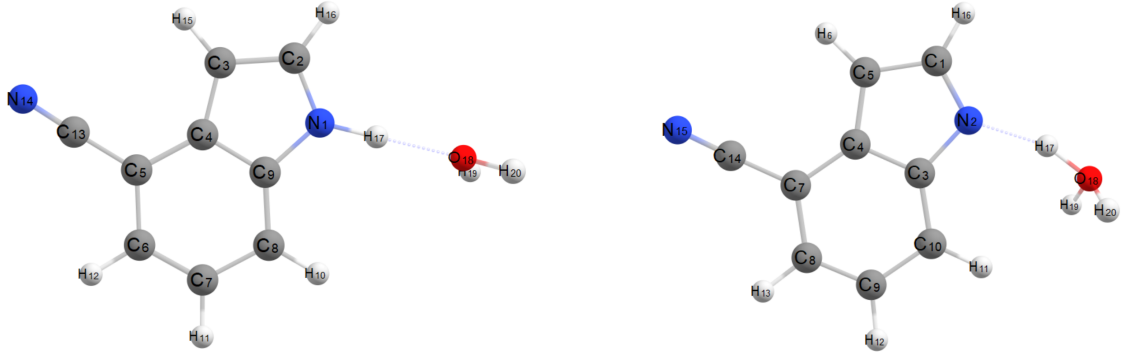
(a) N-H (Å)	1.02	**(b) N-H (Å)**	1.42
Ind	0.338518	**Ind-H**	-0.09526
H_2O	-0.33852	**H_3O**	0.09526



(a) (b)

Table S2: ChelpG charges of 3-CNI and 2 H_2O at the EOMCCSD/6-311+G(d) level of theory

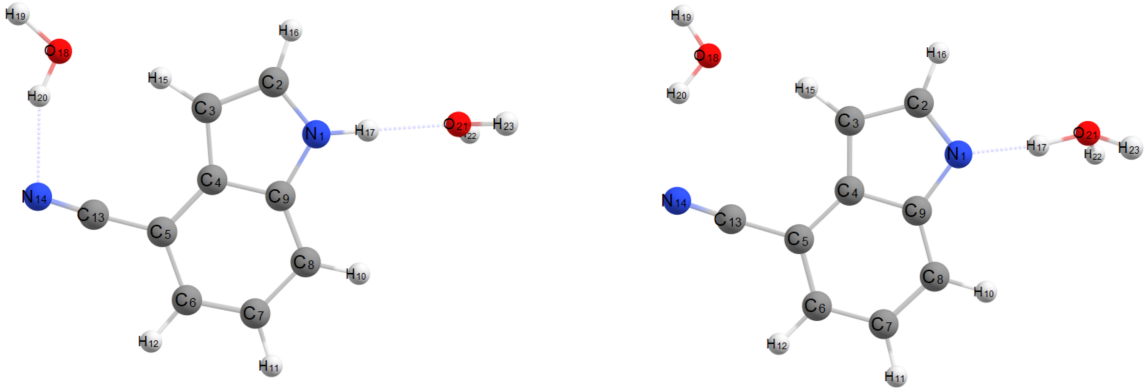
(a) N-H (Å)	1.02	**(b) N-H (Å)**	1.62
3-CNI	0.076471	**3-CNI -H**	0.017786
H_2O (@ NH)	-0.05285	**H_3O**	0.03941
H_2O (@ CN)	-0.02362	**H_2O**	-0.0572



(a) (b)

Table S3: ChelpG charges of 4-CNI + 1 H2O at the EOMCCSD/6-311+G(d) level of theory

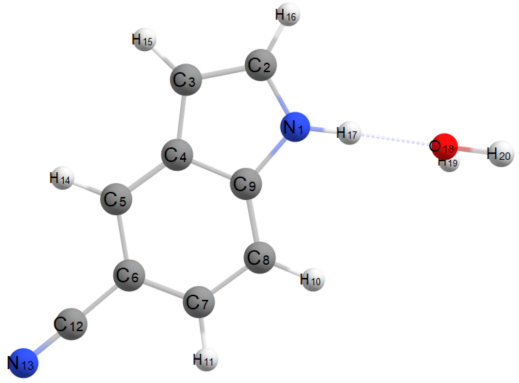
(a) N-H (Å)	1.12	**(b) N-H (Å)**	1.62
4-CNI	0.031122	**4-CNI -H**	-0.1075
H_2O	-0.03112	**H_3O**	0.107503



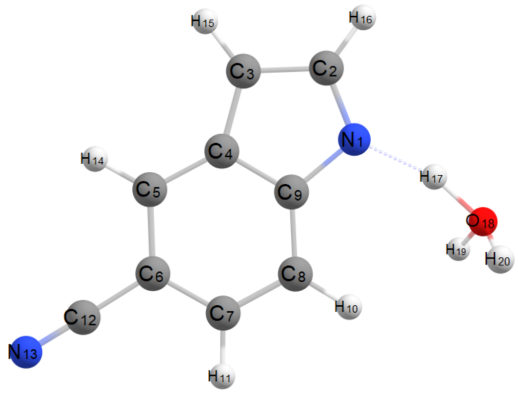
(a) (b)

Table S4: ChelpG charges of 4-CNI + 2 H_2O at the EOMCCSD/6-311+G(d) level of theory

(a) N-H (Å)	1.02	**(b) N-H (Å)**	1.62
4-CNI	0.084639	**4-CNI -H**	0.044612
H_2O (@ NH)	-0.03945	**H_3O**	0.012177
H_2O (@CN)	-0.04519	**H_2O**	-0.05679



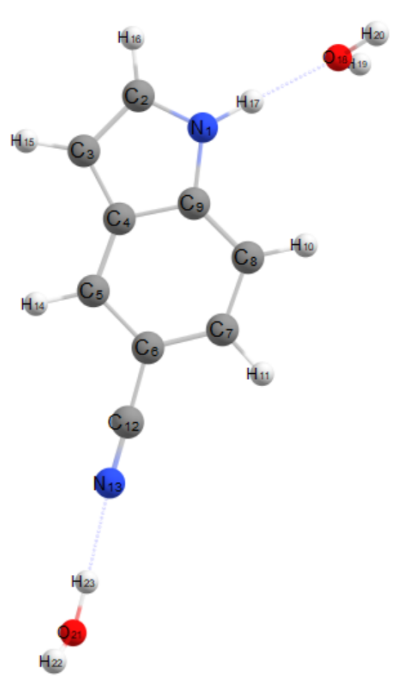
(a)



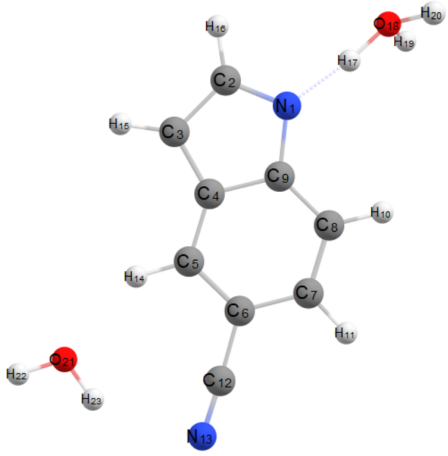
(b)

Table S5: Net molecular charge of 5-CNI and 1 H_2O in the S_1 state as the NH bond is stretched calculated from computing atomic partial charge with ChelpG for all of the atoms in the cluster at the EOMCCSD/6-311+G(d) level of theory.

(a) N-H (Å)	1.02	**(a) N-H (Å)**	1.52
5-CNI	0.044119	**5-CNI -H**	-0.09929
H_2O	-0.04412	**H_3O**	0.099287



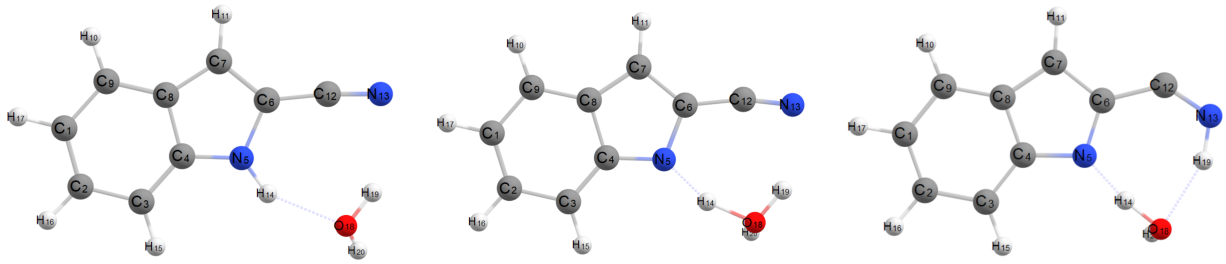
(a)



(b)

Table S6: Net molecular charge of 5-CNI and the 2 H_2O in the S_1 state as the NH bond is stretched calculated from computing atomic partial charge with ChelpG for all of the atoms in the cluster at the EOMCCSD/6-311+G(d) level of theory.

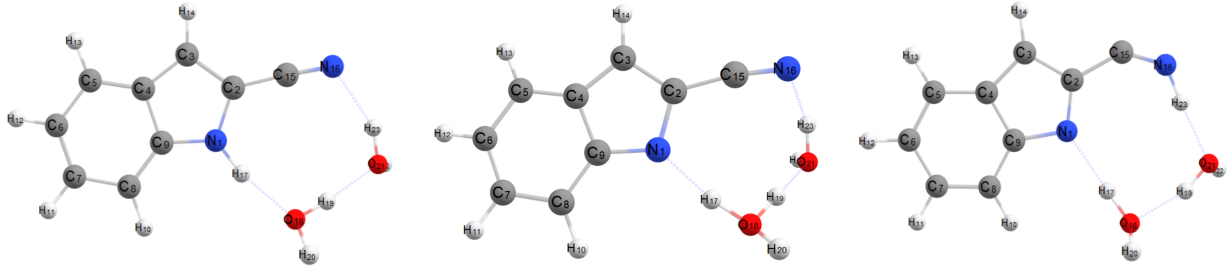
(a) N-H (Å)	1.02	**(b) N-H (Å)**	1.52
5-CNI	0.071838	**5-CNI -H**	0.011693
H_2O (@NH)	-0.04432	**H_3O (@NH)**	0.024521
H_2O (@CN)	-0.02751	**H_2O (@CN)**	-0.03621



(a) (b) (c)

Table S7: Net molecular charge of 2-CNI and the 1 H_2O molecule in the S_1 state as the NH bond is stretched calculated from computing atomic partial charge with ChelpG for all of the atoms in the cluster at the EOMCCSD/6-311+G(d) level of theory.

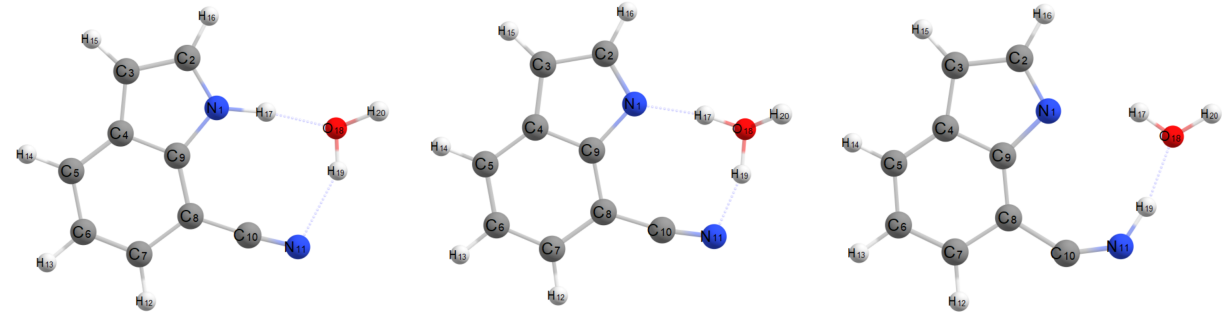
(a) N-H (Å)	1.02	**(b) N-H (Å)**	1.42	**(c) N-H (Å)**	1.72
2-CNI	0.015604	**2-CNI -H**	-0.6388	**2-CNI**	0.110065
H_2O (@NH)	-0.015605	**H_3O**	0.6388	**H_2O(@NH)**	-0.11007



(a) (b) (c)

Table S8: Net molecular charge of 2-CNI and the 2 H_2O in the S_1 state as the NH bond is stretched calculated from computing atomic partial charge with ChelpG for all of the atoms in the cluster at the EOMCCSD/6-311+G(d) level of theory.

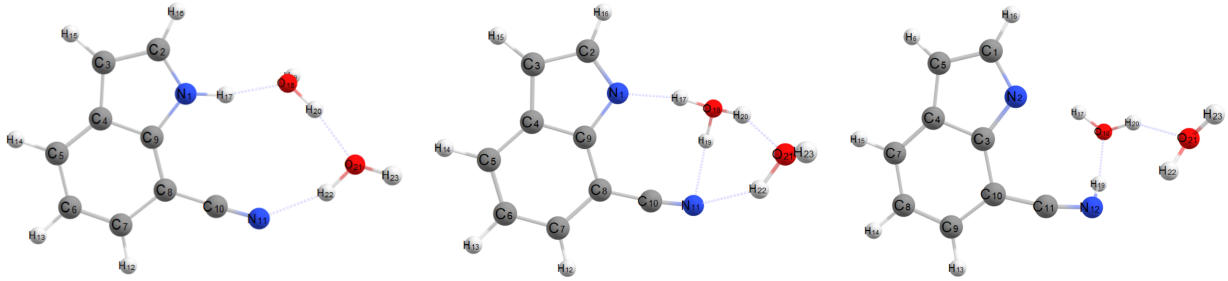
(a) N-H (Å)	1.03	**(b) N-H (Å)**	1.63	**(c) N-H (Å)**	1.83
2-CNI	0.05414	**2CNI**	-0.470456	**2-CNI**	0.108611
H_2O (@NH)	-0.017315	**H_3O**	0.485594	**H_2O (@NH)**	-0.05553
H_2O (@CN)	-0.036826	**H_2O (@ CN)**	-0.015137	**H_2O (@CN)**	-0.05308



(a) (b) (c)

Table S9: Net molecular charge of 7-CNI and the 1 H_2O in the S_1 state as the NH bond is stretched calculated from computing atomic partial charge with ChelpG for all of the atoms in the cluster at the EOMCCSD/6-311+G(d) level of theory.

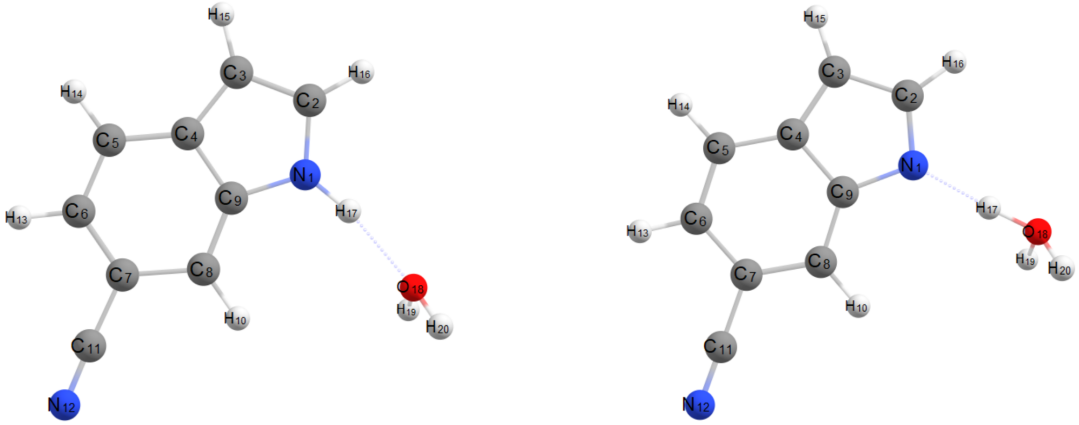
(a) N-H (Å)	1.03	**(b) N-H (Å)**	1.63	**(c) N-H (Å)**	2.03
7-CNI	0.004471	**7-CNI -H**	-0.67243	**7-CNI**	0.112567
H_2O	-0.00447	**H_3O**	0.672428	**H_2O**	-0.11257



(a) **(b)** **(c)**

Table S10: Net molecular charge of 7-CNI and the 2 H_2O in the S_1 state as the NH bond is stretched calculated from computing atomic partial charge with ChelpG for all of the atoms in the cluster at the EOMCCSD/6-311+G(d) level of theory.

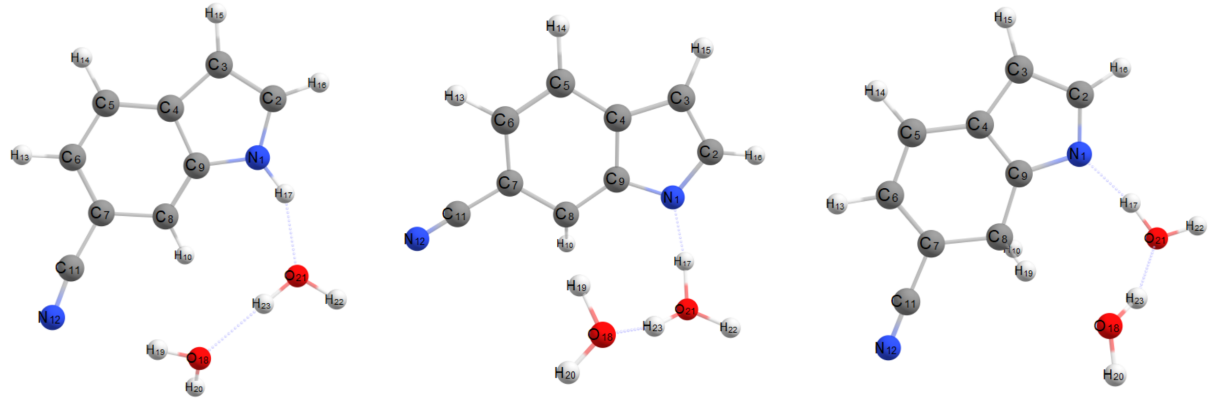
(a) N-H (Å)	1.04	**(b) N-H (Å)**	1.74	**(c) N-H (Å)**	2.54
7-CNI	0.05717	**7-CNI -H**	-0.697595	**7-CNI**	0.025426
H_2O (@NH)	-0.009193	**H_3O**	0.702976	**H_2O(@NH)**	-0.00636
H_2O (@CN)	-0.047976	**H_2O (@CN)**	-0.005381	**H_2O(@CN)**	-0.01907



(a) **(b)**

Table S11: ChelpG charges of 6-CNI and 1 H_2O along the NH bond stretch at the EOMCCSD/6-311+G(d)

(a) N-H (Å)	1.0242	**(b) N-H (Å)**	1.6242
6-CNI	0.032235	**6-CNI -H**	-0.03609
H_2O	-0.03224	**H_3O**	0.036088



(b) **(c)**

(a)

Table S12: ChelpG charge of 6CNI and 2 H_2O along the NH bond stretch at the EOMCCSD/6-311+G(d)

(a) N-H (Å)	1.02	**(b) N-H (Å)**	1.52	**(c) N-H (Å)**	1.62
6-CNI	0.037245	**6-CNI -H**	-0.535217	**6-CNI**	0.155981
H_2O (@NH)	-0.00306	**H_3O (@ NH)**	0.460907	**H_2O (@NH)**	-0.13266
H_2O (@CN)	-0.03419	**H_2O (@ CN)**	-0.119385	**H_2O (@CN)**	-0.02333

S4. Benchmarks

Additional benchmarks were performed at the S_1 minimum and select points along the pathways in order to determine its sensitivity to the electronic structure theory and eventually the best approach to characterize them.

Table S13 shows the vertical energy at the S1 minimum using CC2 and EOM-CCSD levels of theory for all CNI hydrogen bonded with one water molecule. While the results are quantitative different, they show qualitatively similar behavior. One exception is 6CNI which predicts a different character of the S1 state at the CC2 level compared to EOM-CCSD for the bare probe. It is noted here that for 6-CNI the EOM-CCSD vertical energy in this table is slightly higher than the adiabatic energy in Table 2 of the main paper, which cannot be true physically. The reason is that the geometries were optimized at a different level of theory which causes this discrepancy.

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Table S13: Energy (E) and Oscillator strength (*f*) of S_1 minimum of Indole and n-CNI bare and with one water molecule hydrogen bonding to the NH group computed at the CC2 and EOM-CCSD level of theory. Geometries were optimized with CC2/aug-cc-pVDZ for all systems and CC2/cc-pVDZ for indole.

	CC2				**EOMCCSD**			
	bare		**1 H2O**		**bare**		**1 H2O**	
	E (eV)	***f* (a.u.)**	**E (eV)**	***f* (a.u.)**	**E (eV)**	***f* (a.u.)**	**E (eV)**	***f* (a.u.)**
Ind	4.5436	0.044	4.4941	0.052	4.2654	0.028	4.4215	0.047
2CNI	4.0461	0.090	3.9389	0.09	4.1499	0.102	4.0668	0.11
3CNI	4.0859	0.131	4.0702	0.141	4.2358	0.123	4.2314	0.14
4CNI	3.8026	0.147			4.0345	0.179		
5CNI	4.1142	0.035	3.9673	0.036	4.2824	0.025	4.2008	0.036
6CNI	4.7498	0.001	3.9438	0.139	4.4729	0.198	4.1696	0.141
7CNI	3.7921	0.097	3.4903	0.077	4.1219	0.129	3.8122	0.104

Table S14 shows the barrier along the NH PES where the constrained optimizations were done using either CAM-B3LYP or CC2. EOMCCSD/6-311++G(d) was used to do single point calculations at the optimized geometries. The oscillator strengths at the S_1 minimum are shown as well. The results highlight that both CC2 and CAM-B3LYP give similar geometries, since the barriers and oscillator strengths computed with EOMCCSD are similar. The results are also shown pictorially in Figure S33.

Table S14: Energy Barrier and Oscillator strength of n-CNI-(H2O)1 complexes computed at the EOMCCSD/6-311++G(d) level of theory from S_1 minimum geometries optimized using CAM-B3LYP/6-311++G(d) and CC2/aug-cc-pVDZ

	CAM-B3LYP optimized S1 minimum geometry		**CC2 optimized S1 minimum geometry**	
	Barrier (eV)	**f (a.u.)**	**Barrier (eV)**	**f (a.u.)**
Ind			0.11	0.047

2CNI	1.21	0.073	1.57	0.11
3CNI			0.55	0.14
4CNI	1.04	0.183		
5CNI	0.92	0.039	1.09	0.036
6CNI	0.97	0.182	1.13	0.141
7CNI	0.761	0.109	0.88	0.104

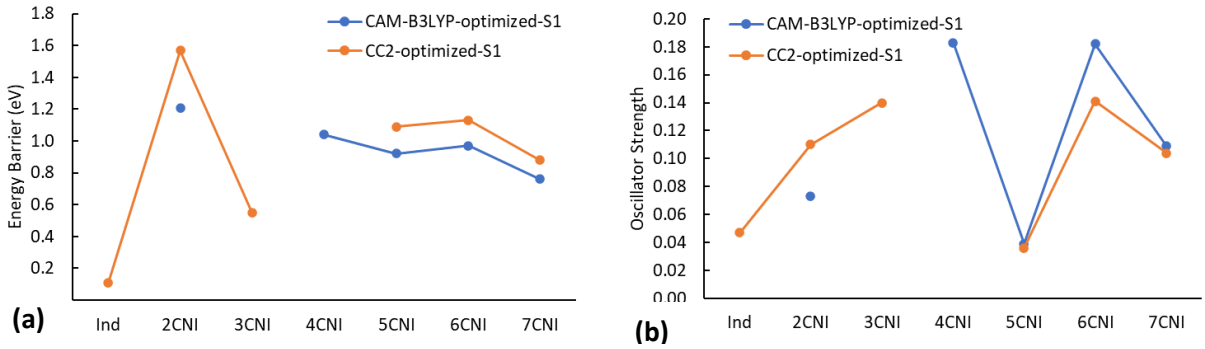
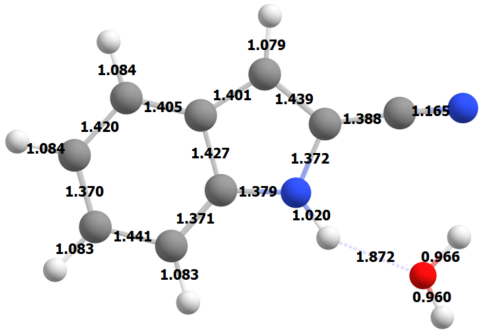
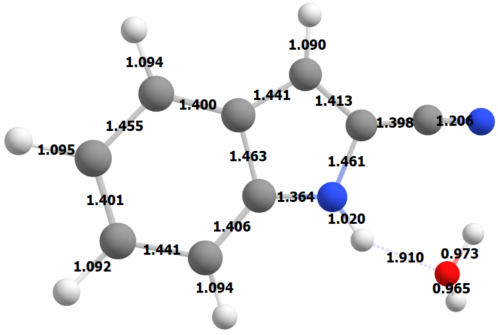
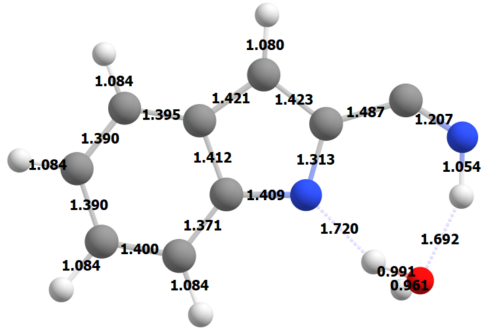
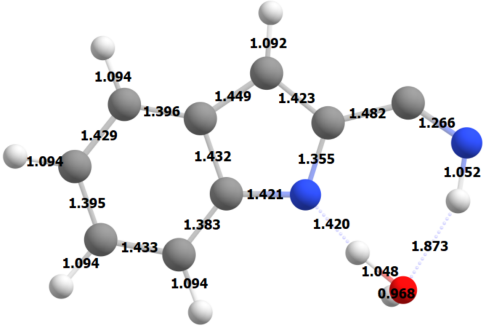


Figure S25: Trend in (a) energy barrier and (b) oscillator strength computed at the EOMCCSD/6-311++G(d) level of theory from S1 minimum geometries of n-CNI-(H2O)1 systems that were optimized at the CAM-B3LYP/6-311++G(d) and CC2/aug-cc-pVDZ level of theory respectively. The values in these plots are reported in Table S14.

Optimized geometries are shown below. The constrained optimizations along NH were performed with ADC(2)/aug-cc-pVDZ to compare with the CAM-B3LYP results shown in the main paper. The bond lengths of the S_1 minimum geometry and final geometry after ESHT/ESPT occurs predicted at the two levels of theory are shown in Figures S34-S39. Although the bond lengths and HB distance differ slightly, the two methods portray the same proton/hydrogen transfer process as well as the same potential energy paths qualitatively at the EOM-CCSD/6-311++G(d) level of theory.

S_1 min		
Post-ESPT		

Method/ Basis set	CAMB3LYP/6-311++G(d)	ADC(2)/aug-cc-pVDZ

Figure S26: The S_1 minimum geometry of the 2-CNI-$(H_2O)_1$ cluster and the last geometry after ESPT takes place, optimized at the CAM-B3LYP/6-311++G(d) and ADC(2)/aug-cc-pVDZ level of theory.

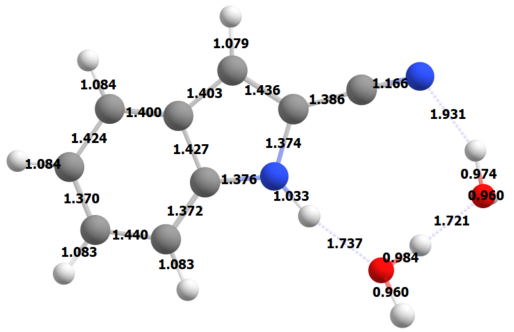
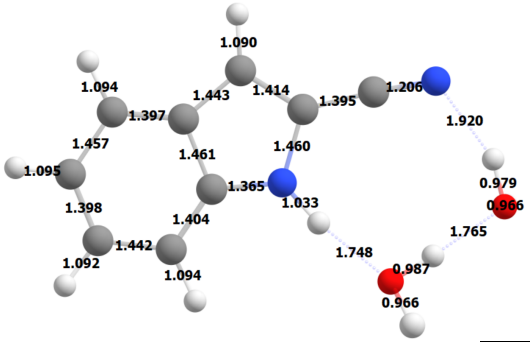
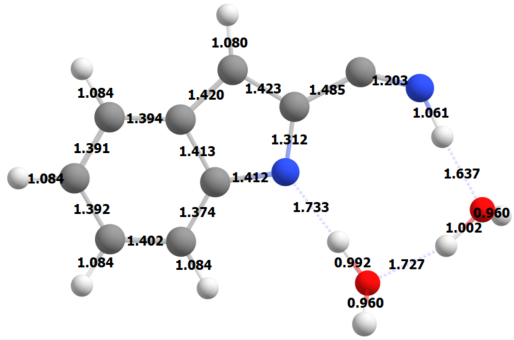
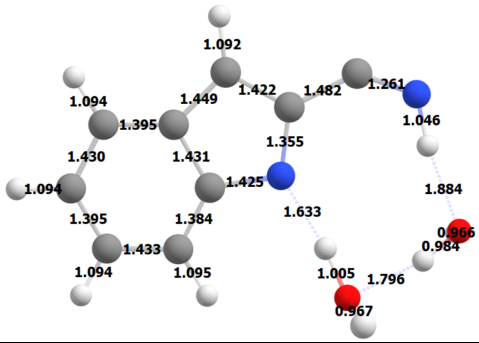
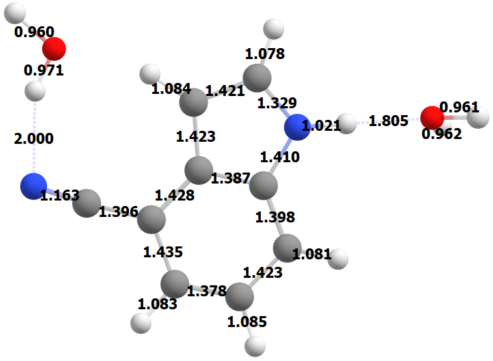
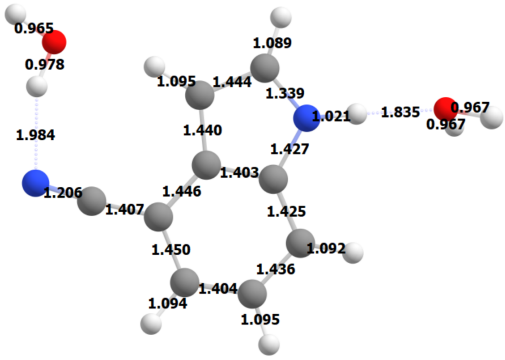
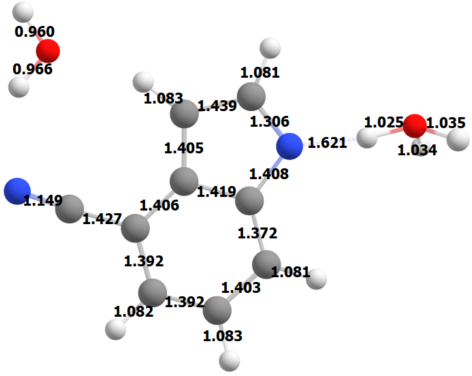
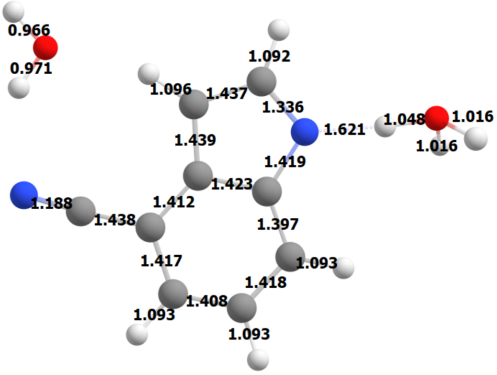
S_1 min		
Post-ESPT		
Method / Basis set	CAMB3LYP/6-311++G(d)	ADC(2)/aug-cc-pVDZ

Figure S27: The S_1 minimum geometry of 2-CNI-$(H_2O)_2$ cluster and the last geometry after ESPT takes place, optimized at the CAM-B3LYP/6-311++G(d) and ADC(2)/aug-cc-pVDZ level of theory.

S_1 min		
Post-ESHT		
Method/	CAMB3LYP/6-311++G(d)	ADC(2)/aug-cc-pVDZ

Basis set		

Figure S28: The S_1 minimum geometry of 4-CNI-$(H_2O)_2$ cluster and the last geometry after ESHT takes place, optimized at the CAM-B3LYP/6-311++G(d) and ADC(2)/aug-cc-pVDZ level of theory.

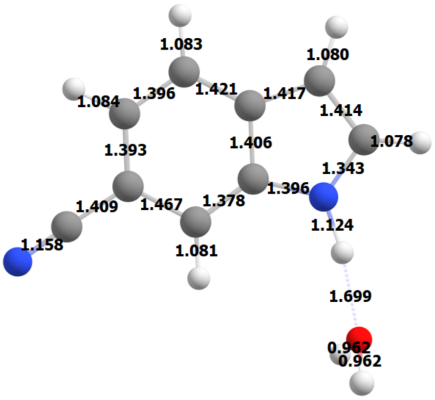
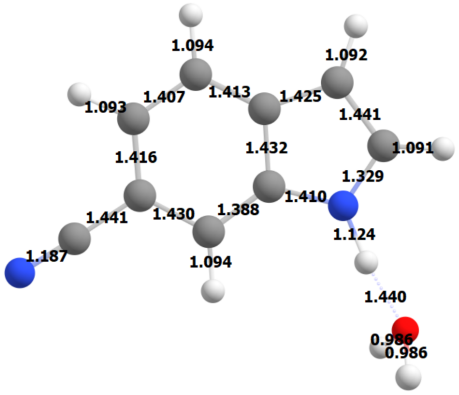
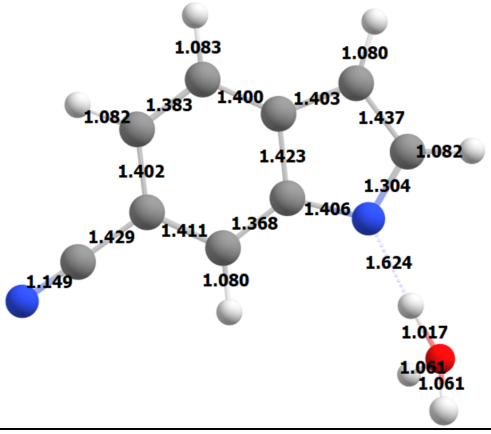
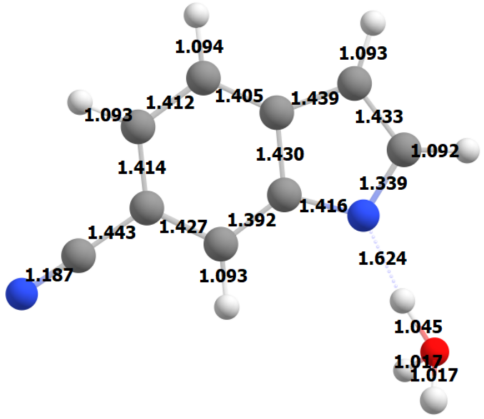
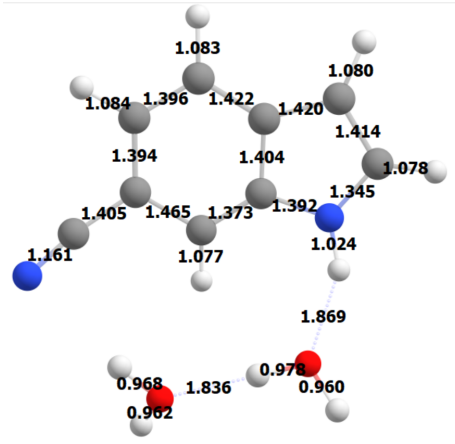
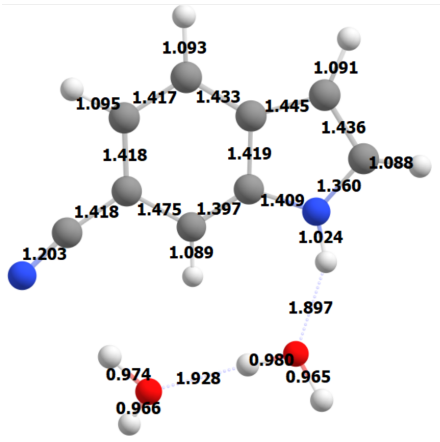
S_1 min		
Post-ESHT		
Method/ Basis set	CAMB3LYP/6-311++G(d)	ADC(2)/aug-cc-pVDZ

Figure S29: The S_1 minimum geometry of 6-CNI-$(H_2O)_1$ cluster and the last geometry after ESHT takes place, optimized at the CAM-B3LYP/6-311++G(d) and ADC(2)/aug-cc-pVDZ level of theory.

S_1 min		

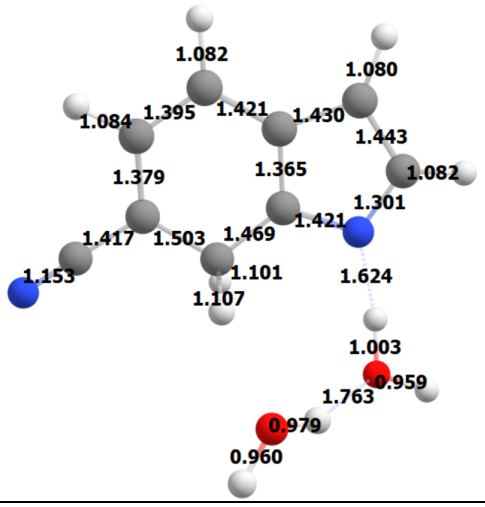
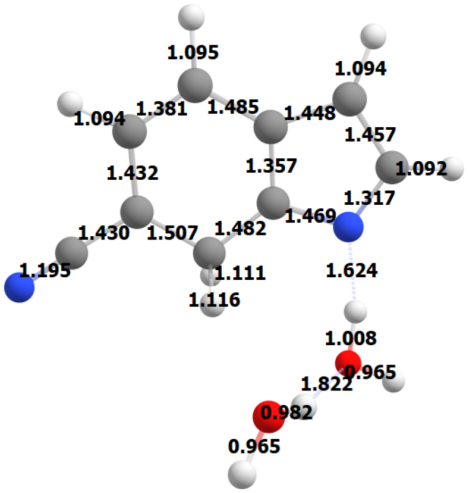
Post-ESPT		
Method/ Basis set	CAMB3LYP/6-311++G(d)	ADC(2)/aug-cc-pVDZ

Figure S30: The S_1 minimum geometry of 6-CNI-$(H_2O)_2$ cluster and last geometry after ESPT takes place, optimized at the CAM-B3LYP/6-311++G(d) and ADC(2)/aug-cc-pVDZ level of theory.

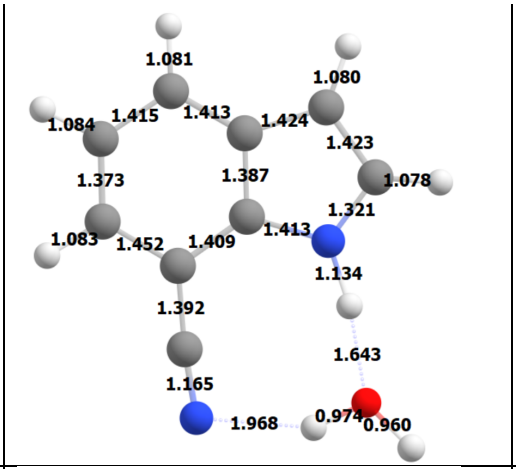
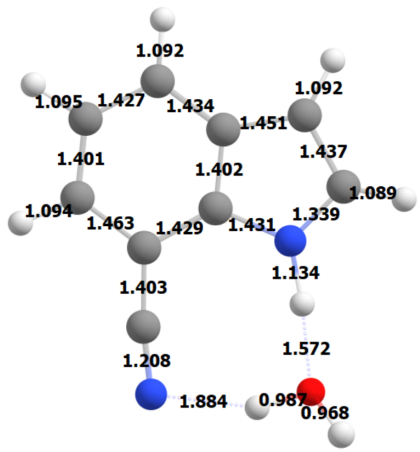
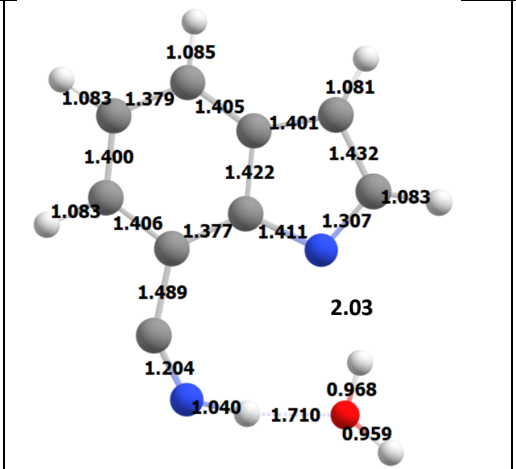
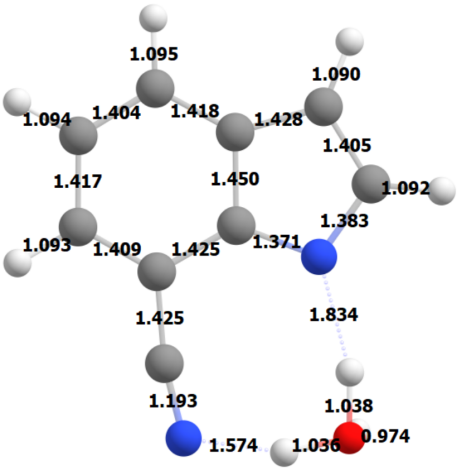
S_1 min		
Post-PCET		
Method/ Basis set	CAMB3LYP/6-311++G(d)	ADC(2)/aug-cc-pVDZ

Figure S31: The S_1 minimum geometry of the 7-CNI-$(H_2O)_1$ cluster and last geometry after ESPCET takes place, optimized at the CAM-B3LYP/6-311++G(d) and ADC(2)/aug-cc-pVDZ level of theory.

S5. Implicit Solvent

This section compares gas phase vs PCM results for 7-CNI. Figure S32a,b shows the CAM-B3LYP/6-311++G(d) PES using constrained optimizations along the NH coordinate, either optimizing in the gas phase or with PCM. Figure S32c,d compares the geometries. These results demonstrate that the implicit solvent has very small effect on the pathway.

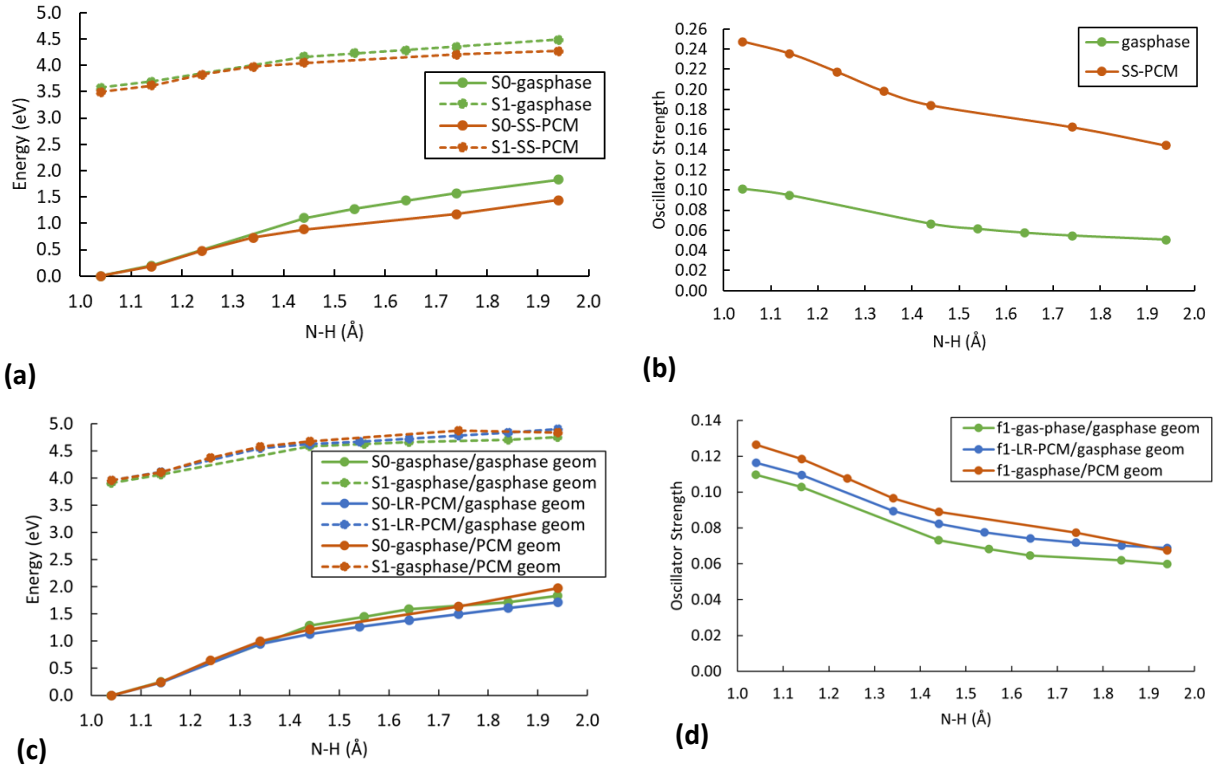
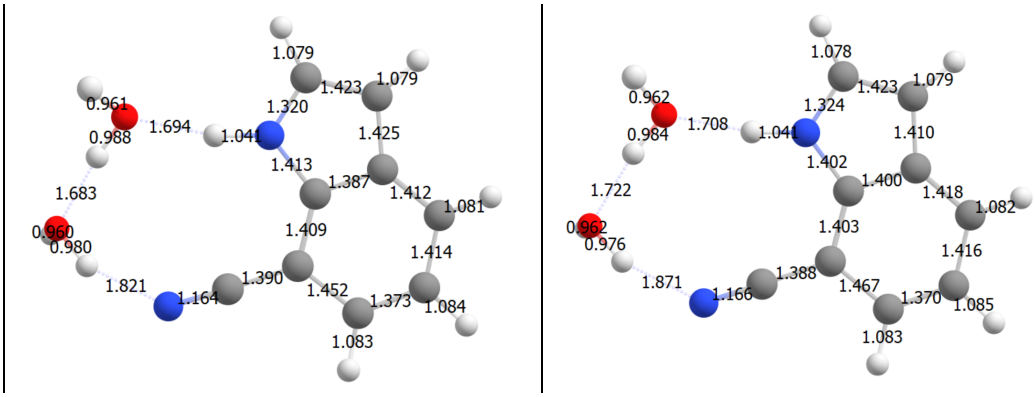


Figure S32: PES of the S_0 (solid curves) and S_1 (dotted curves) along the N-H bond stretch of 7-CNI-$(H_2O)_2$ (a) computed using constrained optimizations in the gas phase and using state-specific (SS) and equilibrium treatment of the PCM solvent at the CAMB3LYP/6-311++G(d) level of theory.
(c) PESs at the EOM-CCSD/6-311++G(d) level of theory obtained by single point calculation on the gas phase geometries (gasphase geom) and on the PCM optimized geometries (PCM geom). Also shown are EOM-CCSD/6-311++G(d) plus Linear-Response (LR) PCM treatment for the energies at the gas phase geometries (Lr-PCM/gasphase geom). **(b,d)** Their corresponding oscillator strengths of the S_1 state as a function of N-H bond distance.

S_1 min



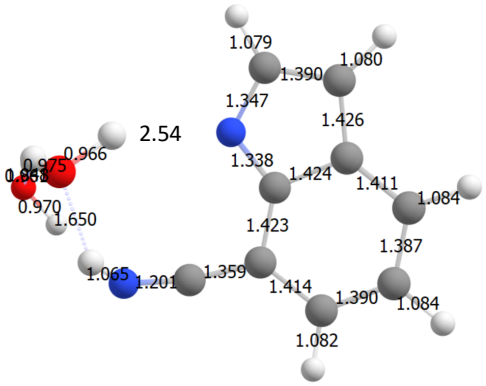
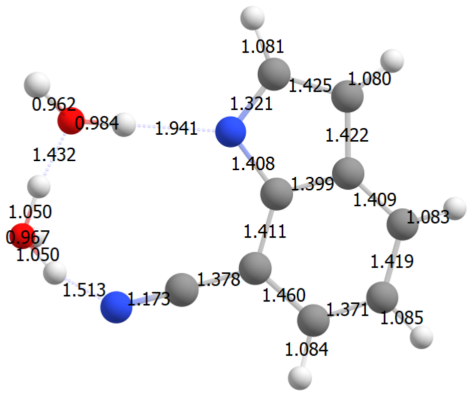
Post-PCET		
Optimized with	(a) gas phase	(b) PCM

Figure S33: Bond lengths of the S_1 minimum and last geometry after ESHT occurs for 7-CNI-(H2O)2 cluster optimized in gas phase and with state specific PCM at the CAM-B3LYP/6-311++G(d) level of theory. The N-H bond distance in last geometry of 7-CN-$(H_2O)_2$ optimized in gas phase is 2.54 Angstroms

S6. Molecular Dynamics Analysis

To assess the site specificity and number of water H2O HB at those sites, Classical Molecular Dynamics simulations of the various n-CNI probes in aqueous solution were performed. We simulate the probes in aqueous solution in the ground and excited states using non-polarizable force field and SPC water model. The box sizes and number of water molecules used per n-CNI probe are reported in Table S15. The Coulomb interactions involving the chromophores at either absorption or emission are described using electrostatic charges of the ground, S0, or second excited state at absorption, $S_2(L_a)$, respectively, of the n-CNI monomer in gas phase computed at the ground state minimum using ChelpG charges of the monomer probes in gas phase at the CCSD and EOMCCSD/6-311++G(d) level of theory respectively and embedding these charges into the coulombic charges of the non-polarizable force field used to model the probes classically. This treatment is similar to that used to simulate the optical spectra of indole to model the excited states in aqueous solution. The $S_2(L_a)$ state is used since it has a large dipole moment compared to the $S_1(L_b)$ state. 10 ns MD simulations with a 2 fs time step of each solvated n-CNI probe were produced on Gromacs 2020. Conditions of the MD simulation such as PBC, NVT/NPT Equilibration are similar to the details described in J. Chem. Phys., 154, 064104 (2021).

Table S15: MD box dimensions and number of water molecules used to solvate the box with the probe

Probe	# H_2O	Length of Cubic box (nm)
2-CNI	3220	4.61849
3-CNI	3059	4.55171
4-CNI	3290	4.65781
5-CNI	3201	4.60652
6-CNI	3189	4.60004
7-CNI	2929	4.48034

A radial distribution function for N of the amino of *n*-CNI probes modeled (Namino) to O of water and Ncyano to H of water is plotted as a function of r HB distance in the main paper using ground state S_0 and excited S_2 state of the *n*-CNI molecule. This can be used to understand the structure and organization of the probe to the waters. The first solvation shell, HB distance from the donor to the acceptor and number of water molecules are HB to that site within that solvation shell.

The HB distance from Hamino to O of water was found to be 1.85 Angstroms and 1.95 Angstroms from Ncyano to H of water for all of the probes in the ground and excited state (except for 2-CNI with 2.05 A

in the ground state). The RDF shows that 1 H2O molecule is hydrogen bonding to the donor or acceptor site of n probes. It also indicates that the polarization of the molecule when it becomes excited from the ground to the polar excited state does not affect the number of water molecules that interact with the probe in the first solvation shell significantly. This could be because we are using charges of the monomer computed at absorption, so it's not the most accurate depiction, however it is a rough approximation. In both of the RDFs computed using the S0 and S2, there is a slight difference in the structure of the waters to probe interaction in the first solvation shell, where 2-CNI and 7-CNI are more similar than the rest at the amino site. The RDF, however, does not indicate whether the water molecules are HB to the Hamino and Ncyano sites at the same time. To validate our QM cluster models with the 2 water molecules simultaneously HB to the H donor and acceptor sites we calculated the number of water molecules HB to the Ncyano and Namino site in each frame of the 10,000 total frames in the 10 ns MD simulations. We performed a search for number of water molecules that are HB to the Hydrogen Donor (Namino) or Acceptor (Ncyano) of the n probes at a HB distance cutoff of 3.5 Angstroms and within an angle cutoff of 90 degrees. The number of water molecules HB to Namino and Ncyano are plotted as a function of simulation time in Figure S43.

We report the statistics of the number of times a water molecule is found to HB to at least 1 H2O in each frame in Table S17. We find that for all of the probes more than 98% of the time at least 1 water molecule is HB to both the Namino and Ncyano at the same time. Orientation of the water molecules HB is not taken into account. These results give us confidence that our QM cluster model with the two water molecules may exist in nature.

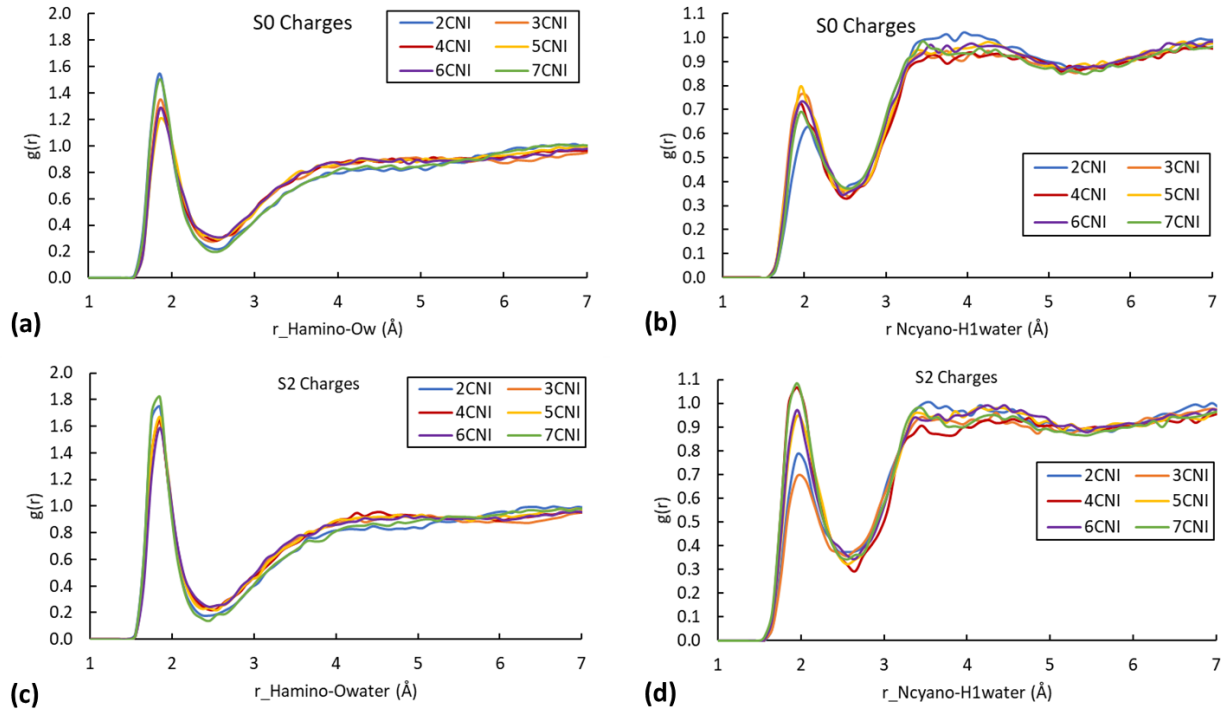


Figure S34: Radial Distribution Function g(r) of (a) H of amino of n HB to O of water and (b) N of cyano HB to H of water, as the *n* probes are simulated in the ground state using ChelpG charges of the monomer in the gas phase at absorption computed at the CCSD/6-311+G(d) level of theory and (c) and (d) are in the S2 excited state.

Table S16: The HB distance, r, radial distribution function g(r), and Integral of g(r) for the first solvation shell of n-CNI probes HB to water molecules, with S_0 charges and S_2 charges embedded in the force field to sample the phase space of the electronic ground state, and the electronic $S_2(L_a)$ excited state. Tabulated data is reflected in Figure S42.

	First Solvation Shell - Hamino to Owater		First Solvation Shell - Ncyano to Hwater	
	S_0 Charges	**S_2 Charges**	**S_0 Charges**	**S_2 Charges**

2-CNI	r (Å)	g(r)	Int g(r)	r (Å)	g(r)	Int g(r)	r (Å)	g(r)	Int g(r)	r (Å)	g(r)	Int g(r)
max	1.85	1.55	0.40	1.85	1.74	0.52	2.05	0.63	0.28	1.95	0.78	0.25
min	2.55	0.22	1.06	2.45	0.18	1.03	2.45	0.35	0.66	2.55	0.37	0.88
3-CNI												
max	1.85	1.35	0.34	1.85	1.63	0.46	1.95	0.76	0.26	1.95	0.69	0.22
min	2.45	0.28	0.99	2.35	0.24	0.97	2.55	0.34	0.88	2.55	0.36	0.82
4-CNI												
max	1.85	1.28	0.31	1.85	1.65	0.46	1.95	0.73	0.23	1.95	1.07	0.38
min	2.55	0.29	1.05	2.45	0.22	1.04	2.55	0.33	0.81	2.65	0.29	1.16
5-CNI												
max	1.85	1.20	0.29	1.85	1.67	0.47	1.95	0.79	0.25	1.95	0.95	0.32
min	2.55	0.29	1.05	2.35	0.23	0.98	2.55	0.36	0.87	2.55	0.32	1.00
6-CNI												
max	1.85	1.28	0.31	1.85	1.59	0.42	1.95	0.73	0.24	1.95	0.97	0.33
min	2.55	0.31	1.06	2.45	0.24	1.02	2.45	0.35	0.76	2.65	0.34	1.09
7-CNI												
max	1.85	1.51	0.39	1.85	1.82	0.54	1.95	0.69	0.21	1.95	1.08	0.39
min	2.55	0.20	1.04	2.45	0.14	1.02	2.55	0.37	0.82	2.55	0.34	1.08

Table S17: Number of times that at least 1 H_2O molecule hydrogen bonds to the amino and cyano H donor/acceptor sites of *n*-CNI probes in the first solvation shell simultaneously, as the probe is simulated in the $S_2(L_a)$ excited state, in a 10 ns classical MD simulation.

Probe	# frames where a H2O molecule is HB to Namino and Ncyano at the same time /10,000 total frames	%
2-CNI	9923	99.23
3-CNI	9886	98.86
4-CNI	9943	99.43
5-CNI	9936	99.36
6-CNI	9904	99.04
7-CNI	9966	99.66

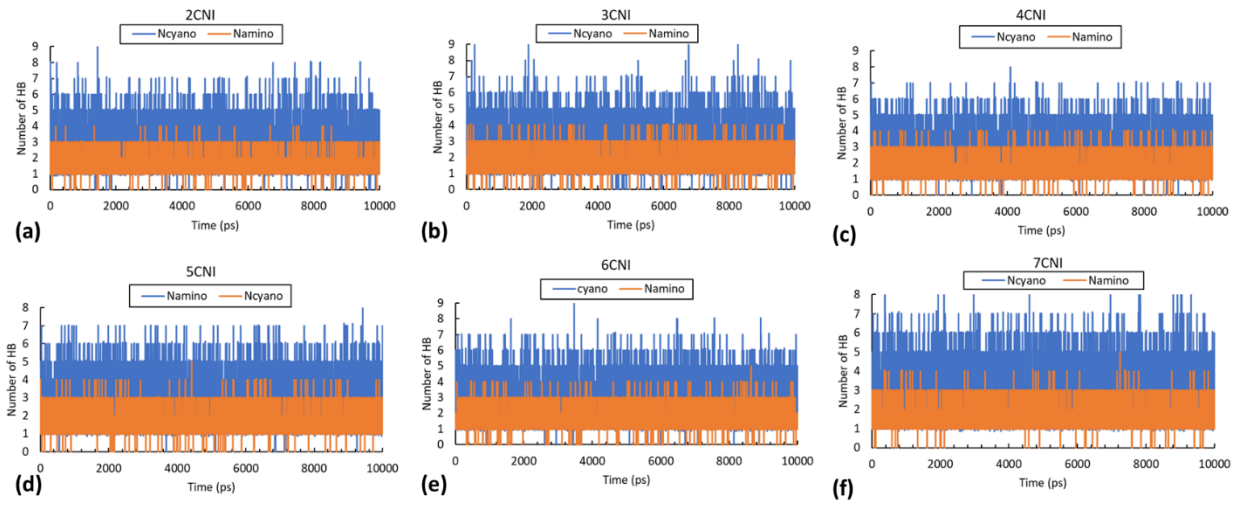


Figure S35: Number of waters Hydrogen bonding (HB) to N amino (orange) and Ncyano (blue) of (a) 2CNI, (b) 3CNI, (c) 4CNI, (d) 5CNI, (e) 6CNI, and (f) CNI probes as a function of MD simulation time (10,000 ps) modeled in the S2(La) excited state at absorption

S7. Cartesian coordinates of all relevant structures

Method: CAM-B3LYP							
S_1 minimum (first) geometry				Last geometry			
2CNI-$(H_2O)_1$							
C	0.000000	0.000000	0.000000	C	0.000000	0.000000000	0.000000000
C	0.000000	0.000000	1.370499	C	0.000000	0.000000000	1.390090000
C	1.244324	0.000000	2.098069	C	1.198833	0.000000000	2.113949000
C	2.406614	-0.000548	1.371563	C	2.365174	0.100422000	1.399612000
N	3.717522	-0.001164	1.800864	N	3.671276	0.217855000	1.914153000
C	4.585755	-0.000253	0.739149	C	4.462319	0.299782000	0.869292000
C	3.777222	0.000657	-0.451219	C	3.749621	0.291259000	-0.361843000
C	2.433898	0.000127	-0.054974	C	2.379765	0.153211000	-0.010926000
C	1.210013	0.000006	-0.744078	C	1.182445	0.091766000	-0.724433000
H	1.184615	-0.000195	-1.827405	H	1.167227	0.127641000	-1.807686000
H	4.169850	0.002351	-1.456671	H	4.184580	0.411412000	-1.343040000
C	5.960922	0.003315	0.930680	C	5.943529	0.350071000	0.985327000
N	7.101665	0.002983	1.167298	N	6.662732	0.271866000	1.951688000
H	4.056433	-0.004159	2.762787	H	4.399579	-0.033321000	3.451843000
H	1.250151	0.001482	3.181517	H	1.204512	-0.020956000	3.197387000
H	-0.931693	0.000131	1.922044	H	-0.941163	-0.046322000	1.925157000
H	-0.941023	-0.000196	-0.537805	H	-0.945709	-0.057801000	-0.527125000
O	5.532085	0.001627	3.914421	O	5.119727	-0.230423000	4.103714000
H	6.362506	0.014494	3.420408	H	6.269679	0.151885000	2.922698000
H	5.724076	-0.193502	4.834762	H	4.998427	-1.144262000	4.376268000
2CNI-$(H_2O)_2$							
N	0.000000	0.000000	0.000000	N	0.015212	-0.005317000	-0.001431000
C	0.000000	0.000000	1.374350	C	0.010361	-0.000948000	1.310790000
C	1.374640	0.000000	1.788142	C	1.316672	-0.000722000	1.871760000
C	2.168038	-0.000575	0.630671	C	2.211099	-0.007281000	0.767485000
C	3.547339	-0.000107	0.389056	C	3.597177	-0.014222000	0.632571000
C	4.014727	-0.002711	-0.955671	C	4.135064	-0.029499000	-0.651177000
C	3.147880	-0.006299	-2.016123	C	3.305077	-0.039604000	-1.767182000
C	1.726084	-0.005905	-1.789801	C	1.907688	-0.032045000	-1.643312000
C	1.285342	-0.002004	-0.490190	C	1.379354	-0.013692000	-0.376204000
H	1.032599	-0.013697	-2.622172	H	1.267362	-0.050462000	-2.517777000
H	3.519787	-0.010458	-3.032882	H	3.747064	-0.056676000	-2.756976000
H	5.083867	-0.003100	-1.133612	H	5.210398	-0.036157000	-0.784360000
H	4.254656	0.000404	1.210130	H	4.243752	-0.009251000	1.502998000
H	1.706245	0.000787	2.815421	H	1.550514	0.002282000	2.925840000
C	-1.181355	-0.016153	2.099922	C	-1.214862	-0.016313000	2.145716000
N	-2.203304	-0.038536	2.660139	N	-2.399546	-0.054551000	1.939922000
H	-0.870512	-0.002887	-0.557030	H	-1.231861	0.171887000	-1.468317000
O	-2.492421	-0.026258	-1.177839	O	-1.888791	0.295992000	-2.182190000

H	-3.178321	-0.296040	-0.526646	H	-3.317444	-0.036171000	-1.242779000
H	-2.862879	0.677696	-1.715542	H	-1.797395	1.192691000	-2.514427000
O	-4.248919	-0.621473	0.780905	O	-3.891705	-0.149152000	-0.457747000
H	-4.755743	-1.429533	0.891399	H	-4.560714	-0.810550000	-0.646903000
H	-3.775095	-0.441728	1.612546	H	-2.906196	-0.079938000	1.030440000

4CNI-$(H_2O)_1$

N	0.000000	0.000000	0.000000	C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.330204	N	0.000000	0.000000	1.323700
C	1.353240	0.000000	1.766170	C	1.331198	0.000000	1.780808
C	2.165838	0.000420	0.610581	C	2.181498	-0.000403	0.685628
C	3.585687	-0.000539	0.442280	C	1.343505	-0.000444	-0.470115
C	4.057093	-0.001823	-0.912784	H	1.661126	-0.000633	-1.502307
C	3.179102	-0.001977	-1.972432	C	3.591339	-0.000709	0.842457
C	1.759228	-0.001025	-1.816197	C	4.072146	-0.000211	2.198102
C	1.317477	0.000169	-0.493869	C	3.205611	0.000142	3.263189
H	1.087756	-0.001825	-2.663383	C	1.787510	-0.000023	3.109586
H	3.583351	-0.002954	-2.978980	H	1.135597	0.003801	3.975884
H	5.124098	-0.002602	-1.095400	H	3.618875	0.000616	4.266488
C	4.434725	0.000314	1.553898	H	5.140898	-0.000330	2.372495
N	5.114252	0.001084	2.496197	C	4.442377	-0.001279	-0.271264
H	1.683606	-0.000320	2.793943	N	5.126925	-0.001595	-1.208507
H	-0.913289	0.000239	1.903503	H	-0.912720	-0.000130	-0.576681
H	-0.914101	0.000026	-0.641765	H	-1.122361	-0.002543	2.487587
O	-2.311107	-0.002338	-1.623749	O	-1.555744	-0.001637	3.450131
H	-2.685951	-0.782327	-2.042908	H	-1.262893	0.789922	3.928657
H	-2.684837	0.774842	-2.049072	H	-1.261933	-0.791627	3.930600

4CNI-$(H_2O)_2$

N	0.004643	0.000204	-0.008372	N	0.000117	0.000578	-0.000306
C	0.001724	0.000509	1.320559	C	0.000017	0.000572	1.305686
C	1.350171	0.000534	1.769821	C	1.324048	0.000161	1.869212
C	2.166188	-0.000457	0.604568	C	2.185228	-0.000079	0.759321
C	3.584379	-0.001788	0.440178	C	3.583271	-0.000501	0.605735
C	4.062755	-0.002056	-0.912454	C	4.119150	-0.000573	-0.678551
C	3.186115	-0.001391	-1.975123	C	3.276607	-0.000235	-1.786924
C	1.771233	-0.000334	-1.824435	C	1.880106	0.000146	-1.656750
C	1.326244	0.000001	-0.499042	C	1.352958	0.000212	-0.390188
H	1.101192	-0.000276	-2.672624	H	1.242296	0.000436	-2.529584
H	3.595077	-0.002039	-2.979946	H	3.714413	-0.000277	-2.777184
H	5.130160	-0.003502	-1.092885	H	5.193091	-0.000870	-0.812876
C	4.413651	-0.006260	1.562801	C	4.423565	-0.000836	1.758965
N	5.044796	-0.009744	2.540050	N	5.060601	-0.000951	2.714889
H	1.677653	0.001195	2.803435	H	1.598448	0.000098	2.917186
H	-0.913775	-0.000480	1.890569	H	-0.926003	0.000876	1.863761
H	-0.829631	-0.001554	-0.597460	H	-1.385240	0.001175	-0.842553
O	2.893077	-0.036581	4.500035	O	2.776233	0.000300	4.637676
H	3.000221	0.329426	5.381199	H	2.696371	0.001365	5.594778
H	3.767408	-0.056510	4.077794	H	3.715135	-0.000409	4.412369
O	-2.298810	-0.010986	-1.646320	O	-2.323997	0.002292	-1.255082

H	-2.666851	-0.794090	-2.065602	H	-2.486982	-0.840287	-1.831379
H	-2.672795	0.763333	-2.076476	H	-2.480108	0.839327	-1.843518

5CNI-(H_2O)$_1$

N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.324198	C	0.000000	0.000000	1.318383
C	1.357945	0.000000	1.764786	C	1.349836	0.000000	1.791479
C	2.184763	-0.000063	0.619278	C	2.197790	-0.000393	0.646516
C	3.584491	-0.000165	0.449719	C	3.594272	-0.001486	0.485286
C	4.065681	-0.000360	-0.912943	C	4.071555	-0.003953	-0.877487
C	3.166837	-0.000286	-1.981782	C	3.190720	-0.002965	-1.950517
C	1.768167	-0.000008	-1.811169	C	1.788672	-0.000844	-1.779496
C	1.322125	-0.000006	-0.482068	C	1.335725	-0.000418	-0.445464
H	1.094153	0.000441	-2.656951	H	1.131670	0.002909	-2.642093
H	3.566360	-0.000424	-2.989658	H	3.599042	-0.003980	-2.954906
C	5.453615	-0.000676	-1.181941	C	5.466132	-0.008543	-1.140069
N	6.592173	0.001000	-1.382650	N	6.603527	-0.016617	-1.337690
H	4.268909	0.000266	1.285806	H	4.281115	-0.002603	1.319265
H	1.668283	-0.000001	2.798920	H	1.649483	0.000124	2.829403
H	-0.912619	-0.000139	1.898946	H	-0.911787	-0.000436	1.897090
H	-0.832210	-0.000505	-0.593105	H	-1.051552	-0.010272	-1.100188
O	-2.265303	-0.009280	-1.682536	O	-1.554512	-0.023955	-2.125897
H	-2.612597	-0.791015	-2.121710	H	-1.254713	-0.815980	-2.600530
H	-2.624110	0.766264	-2.123410	H	-1.274257	0.767723	-2.612980

5CNI-(H_2O)$_2$

N	0.003026	0.002305	-0.009295	N	0.495326	0.042887	0.095114
C	0.001910	0.004460	1.313235	C	0.860197	-0.114289	1.343067
C	1.358125	0.001256	1.759192	C	2.282958	-0.173480	1.493142
C	2.188514	-0.003162	0.615557	C	2.805201	-0.036344	0.195100
C	3.587031	-0.008600	0.451518	C	4.100120	-0.013600	-0.321754
C	4.073738	-0.015835	-0.910027	C	4.237184	0.144327	-1.702028
C	3.173252	-0.014603	-1.983635	C	3.118515	0.274699	-2.534812
C	1.780038	-0.007037	-1.815145	C	1.818497	0.251941	-2.016734
C	1.328643	-0.002490	-0.487180	C	1.676056	0.097040	-0.660368
H	1.108128	-0.007165	-2.662718	H	0.962400	0.353319	-2.668028
H	3.574281	-0.021172	-2.990912	H	3.265994	0.395398	-3.600471
C	5.455356	-0.027250	-1.180135	C	5.553427	0.171803	-2.263804
N	6.593898	-0.036394	-1.384101	N	6.627396	0.188315	-2.671885
H	4.267894	-0.012768	1.290457	H	4.982152	-0.112580	0.301856
H	1.664583	0.001869	2.794414	H	2.826882	-0.297765	2.416900
H	-0.911522	0.007618	1.886935	H	0.126403	-0.185625	2.133497
H	-0.828869	0.001796	-0.602843	H	-0.970772	0.133645	-0.303120
O	-2.269942	-0.007303	-1.673920	O	-2.009485	0.182301	-0.451159
H	-2.642126	-0.790216	-2.090102	H	-2.346640	-0.575789	-1.059708
H	-2.651649	0.766990	-2.097475	H	-2.296769	1.079086	-0.865946
O	9.438046	-0.406932	-1.998763	O	7.141261	-0.184634	0.375417
H	9.724022	0.506323	-1.915165	H	7.939026	-0.269843	0.904721
H	8.487124	-0.410100	-1.805137	H	7.407002	-0.084142	-0.546039

6CNI-(H_2O)$_1$

N	0.000786	0.000817	-0.002105	N	0.088214	-0.000106	-0.085936
C	-0.000241	0.001556	1.342771	C	0.091948	-0.000044	1.218116
C	1.347825	0.000304	1.768326	C	1.419801	-0.000006	1.768123
C	2.164505	-0.001401	0.611660	C	2.284354	-0.000046	0.663528
C	3.571724	-0.003399	0.409387	C	3.676295	-0.000038	0.510891
C	4.045365	-0.004950	-0.903156	C	4.201338	-0.000088	-0.768489
C	3.188311	-0.004692	-2.002126	C	3.350268	-0.000143	-1.882358
C	1.732979	-0.002622	-1.810973	C	1.944968	-0.000147	-1.750405
C	1.305314	-0.001094	-0.502020	C	1.437276	-0.000106	-0.480437
H	1.061332	-0.001971	-2.657477	H	1.307505	-0.000178	-2.622459
C	3.704244	-0.006423	-3.312314	C	3.927503	-0.000197	-3.189053
N	4.089059	-0.007923	-4.404576	N	4.402139	-0.000247	-4.235352
H	5.114504	-0.006569	-1.080043	H	5.272458	-0.000086	-0.922470
H	4.258095	-0.003626	1.246722	H	4.332704	0.000005	1.372808
H	1.672708	0.000568	2.798053	H	1.679814	0.000047	2.815929
H	-0.914036	0.003133	1.913809	H	-0.832341	-0.000024	1.779805
H	-0.828141	0.000983	-0.603657	H	-1.266218	-0.000127	-0.982338
O	-2.076464	-0.000717	-1.914500	O	-2.143936	-0.000386	-1.496970
H	-2.277864	-0.780082	-2.440877	H	-2.194791	-0.876048	-2.093949
H	-2.280886	0.776149	-2.443382	H	-2.194956	0.875012	-2.094600

6CNI-(H_2O)$_2$

N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.344526	C	0.000000	0.000000	1.311192
C	1.347712	0.000000	1.771482	C	1.336601	0.000000	1.834602
C	2.167928	0.010412	0.612216	C	2.197630	-0.002457	0.683646
C	3.572162	0.040610	0.389822	C	3.601927	-0.091457	0.527743
C	4.032883	0.131451	-0.925312	C	4.099591	-0.226927	-0.771123
C	3.157225	0.124317	-2.010489	C	3.264949	-0.224387	-1.875591
C	1.719026	-0.059727	-1.799625	C	1.784422	-0.033345	-1.773707
C	1.302052	-0.012989	-0.492672	C	1.361031	-0.008140	-0.401773
H	1.048982	-0.200762	-2.631231	H	1.222837	-0.737069	-2.410045
C	3.543845	0.415606	-3.328979	C	3.807693	-0.364198	-3.175932
N	3.693417	0.671874	-4.451649	N	4.250716	-0.476893	-4.234533
H	5.095161	0.246824	-1.107472	H	5.166116	-0.339806	-0.928368
H	4.268928	0.058512	1.218580	H	4.267245	-0.045064	1.379225
H	1.669840	-0.008980	2.802115	H	1.621082	-0.077529	2.875383
H	-0.911478	0.014217	1.919159	H	-0.912431	0.021866	1.890631
H	-0.789934	0.133373	-0.638191	H	-0.960215	0.919746	-0.932854
O	0.363134	1.231397	-4.440582	O	0.967959	2.326910	-2.623855
H	1.314270	1.390421	-4.362068	H	1.522540	1.035598	-2.258748
H	0.218307	0.851960	-5.312128	H	0.758996	2.352892	-3.563466
O	-1.393380	0.729832	-2.302971	O	-1.285886	1.660782	-1.515541
H	-2.234850	1.140580	-2.514973	H	-2.158789	1.960791	-1.253564
H	-0.768602	0.948630	-3.022234	H	0.058475	2.357496	-2.006957

7CNI-(H_2O)$_1$

N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.321154	C	0.000000	0.000000	1.307197

C	1.352372	0.000000	1.764480	C	1.317090	0.000000	1.868220
C	2.184005	-0.001018	0.608387	C	2.190927	-0.000437	0.773505
C	3.586409	-0.004417	0.438699	C	3.588707	0.069306	0.651666
C	4.050946	-0.010860	-0.897614	C	4.130402	0.247666	-0.603502
C	3.205592	-0.015144	-1.979198	C	3.296275	0.300892	-1.726107
C	1.761852	-0.013278	-1.822574	C	1.897723	0.187579	-1.638120
C	1.327704	-0.003054	-0.482681	C	1.358745	0.050591	-0.377921
C	0.844611	-0.029125	-2.869229	C	1.150866	0.257914	-2.924428
N	0.002463	-0.041544	-3.673897	N	0.028895	0.222300	-3.359954
H	3.609582	-0.021199	-2.984161	H	3.723865	0.432731	-2.712581
H	5.119798	-0.013147	-1.080454	H	5.203653	0.327616	-0.726175
H	4.264262	-0.002526	1.281161	H	4.227036	-0.030322	1.522947
H	1.664962	-0.001195	2.797790	H	1.567864	-0.061097	2.917542
H	-0.913194	-0.001207	1.894816	H	-0.926602	-0.004295	1.868131
H	-0.926151	0.005605	-0.654461	H	-1.760034	-0.191873	-1.001444
O	-2.121363	-0.035915	-1.781270	O	-2.193445	-0.318943	-1.857606
H	-1.675443	-0.076434	-2.646103	H	-0.887322	0.066182	-2.892447
H	-2.935235	0.463881	-1.877797	H	-3.143591	-0.207085	-1.798486

7CNI-(H_2O)$_2$

N	0.000000	0.000000	0.000000	C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.319780	N	0.000000	0.000000	1.347490
C	1.350857	0.000000	1.766886	C	1.231855	0.000000	1.870584
C	2.183928	-0.000393	0.610494	C	2.129116	-0.041843	0.765887
C	3.586387	0.006655	0.448168	C	1.326641	-0.049816	-0.413010
C	4.056496	0.018345	-0.885071	H	1.656544	-0.021884	-1.441169
C	3.214305	0.029261	-1.968929	C	3.512251	0.019252	1.037811
C	1.769582	0.030181	-1.819238	C	3.943354	0.066658	2.355620
C	1.328834	0.003940	-0.481404	C	3.067293	0.153098	3.430748
C	0.878740	0.081855	-2.884878	C	1.669516	0.142671	3.217150
N	0.100418	0.131158	-3.748848	C	0.687258	0.462296	4.099741
H	3.621883	0.039504	-2.972456	N	-0.313572	0.779661	4.682949
H	5.125945	0.019351	-1.064517	H	3.444293	0.262386	4.439271
H	4.259872	-0.000418	1.294072	H	5.008973	0.069678	2.556617
H	1.663033	0.003931	2.800229	H	4.226153	-0.009990	0.222523
H	-0.916543	-0.001047	1.888264	H	-0.899276	0.104932	-0.586254
H	-0.872387	-0.029962	-0.566423	H	-1.262675	2.019992	2.230550
O	-2.448985	-0.116623	-1.180161	O	-1.641571	2.310771	3.070289
H	-2.946042	-0.937567	-1.139691	H	-0.759263	1.672545	4.309984
H	-2.577906	0.251926	-2.087434	H	-2.421295	1.753367	3.250443
O	-2.594723	0.662080	-3.720009	O	-3.118056	0.349458	4.229773
H	-1.666792	0.499518	-3.991462	H	-2.295752	0.049426	4.647470
H	-2.875761	1.505798	-4.081166	H	-3.618809	-0.424285	3.958328

Method: CAM-B3LYP/6-311++G(d) + PCM							
S_1 minimum (first) geometry				Last geometry			
7CNI-(H_2O)$_2$							
N	0.000000	0.000000	0.000000	N	0.000000	0.000000	0.000000

C	0.000000	0.000000	1.324367	C	0.000000	0.000000	1.320640
C	1.349957	0.000000	1.774214	C	1.325567	0.000000	1.843732
C	2.175338	0.000805	0.631172	C	2.199315	0.003417	0.721402
C	3.584030	0.005438	0.467560	C	3.601599	-0.024269	0.588928
C	4.067676	0.011847	-0.863004	C	4.111652	-0.033868	-0.734841
C	3.235775	0.012902	-1.951011	C	3.302091	-0.039410	-1.841304
C	1.776024	0.006458	-1.802620	C	1.847845	-0.042618	-1.712830
C	1.318831	0.000163	-0.476462	C	1.351926	-0.014325	-0.391987
C	0.915739	0.012309	-2.892166	C	0.996707	-0.121443	-2.794124
N	0.186270	0.020062	-3.801821	N	0.249735	-0.192726	-3.695591
H	3.645998	0.018235	-2.953499	H	3.733480	-0.056658	-2.835256
H	5.139027	0.016450	-1.032369	H	5.186878	-0.033649	-0.883736
H	4.251563	0.004901	1.319198	H	4.257834	0.012664	1.449232
H	1.658676	0.000494	2.808105	H	1.599823	-0.007284	2.888803
H	-0.915519	-0.000376	1.893873	H	-0.921454	0.010991	1.886650
H	-0.871132	-0.003841	-0.569128	H	-1.616759	0.191644	-1.056024
O	-2.443943	0.015910	-1.235038	O	-2.437888	0.351642	-1.574203
H	-3.045798	-0.696184	-0.998766	H	-3.053170	-0.371971	-1.418877
H	-2.570362	0.215537	-2.189994	H	-2.263327	0.729688	-2.944415
O	-2.562249	0.518379	-3.885287	O	-1.990212	0.954187	-3.933176
H	-1.614640	0.427956	-4.102438	H	-1.029961	0.540633	-4.030778
H	-2.859903	1.377140	-4.200844	H	-1.961872	1.913352	-4.055510

Method: ADC(2)

S_1 minimum (first) geometry				Last geometry
Ind				
N	-1.9720159	0.0011512	0.1162743	
C	-1.9863166	0.0012711	1.4413484	
C	-0.6264899	0.0005058	1.9250353	
C	0.2155434	-0.0000703	0.7831919	
C	1.6218744	-0.0009231	0.6009343	
C	2.1185137	-0.0013008	-0.7164690	
C	1.2430318	-0.0008215	-1.8219694	
C	-0.1738431	0.0000466	-1.6668136	
C	-0.6456043	0.0003760	-0.3630829	
H	-0.8469539	0.0004297	-2.5265142	
H	1.6572264	-0.0011373	-2.8341916	
H	3.1980228	-0.0020108	-0.8885810	
H	2.2994841	-0.0012966	1.4592983	
H	-0.3388019	0.0003397	2.9784704	
H	-2.9296888	0.0017888	1.9920625	
H	-2.8339821	0.0016514	-0.4789936	
2CNI				
C	-2.4327390	-0.0002838	-0.7165567	
C	-2.4643117	-0.0007584	0.6914333	
C	-1.2241094	-0.0006930	1.4191042	
C	-0.0316377	-0.0001576	0.6686592	
N	1.2669710	-0.0000465	1.0891023	
C	2.2007771	0.0002558	-0.0301619	

C	1.4018152	0.0006626	-1.1962891
C	0.0218192	0.0003354	-0.7970725
C	-1.2008296	0.0002032	-1.4867430
H	-1.2417202	0.0004264	-2.5794403
H	1.7871294	0.0010593	-2.2157412
C	3.5831435	0.0009406	0.1965614
N	4.7636836	0.0012242	0.4265117
H	1.5693535	-0.0008434	2.0617735
H	-1.2041047	-0.0009381	2.5131732
H	-3.4171361	-0.0011128	1.2245381
H	-3.3781042	-0.0002739	-1.2688523

2CNI-(H_2O)$_1$

6	-3.447716	-0.002502	-0.156923	6	-3.381161	-0.032403	-0.110825
6	-3.078241	0.006662	1.194674	6	-2.928101	-0.001246	1.208668
6	-1.680034	0.010230	1.541880	6	-1.524788	0.027791	1.497352
6	-0.748868	0.003610	0.488385	6	-0.657622	0.019654	0.419834
7	0.614017	0.004086	0.531306	7	0.762561	0.047851	0.458685
6	1.190199	-0.003420	-0.810841	6	1.191373	0.036770	-0.826391
6	0.096468	-0.008669	-1.705887	6	0.100135	0.002591	-1.739132
6	-1.116707	-0.005005	-0.927875	6	-1.107399	-0.009409	-0.939075
6	-2.480229	-0.009236	-1.243993	6	-2.475168	-0.036075	-1.216147
1	-2.827903	-0.016976	-2.280957	1	-2.854891	-0.057169	-2.242226
1	0.173643	-0.013411	-2.793151	1	0.190145	-0.007032	-2.827565
6	2.580682	0.004107	-0.951803	6	2.634558	0.064925	-1.161606
7	3.787052	0.009107	-0.952637	7	3.665219	0.098964	-0.426892
1	1.214285	0.002172	1.355831	1	1.698151	0.007001	1.525960
1	-1.350118	0.019540	2.585057	1	-1.155109	0.058645	2.527004
1	-3.838905	0.012060	1.978276	1	-3.644973	0.003776	2.034463
1	-4.510427	-0.004717	-0.420298	1	-4.457053	-0.052910	-0.308925
8	2.980417	0.078630	2.078377	8	2.499758	0.052832	2.200049
1	3.589245	0.050312	1.319837	1	3.488984	0.106585	0.610604
1	3.481130	-0.291054	2.816368	1	2.605652	-0.829014	2.583841

2CNI-(H_2O)$_2$

7	-0.217045	0.039080	-0.293736	N	-0.463640	-0.083409495	-0.013605003
6	-0.609099	0.039289	1.112710	C	-0.652172	-0.089102328	1.328320774
6	0.591058	0.000822	1.859318	C	0.581964	-0.085302505	2.034688375
6	1.693457	-0.022185	0.928476	C	1.631692	-0.084145874	1.035623861
6	3.083993	-0.055623	1.062433	C	3.026440	-0.087148845	1.065868733
6	3.901927	-0.071548	-0.142982	C	3.721620	-0.094729065	-0.183451698
6	3.356985	-0.051798	-1.430025	C	3.040504	-0.098952554	-1.400972881
6	1.924197	-0.014620	-1.589301	C	1.607504	-0.093867208	-1.436552935
6	1.140964	0.000547	-0.423615	C	0.946629	-0.085541569	-0.220823210
1	1.458708	-0.005615	-2.579468	H	1.056070	-0.100563101	-2.382028630
1	4.005752	-0.066641	-2.308587	H	3.599189	-0.108014621	-2.341092387
1	4.989591	-0.100664	-0.021374	H	4.815895	-0.098618484	-0.179455186
1	3.564909	-0.069520	2.044839	H	3.582896	-0.084593223	2.008225010
1	0.655447	-0.011498	2.947517	H	0.682613	-0.087889445	3.122386650
6	-1.963452	0.048401	1.448276	C	-1.991882	-0.130331112	1.960132560
7	-3.151470	0.058749	1.656640	N	-3.178293	-0.207771870	1.539841698

1	-0.913819	0.087400	-1.055479
8	-2.276416	0.144699	-2.149432
1	-3.139103	-0.028161	-1.701719
1	-2.437072	0.938147	-2.676139
8	-4.623842	-0.222281	-0.768175
1	-5.119149	-1.050803	-0.797826
1	-4.349245	-0.133386	0.167805

3CNI

N	-0.2170447	0.0390801	-0.2937355
C	-0.6090989	0.0392890	1.1127100
C	0.5910582	0.0008220	1.8593175
C	1.6934561	-0.0221852	0.9284759
C	3.0839917	-0.0556233	1.0624334
C	3.9019257	-0.0715478	-0.1429822
C	3.3569840	-0.0517983	-1.4300242
C	1.9241960	-0.0146200	-1.5893002
C	1.1409639	0.0005475	-0.4236144
H	1.4587073	-0.0056154	-2.5794674
H	4.0057503	-0.0666409	-2.3085865
H	4.9895887	-0.1006645	-0.0213736
H	3.5649081	-0.0695195	2.0448385
H	0.6554472	-0.0114981	2.9475163
C	-1.9634508	0.0484013	1.4482757
N	-3.1514687	0.0587492	1.6566394
H	-0.9138189	0.0873997	-1.0554784
O	-2.2764152	0.1446993	-2.1494314
H	-3.1391015	-0.0281614	-1.7017182
H	-2.4370713	0.9381462	-2.6761378
O	-4.6238401	-0.2222805	-0.7681749
H	-5.1191475	-1.0508021	-0.7978256
H	-4.3492434	-0.1333862	0.1678047

3CNI-$(H_2O)_1$

N	-0.2170447	0.0390801	-0.2937355
C	-0.6090989	0.0392890	1.1127100
C	0.5910582	0.0008220	1.8593175
C	1.6934561	-0.0221852	0.9284759
C	3.0839917	-0.0556233	1.0624334
C	3.9019257	-0.0715478	-0.1429822
C	3.3569840	-0.0517983	-1.4300242
C	1.9241960	-0.0146200	-1.5893002
C	1.1409639	0.0005475	-0.4236144
H	1.4587073	-0.0056154	-2.5794674
H	4.0057503	-0.0666409	-2.3085865
H	4.9895887	-0.1006645	-0.0213736
H	3.5649081	-0.0695195	2.0448385
H	0.6554472	-0.0114981	2.9475163
C	-1.9634508	0.0484013	1.4482757
N	-3.1514687	0.0587492	1.6566394
H	-0.9138189	0.0873997	-1.0554784
H	-1.278595	0.179822190	-1.404581612
O	-1.66390	0.289735900	-2.326777902
H	-3.293104	-0.235248981	-1.782379010
H	-1.730618	1.244524540	-2.464878945
O	-4.091075	-0.386335621	-1.227555646
H	-4.397890	-1.272890819	-1.456059469
H	-3.398968	-0.236211240	0.518089748

O -2.2764152 0.1446993 -2.1494314 H -3.1391015 -0.0281614 -1.7017182 H -2.4370713 0.9381462 -2.6761378 O -4.6238401 -0.2222805 -0.7681749 H -5.1191475 -1.0508021 -0.7978256 H -4.3492434 -0.1333862 0.1678047	
4CNI	
N -2.1728977 0.0003761 -0.0166878 C -2.1849927 0.0016108 1.3240840 C -0.8040941 0.0018007 1.7548840 C 0.0176631 0.0000183 0.5914912 C 1.4557289 -0.0005851 0.4234785 C 1.9206565 -0.0004556 -0.9465028 C 1.0216243 -0.0011757 -2.0263571 C -0.4118754 -0.0039327 -1.8798408 C -0.8423453 -0.0006895 -0.5279843 H -1.0927453 -0.0012008 -2.7336326 H 1.4342817 -0.0007624 -3.0406632 H 2.9966243 0.0010443 -1.1425650 C 2.2947794 -0.0007867 1.5581476 N 2.9545261 -0.0005222 2.5650001 H -0.4724806 0.0031795 2.7954060 H -3.1071546 0.0023116 1.9029788 H -3.0072985 -0.0002304 -0.6012364	
4CNI-$(H_2O)_1$	
N -1.4816142 -0.0004565 0.3235629 C -1.4713431 -0.0000515 1.6626768 C -0.0855166 0.0005390 2.0766408 C 0.7227932 0.0004592 0.8954703 C 2.1549983 0.0009384 0.7033004 C 2.5954506 0.0007066 -0.6772972 C 1.6791889 0.0000732 -1.7400846 C 0.2490331 -0.0003691 -1.5658929 C -0.1572592 -0.0001591 -0.2040720 H -0.4502983 -0.0009932 -2.4045604 H 2.0750200 -0.0000634 -2.7613590 H 3.6682319 0.0010395 -0.8912880 C 3.0178392 0.0015939 1.8202829 N 3.7010912 0.0021771 2.8116687 H 0.2644960 0.0009629 3.1111894 H -2.3855618 -0.0001801 2.2541224 H -2.3298685 -0.0008135 -0.2642262 O -3.7831447 -0.0015785 -1.3482019 H -3.9924239 -0.7674792 -1.9002532 H -3.9911122 0.7636542 -1.9016790	
4CNI-$(H_2O)_2$	
N -1.865002 0.007816485 0.915973142	N -1.942153 -0.000196827 0.820592410

C	-1.016741	0.025237016	1.952029224
C	0.323417	0.030876413	1.414063085
C	0.206449	0.015544581	-0.020911710
C	1.201219	0.013340392	-1.070419877
C	0.680021	-0.004433670	-2.423159159
C	-0.701694	-0.018398881	-2.674652930
C	-1.703564	-0.016438672	-1.645514727
C	-1.162768	0.001167694	-0.326714971
H	-2.774415	-0.027604119	-1.858618600
H	-1.032552	-0.031524059	-3.718869175
H	1.380828	-0.006977070	-3.263127790
C	2.566440	0.027496108	-0.730852610
N	3.709814	0.040548809	-0.348206393
H	1.244475	0.044599065	2.006724677
H	-1.358999	0.032677607	2.985708663
H	-2.883563	0.000174124	0.990242532
O	3.299469	0.052720730	2.541692317
H	4.076019	0.081332081	3.113826266
H	3.665155	0.048886764	1.635048615
O	-4.717305	-0.012108270	1.063863551
H	-5.234007	-0.783942710	0.795894225
H	-5.243577	0.746538211	0.777473893

5CNI

N	-2.2850808	-0.0004136	0.2299807
C	-2.2843492	0.0000987	1.5691445
C	-0.9065322	0.0005065	2.0037456
C	-0.0726455	0.0001226	0.8574146
C	1.3539540	0.0006860	0.6953525
C	1.8314209	0.0001532	-0.6786280
C	0.9103732	-0.0003052	-1.7784006
C	-0.5030229	-0.0005610	-1.6190011
C	-0.9485124	-0.0004904	-0.2682801
H	-1.1767871	-0.0009992	-2.4786736
H	1.3256484	-0.0005985	-2.7915100
C	3.2288541	0.0003742	-0.9597537
N	4.4057097	0.0004587	-1.1801316
H	2.0397971	0.0006096	1.5453093
H	-0.5966756	0.0011385	3.0500853
H	-3.2028386	0.0001381	2.1545031
H	-3.1193131	-0.0009182	-0.3511570

5CNI-$(H_2O)_1$

N	-1.5730728	-0.0036233	0.5313969
C	-1.5686688	-0.0012797	1.8655684
C	-0.1849266	0.0023210	2.2925134
C	0.6465647	0.0020175	1.1315950
C	2.0698732	0.0046397	0.9533795
C	2.5229118	0.0030550	-0.4322359
C	1.5987212	-0.0007071	-1.5138971
C	0.1845292	-0.0032083	-1.3348200
C	-1.087627	-0.000043464	1.851227950
C	0.280598	0.000041170	1.419004113
C	0.224687	0.000182138	-0.021710643
C	1.198437	0.000285739	-1.042935665
C	0.766546	0.000248420	-2.393413138
C	-0.608322	-0.000002775	-2.697930012
C	-1.601856	-0.000227197	-1.686169947
C	-1.157009	-0.000055649	-0.361689629
H	-2.667118	-0.000644906	-1.930196693
H	-0.916264	-0.000185717	-3.747000475
H	1.509065	0.000308505	-3.195629132
C	2.593968	0.000186075	-0.694244781
N	3.730711	0.000023911	-0.349007988
H	1.178319	0.000171363	2.047741740
H	-1.450348	-0.000189970	2.881608983
H	-3.762103	-0.000146266	0.890445859
O	3.253370	0.000090819	2.613197093
H	3.891648	0.000036535	3.337853271
H	3.795646	0.000044945	1.807851642
O	-4.772721	0.000154787	1.037347306
H	-5.157413	-0.801124431	0.533648054
H	-5.156934	0.801661835	0.533636241

C	-0.2362468	-0.0017634	0.0246955
H	-0.5066725	-0.0063746	-2.1802599
H	2.0020370	-0.0017495	-2.5320234
C	3.9202469	0.0052140	-0.7283100
N	5.0953595	0.0070859	-0.9549859
H	2.7705058	0.0077373	1.7911441
H	0.1354418	0.0047585	3.3360765
H	-2.4849830	-0.0021581	2.4541860
H	-2.4144759	-0.0063809	-0.0642022
O	-3.8536519	-0.0039429	-1.1781427
H	-4.0661687	-0.7683904	-1.7307172
H	-4.0573242	0.7627493	-1.7309610

6CNI

N	-2.0823410	0.0028666	0.4214153
C	-2.1149337	0.0040930	1.8135213
C	-0.7653524	0.0025343	2.2363911
C	0.0773827	0.0005288	1.0628268
C	1.4851362	-0.0012720	0.8528543
C	1.9670932	-0.0028122	-0.4890981
C	1.0998618	-0.0025834	-1.6224548
C	-0.3552165	-0.0004762	-1.4180955
C	-0.7841012	0.0008864	-0.0885084
H	-1.0427575	-0.0001461	-2.2683582
C	1.6303545	-0.0041978	-2.9395883
N	2.0533059	-0.0054705	-4.0614461
H	3.0475925	-0.0043315	-0.6638316
H	2.1892785	-0.0015879	1.6893953
H	-0.4373986	0.0029164	3.2766014
H	-3.0522749	0.0056030	2.3638995
H	-2.9156295	0.0034491	-0.1655241

6CNI-$(H_2O)_1$

N	-1.4584516	-0.0031216	0.7227113
C	-1.4786541	-0.0005730	2.0873041
C	-0.1116050	0.0017672	2.5115005
C	0.7241782	0.0006621	1.3326655
C	2.1395581	0.0023511	1.1243733
C	2.6034475	0.0006521	-0.2157844
C	1.7278072	-0.0026387	-1.3309928
C	0.2651134	-0.0043646	-1.1315366
C	-0.1455684	-0.0025203	0.2075127
H	-0.4263483	-0.0085658	-1.9772444
C	2.2432925	-0.0040960	-2.6558404
N	2.6334794	-0.0053290	-3.7898574
H	3.6815861	0.0019055	-0.4059628
H	2.8432102	0.0048777	1.9610038
H	0.2171099	0.0039788	3.5520349
H	-2.4072098	-0.0004638	2.6538709
H	-2.2904933	-0.0039150	0.1097616
O	-3.5610680	0.0076449	-1.1906108

N	-1.938924	0.000414228	-0.266484844
C	-2.632746	0.000334087	0.878788116
C	-1.765517	0.000093134	2.019479415
C	-0.422279	0.000218954	1.502774157
C	0.853592	-0.000079082	2.089961743
C	1.978708	-0.000229179	1.236881294
C	1.815067	-0.000134004	-0.167545685
C	0.527066	0.000059791	-0.781749860
C	-0.565695	0.000292553	0.080476674
H	0.415397	-0.000090700	-1.869384409
C	2.991679	-0.000185612	-1.002681330
N	3.970006	-0.000219753	-1.674636501
H	2.989456	-0.000342848	1.653119447
H	0.984915	-0.000214604	3.176126061
H	-2.075883	-0.000213202	3.067452863
H	-3.725151	0.000482170	0.873094495
H	-2.628118	0.000225503	-1.737210913
O	-3.194881	-0.000449075	-2.615699432

H	-3.6200855	-0.7583258	-1.7787777
H	-3.5792986	0.7700742	-1.7861312

6CNI-(H_2O)$_2$

N	-1.306173	-0.210633477	1.732486551
C	-1.043143	0.034472418	3.044517236
C	0.375312	0.233432118	3.146765387
C	0.943793	0.095420354	1.825226894
C	2.266882	0.208063836	1.286244259
C	2.418657	0.097680773	-0.118718295
C	1.324883	-0.183929785	-0.975844244
C	-0.010400	-0.463527800	-0.415285993
C	-0.133114	-0.206391354	0.951872715
H	-0.831650	-0.804107510	-1.044254431
C	1.394851	-0.113563893	-2.390243122
N	1.270424	-0.067228577	-3.585606522
H	3.404799	0.266434895	-0.563518975
H	3.127287	0.429719271	1.923290210
H	0.905305	0.447402309	4.076371661
H	-1.825858	0.080192848	3.798601754
H	-2.221808	-0.283021734	1.279226206
O	-1.952527	0.399963820	-2.893870485
H	-0.992502	0.450115246	-3.049504645
H	-2.287862	-0.012800771	-3.700841941
O	-3.220056	-0.037464469	-0.315139720
H	-4.127888	0.256303557	-0.459588449
H	-2.764959	0.145633278	-1.163718574

7CNI

N	-1.8258237	0.0021649	0.3549998
C	-1.8740806	0.0094825	1.6952329
C	-0.5060609	0.0117175	2.1522997
C	0.3618694	0.0052574	1.0006323
C	1.7874941	0.0041481	0.8316815
C	2.2452548	-0.0031464	-0.5231904
C	1.3923287	-0.0089838	-1.6341069
C	-0.0645951	-0.0080010	-1.4786077
C	-0.4844344	-0.0006391	-0.1211904
C	-1.0329401	-0.0134031	-2.5038621
N	-1.9528480	-0.0174779	-3.2817141
H	1.8090812	-0.0144224	-2.6454940
H	3.3243242	-0.0042359	-0.7101896
H	2.4740183	0.0086034	1.6812811
H	-0.2106678	0.0173517	3.2034565
H	-2.8090599	0.0126692	2.2524056
H	-2.6338603	-0.0010849	-0.2736341

7CNI-(H_2O)$_1$

H	-2.910777	-0.799963531	-3.176347543
H	-2.912859	0.799838451	-3.176251368

N	-2.061975	-0.344283752	0.126618107
C	-2.733897	-0.066865990	1.224311459
C	-1.835880	0.277465872	2.318500885
C	-0.496792	0.184411682	1.774193891
C	0.847764	0.408839675	2.364013288
C	1.946645	0.226263909	1.547230190
C	1.796028	-0.165374858	0.178159916
C	0.462398	-0.382201725	-0.489861554
C	-0.644172	-0.184960953	0.476736069
H	0.418964	-1.392820238	-0.949760591
C	2.965152	-0.352306517	-0.624118037
N	3.928347	-0.521039334	-1.311493368
H	2.960577	0.373839049	1.931679398
H	0.955728	0.707521390	3.412134560
H	-2.127087	0.549338781	3.337256417
H	-3.824680	-0.101742577	1.264951224
H	-2.342116	-0.639695766	-1.445773734
O	-0.617481	1.403655296	-2.918921973
H	0.349272	0.318316814	-1.350697479
H	-0.252911	1.429416932	-3.812350110
O	-2.282653	-0.764679295	-2.444215129
H	-3.191807	-0.850605122	-2.756210391
H	-1.264507	0.664827941	-2.933145275

N	-0.6664213	-0.0228798	1.3096160	C	0.156507	-0.053303709	-2.396761347
C	-0.0106916	-0.0281058	2.4771388	N	-0.635598	-0.009168642	-1.263576684
C	1.3960432	-0.0120660	2.1822117	C	0.247435	0.042195840	-0.215654880
C	1.5548589	0.0041681	0.7404248	C	1.620106	0.032084700	-0.681927960
C	2.7016052	0.0201475	-0.1206673	C	1.531075	-0.029661066	-2.105415891
C	2.4169058	0.0246579	-1.5189933	H	2.348999	-0.056282396	-2.825540836
C	1.1190831	0.0126647	-2.0478275	C	2.676030	0.077629436	0.263612632
C	-0.0578961	-0.0051631	-1.1791773	C	2.382362	0.130453151	1.635399001
C	0.2555118	-0.0048779	0.2150153	C	1.046508	0.140201459	2.109314990
C	-1.3989591	-0.0385995	-1.5917356	C	-0.014719	0.096064881	1.184224006
N	-2.5882107	-0.0688952	-1.8034372	C	-1.393167	0.105326213	1.545029060
H	0.9687277	0.0148068	-3.1314684	N	-2.581890	0.109013355	1.647734217
H	3.2540129	0.0371511	-2.2253673	H	0.832978	0.180771827	3.180915595
H	3.7221365	0.0282641	0.2691495	H	3.198364	0.164612989	2.363182302
H	2.1898541	-0.0144628	2.9323409	H	3.719100	0.070165632	-0.070844505
H	-0.5264200	-0.0445759	3.4361137	H	-0.308328	-0.103953806	-3.384097898
H	-1.7941115	-0.0165932	1.1896964	H	-2.462975	-0.044071808	-1.111017937
O	-3.3383636	-0.0714404	0.9006982	O	-3.441392	0.045876245	-0.775105028
H	-3.3565097	-0.1235010	-0.0843074	H	-3.307775	0.060660129	0.251852918
H	-3.8841199	0.6986597	1.1132124	H	-3.734566	0.936130994	-1.038674473

Method: CC2

S_1 minimum (first) geometry

Ind

N	0.0076909	-0.0997111	-0.0016380
C	-0.0365614	-0.0000654	1.4231652
C	1.2829411	-0.0000005	1.8731735
C	2.1520171	-0.0997082	0.7243839
C	3.5643234	-0.0011884	0.6000000
C	4.0656940	-0.0020679	-0.8101031
C	3.2113210	-0.0025075	-2.0000000
C	1.7803257	-0.0020282	-1.8058543
C	1.2938746	-0.0011284	-0.5000000
H	1.1034182	-0.0023449	-2.6659958
H	3.6558822	-0.0032099	-2.9628963
H	5.1513658	-0.0024088	-0.9623675
H	4.2528139	-0.0009933	1.3951223
H	1.5959389	0.0004648	2.9186066
H	-0.9895679	0.0004806	1.9489709
H	-0.8162293	-0.0010978	-0.5980879

Ind-$(H_2O)_1$

N	-0.2456900	0.2390321	0.0500000
C	-0.9982334	1.4479099	0.0715174
C	-0.0798046	2.4971023	0.0558796
C	1.2534270	1.9328283	0.0131584

C	2.5680718	2.4791833	-0.0181007
C	3.6723055	1.5487999	-0.0579471
C	3.5055100	0.1299606	-0.0670677
C	2.1803912	-0.4409140	-0.0356389
C	1.1008161	0.4787831	0.0030000
H	2.0099292	-1.5207465	-0.0416760
H	4.3868699	-0.5171617	-0.1000000
H	4.6901554	1.9566017	-0.0823973
H	2.7468766	3.5587127	-0.0125248
H	-0.3281672	3.5600122	0.0730486
H	-2.0857853	1.4249494	0.1015237
H	-0.6244909	-0.7181374	0.0406412
O	-0.5428032	-2.6140133	0.0235819
H	-0.0126555	-2.8644688	-0.7484278
H	0.0320637	-2.8742049	0.7595372

2CNI

C	-2.4327390	-0.0002838	-0.7165567
C	-2.4643117	-0.0007584	0.6914333
C	-1.2241094	-0.0006930	1.4191042
C	-0.0316377	-0.0001576	0.6686592
N	1.2669710	-0.0000465	1.0891023
C	2.2007771	0.0002558	-0.0301619
C	1.4018152	0.0006626	-1.1962891
C	0.0218192	0.0003354	-0.7970725
C	-1.2008296	0.0002032	-1.4867430
H	-1.2417202	0.0004264	-2.5794403
H	1.7871294	0.0010593	-2.2157412
C	3.5831435	0.0009406	0.1965614
N	4.7636836	0.0012242	0.4265117
H	1.5693535	-0.0008434	2.0617735
H	-1.2041047	-0.0009381	2.5131732
H	-3.4171361	-0.0011128	1.2245381
H	-3.3781042	-0.0002739	-1.2688523

2CNI-$(H_2O)_1$

N	-0.7209272	-0.6267393	-0.0250179
C	-1.7068776	0.4518160	0.0067872
C	-0.9690584	1.6587296	0.0243217
C	0.4325573	1.3241050	0.0048387
C	1.6154900	2.0760052	0.0123502
C	2.8877104	1.3728829	-0.0151173
C	2.9847266	-0.0328552	-0.0469259
C	1.7851068	-0.8247317	-0.0537752
C	0.5512065	-0.1389220	-0.0270658
H	1.8198992	-1.9183769	-0.0814544
H	3.9636824	-0.5173603	-0.0676730
H	3.8048801	1.9717624	-0.0108315
H	1.5980048	3.1698206	0.0378035
H	-1.4003815	2.6600806	0.0469682
C	-3.0661075	0.1286714	0.0020341

N	-4.2117545	-0.2747745	-0.0023322
H	-1.0264476	-1.6120060	-0.0315663
O	-2.4411069	-2.8754770	-0.1118272
H	-3.2552252	-2.3386757	-0.0869282
H	-2.6453777	-3.6539551	0.4254112

3CNI

N	-1.9635845	-0.0304137	-0.1938079
C	-2.0578512	-0.1623701	1.2592399
C	-0.6863428	-0.0427504	1.6876060
C	0.1766443	0.0010446	0.5254188
C	1.5583730	-0.0094283	0.3408717
C	2.0763529	0.0112808	-1.0184470
C	1.2449409	0.0196144	-2.1451912
C	-0.1800353	0.0163579	-1.9702821
C	-0.6776345	0.0096277	-0.6516941
H	-0.8573060	0.0312546	-2.8300972
H	1.6729928	0.0303951	-3.1498506
H	3.1626956	0.0167569	-1.1529328
H	2.2438169	-0.0344281	1.1933533
C	-0.2175932	-0.0132121	3.0196731
N	0.2178121	0.0189654	4.1348020
H	-2.9403532	0.2557666	1.7560069
H	-2.7729278	-0.1184613	-0.8046689

3CNI-$(H_2O)_1$

N	-0.5085738	1.2499459	0.0200000
C	-1.7768803	0.8627260	0.0453270
C	-1.8274917	-0.5919873	0.0491645
C	-0.4737291	-1.0552323	0.0143121
C	0.1195809	-2.3378430	0.0008914
C	1.5313543	-2.4039918	-0.0361711
C	2.3145458	-1.2317146	-0.0588155
C	1.7284036	0.0711656	-0.0500000
C	0.3420607	0.1190955	-0.0091825
H	2.3358866	0.9804118	-0.0631456
H	3.4051267	-1.3159805	-0.0873960
H	2.0254190	-3.3795119	-0.0474950
H	-0.4949418	-3.2440801	0.0186425
C	-3.0006920	-1.3929983	0.0814159
N	-3.9669609	-2.1017478	0.1080640
H	-2.5984868	1.5831976	0.0656856
H	-0.1448964	2.3022608	-0.0000984
O	0.5250564	3.6006319	-0.0200100
H	0.2527754	4.1443072	0.7597309
H	0.2124433	4.1413456	-0.7865821

4CNI

N	2.3772319	-0.4523427	-0.0000149
C	2.0064880	-1.7439776	-0.0000600

C	0.5578603	-1.7679450	-0.0000465
C	0.0979851	-0.4187533	-0.0000169
C	-1.2378198	0.1444094	-0.0000149
C	-1.2987880	1.5919226	0.0000681
C	-0.1311109	2.3771563	0.0001337
C	1.2055405	1.8338006	0.0001055
C	1.2384208	0.4157617	0.0000036
H	2.0982382	2.4631868	0.0001840
H	-0.2424653	3.4670323	0.0002132
H	-2.2764000	2.0829433	0.0000757
C	-2.3599450	-0.7113211	-0.0000982
N	-3.2818103	-1.4970021	-0.0001620
H	-0.0562494	-2.6718880	-0.0000718
H	2.7279305	-2.5604181	-0.0001207
H	3.3433551	-0.1272428	0.0000003

5CNI

N	2.5542700	0.7102093	-0.0002652
C	3.0575973	-0.5376893	-0.0000242
C	1.9485281	-1.4621511	0.0002571
C	0.7423427	-0.7160701	0.0001792
C	-0.6383269	-1.1055558	0.0001865
C	-1.6067176	-0.0170563	0.0000489
C	-1.1697687	1.3555080	-0.0002631
C	0.2010128	1.7424419	-0.0004287
C	1.1269196	0.6636696	-0.0001532
H	0.4976704	2.7941144	-0.0007120
H	-1.9384311	2.1359727	-0.0003767
C	-3.0044497	-0.2875935	0.0001543
N	-4.1846968	-0.5315666	0.0002179
H	-0.9500802	-2.1526528	0.0004245
H	2.0563348	-2.5485981	0.0004796
H	4.1301310	-0.7315821	-0.0000538
H	3.1084056	1.5631857	-0.0004641

5CNI-$(H_2O)_1$

N	-1.6685316	0.0496988	-0.0184329
C	-2.1238222	-1.2080193	-0.0524454
C	-0.9728519	-2.0896843	-0.0587533
C	0.2093874	-1.2881835	-0.0264486
C	1.6057461	-1.6139754	-0.0168727
C	2.5147903	-0.4728591	0.0198156
C	2.0212586	0.8649817	0.0447106
C	0.6309837	1.1870230	0.0355700
C	-0.2355386	0.0588188	-0.0011070
H	0.2758282	2.2199751	0.0549709
H	2.7525303	1.6804777	0.0720889
C	3.9271993	-0.6796465	0.0316627
N	5.1154124	-0.8759478	0.0408561
H	1.9717155	-2.6431177	-0.0365641

H	-1.0324980	-3.1801489	-0.0841302
H	-3.1879247	-1.4427702	-0.0706914
H	-2.2516540	0.9013392	-0.0063988
O	-3.2016660	2.4494525	0.0147485
H	-3.1873207	3.0237624	0.7946990
H	-3.1630442	3.0588235	-0.7372778

6CNI

N	-2.0823410	0.0028666	0.4214153
C	-2.1149337	0.0050000	1.8135213
C	-0.7653524	0.0025343	2.2363911
C	0.0773827	0.0005288	1.0628268
C	1.4851362	-0.0012720	0.8528543
C	1.9670932	-0.0028122	-0.4890981
C	1.0998618	-0.0025834	-1.6224548
C	-0.3552165	-0.0004762	-1.4180955
C	-0.7841012	0.0008864	-0.0885084
H	-1.0427575	-0.0001461	-2.2683582
C	1.6303545	-0.0050000	-2.9395883
N	2.0533059	-0.0054705	-4.0614461
H	3.0475925	-0.0043315	-0.6638316
H	2.1892785	-0.0015879	1.6893953
H	-0.4373986	0.0029164	3.2766014
H	-3.0522749	0.0056030	2.3638995
H	-2.9156295	0.0034491	-0.1655241

6CNI-$(H_2O)_1$

N	1.4988295	-0.6709578	-0.0219187
C	2.5623567	0.1843594	-0.0570794
C	2.0177076	1.5120982	-0.0657266
C	0.5748510	1.4026450	-0.0338574
C	-0.4869191	2.3631452	-0.0259678
C	-1.8167075	1.8667043	0.0094238
C	-2.1197577	0.4802465	0.0365858
C	-1.0318268	-0.5212380	0.0288167
C	0.2617057	0.0152013	-0.0063945
H	-1.2436632	-1.5931102	0.0489242
C	-3.4685561	0.0338620	0.0716721
N	-4.5973812	-0.3921713	0.1018280
H	-2.6501923	2.5773859	0.0162674
H	-0.2890427	3.4384836	-0.0462549
H	2.6091784	2.4296768	-0.0919782
H	3.5911150	-0.1705613	-0.0731908
H	1.5539887	-1.7046696	-0.0069968
O	1.3221129	-3.5032737	0.0288459
H	0.8438345	-3.8887044	-0.7211866
H	0.8683666	-3.8591220	0.8081876

7CNI

N	-0.5027001	-1.7011151	0.0001623

C	-1.8363354	-1.8545848	-0.0000390
C	-2.4036161	-0.5233796	-0.0002490
C	-1.3231210	0.4339022	-0.0001788
C	-1.2688135	1.8686981	-0.0002989
C	0.0471382	2.4335913	-0.0001715
C	1.2227779	1.6716411	0.0000731
C	1.1857406	0.2044913	0.0002194
C	-0.1362681	-0.3202209	0.0000606
C	2.2837476	-0.6801202	0.0004392
N	3.1384749	-1.5398915	0.0006547
H	2.1981014	2.1678881	0.0001488
H	0.1480407	3.5245016	-0.0002737
H	-2.1713896	2.4843341	-0.0004982
H	-3.4757905	-0.3123666	-0.0004425
H	-2.3177025	-2.8315412	-0.0000372
H	0.1906999	-2.4554777	0.0003419

7CNI-(H_2O)$_1$

N	0.5692227	-1.2628240	0.0585883
C	1.9073863	-1.3394246	0.0530963
C	2.4161070	0.0097113	0.0055112
C	1.2847854	0.9172456	-0.0182392
C	1.1757014	2.3459560	-0.0615781
C	-0.1583982	2.8600257	-0.0645147
C	-1.3017592	2.0511611	-0.0262199
C	-1.2045554	0.5891074	0.0199105
C	0.1399198	0.1057962	0.0173543
C	-2.2766705	-0.3158809	0.0797347
N	-3.1114261	-1.1969864	0.1338790
H	-2.2967671	2.5067178	-0.0289866
H	-0.3031093	3.9456349	-0.0975156
H	2.0540510	2.9952459	-0.0907034
H	3.4760206	0.2759279	-0.0071407
H	2.4359209	-2.2916620	0.0828442
H	-0.0853721	-2.0887372	0.0767748
O	-1.2462596	-3.3289652	0.1811819
H	-2.0800831	-2.8042732	0.2119684
H	-1.3947145	-3.9737761	-0.5259455