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

Electronic supplementary information for: Rotationally Resolved Electronic Spectroscopy of 3-Cyanoindole and the 3-Cyanoindole-water Complex

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ELECTRONIC SUPPORTING INFORMATION

The supporting online material contains:

- A figure with the molecular orbitals of the 3-cyanoindole-water cluster.
- A table with the CC2/cc-pVTZ computed and experimental molecular parameters of different 1:1 3-cyanoindole-water complexes.
- A table with the CC2/cc-pVTZ computed stabilization energies of the different 1:1 3-cyanoindole-water complexes.
- Tables with the Cartesian coordinates of the CC2/cc-pVTZ and SCS-CC2/cc-pVTZ optimized structures of 3-cyanoindole (Table S3 - S6) and the 3-cyanoindole water complexes (Table S7-S22) 1a, 1b, 2, 3 in their S_0 and S_1 states, respectively.

TABLE S1. CC2/cc-pVTZ computed and experimental molecular parameters of different 1:1 3-cyanoindole-water complexes. For details see text.

	CC2/cc-pVTZ				experiment		
	1a	1b	2	3	$\sigma = 1$	$\sigma = 0$	$\Delta\sigma$
A'' / MHz	1100	1113	1305	2025	1104.10	1100.04	-4.06
B'' / MHz	750	747	750	567	728.29	728.01	-0.28
C'' / MHz	447	448	477	444	439.07	438.99	-0.08
$\Delta I''$ / uÅ^2	-2.34	-2.34	-1.91	-2.12	-0.6380	-2.3774	
A' / MHz	1121	1119	1279	2009	1099.63	1096.97	-2.66
B' / MHz	739	740	731	560	724.63	724.33	-0.30
C' / MHz	446	447	466	439	437.28	437.20	0.00
$\Delta I'$ / uÅ^2	-2.33	-3.31	-1.88	-3.75	-1.2938	-2.0979	
ΔA / MHz	21.01	6.01	-26.06	-16.33	-4.47	-3.07	
ΔB / MHz	-10.97	-6.57	-28.29	-6.91	-3.65	-3.68	
ΔC / MHz	-0.55	-1.03	-10.91	-4.40	-1.79	-1.79	
$\Delta\nu_{Lor.}$/MHz	-	-	-	-	43.51	43.51	
τ / ns	-	-	-	-	3.66	3.66	
θ / $^\circ$	-20	-16	-25	+34	$\pm$48.26	$\pm$48.26	
ν_0 / cm^{-1}	36335	36280	36093	36501	35262.2	35261.9	
$\Delta\nu_0$ /MHz	-	-	-	-	-8977.46		

TABLE S2. Summary of stabilization energies (including ZPE and BSSE corrections) and adiabatic excitation (including ZPE) and vertical excitation and emission energies of four most stable isomers of the 3-cyanoindole-water cluster at CC2/cc-pVTZ level of theory.

	1a	1b	2	3
$\Delta E_{stab.}$(S_0) /kJ mol^{-1}	-32.08	-32.06	-24.20	-25.38
$\Delta E_{stab.}$(S_0) /cm^{-1}	-2681.70	-2679.89	-2023.1	-2122.01
$\Delta E_{stab.}$(S_1) /kJ mol^{-1}	-29.94	-30.57	-24.96	-21.26
$\Delta E_{stab.}$(S_1) /cm^{-1}	-2502.6	-2555.6	-2086.3	-1777.0
$\Delta E_{adiabatic}$ /cm^{-1}	36335	36280	36093	36501
$\Delta E_{vertical}$ @ opt. S_0	39299	39357	39322	39503
$\Delta E_{vertical}$ @ opt. S_1	36002	33724	32614	34073

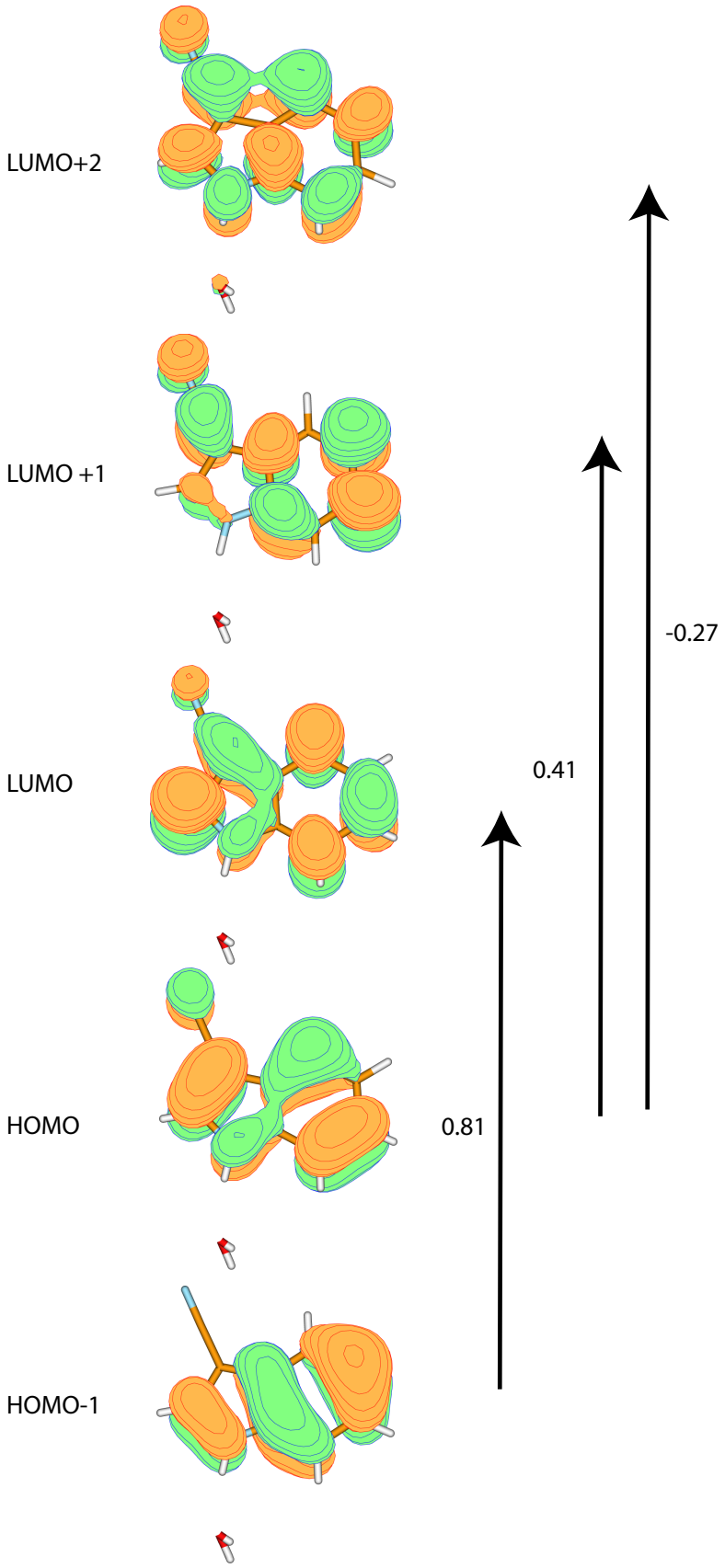

FIG. S1. Molecular orbitals of 3-cyanoindole water cluster (1a) with the coefficients of the respective excitations according to SCS-CC2/cc-pVTZ calculations. Only π-orbitals were considered.

TABLE S3. CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole (in bohr).

c	-2.31860350	-4.71208238	-0.00237471
c	0.34505222	-4.71876513	-0.00206834
c	1.72123137	-2.48274302	-0.00176550
c	0.34710443	-0.22946807	-0.00165995
n	1.16269474	2.24767183	-0.00132971
c	-0.87176619	3.84603113	-0.00129166
c	-3.06707244	2.42460399	-0.00158323
c	-2.33217045	-0.18705951	-0.00182482
c	-3.67829789	-2.46885021	-0.00226125
h	-3.31687886	-6.49569444	-0.00274291
h	1.34135663	-6.50360103	-0.00201287
h	3.76654136	-2.49512894	-0.00159832
h	-0.63823912	5.86825568	-0.00106641
c	-5.56529264	3.37276034	-0.00158999
h	-5.72373272	-2.46842242	-0.00254132
h	2.98035993	2.80824638	-0.00113812
n	-7.67456788	4.11051580	-0.00157987

TABLE S4. CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole (in bohr).

c	-0.38812082	-3.83487540	0.07146021
c	2.24004126	-3.38839598	0.00288695
c	3.17310639	-0.86722703	0.04338136
c	1.37256577	1.08308504	0.15215508
n	1.67347712	3.62885202	0.21556824
c	-0.67867807	4.94852297	0.32807896
c	-2.54939811	3.06977902	0.32895680
c	-1.34402699	0.64277833	0.22315865
c	-2.22844909	-1.84134292	0.18255211
h	-1.06325777	-5.76575037	0.03981881
h	3.53418536	-4.96348344	-0.08016863
h	5.17607565	-0.46207249	-0.00721536
h	-0.77182565	6.97566037	0.37016868
c	-5.18127510	3.44123174	0.41813629
h	-4.22697939	-2.26530633	0.23265957
h	3.36919202	4.50248639	0.19263515
n	-7.40694457	3.68306709	0.49123914

TABLE S5. SCS CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole (in bohr).

c	-2.31879816	-4.72113457	-0.00223036
c	0.35084906	-4.72497653	-0.00204012
c	1.72285892	-2.48740682	-0.00185721
c	0.34295897	-0.22964943	-0.00191268
n	1.16487242	2.25154597	-0.00133592
c	-0.87606086	3.84890934	-0.00120510
c	-3.06839866	2.43030251	-0.00161916
c	-2.33063849	-0.18983957	-0.00209655
c	-3.67806966	-2.47828788	-0.00239326
h	-3.31566816	-6.50613706	-0.00222625
h	1.34852910	-6.50978426	-0.00207969
h	3.76838477	-2.49588137	-0.00159686
h	-0.64279591	5.87132784	-0.00085618
c	-5.57583118	3.39006973	-0.00154992
h	-5.72349295	-2.48080295	-0.00289781
h	2.98007428	2.81184887	-0.00104787
n	-7.67105447	4.13616617	-0.00148406

TABLE S6. SCS CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole (in bohr).

c	-2.31314536	-4.74038251	-0.00233793
c	0.38627504	-4.78743558	-0.00205848
c	1.80161090	-2.49354956	-0.00169251
c	0.39305489	-0.22927146	-0.00169440
n	1.16962481	2.22845791	-0.00141271
c	-0.89351095	3.91681323	-0.00117351
c	-3.08481895	2.45938963	-0.00160334
c	-2.37889064	-0.15462168	-0.00203060
c	-3.74520547	-2.43441622	-0.00234170
h	-3.32359336	-6.51822115	-0.00254925
h	1.35257002	-6.58558124	-0.00215590
h	3.84429582	-2.48901068	-0.00142463
h	-0.62582255	5.93100026	-0.00072382
c	-5.60068821	3.38749672	-0.00161580
h	-5.78725044	-2.46090772	-0.00253656
h	2.99036628	2.78121524	-0.00143713
n	-7.70715283	4.10529481	-0.00164073

TABLE S7. CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 1a (in bohr).

c	-0.47709694	-3.87415680	0.07362869
c	2.14308746	-3.39487669	0.00581837
c	3.08664693	-0.94506230	0.04400719
c	1.32829895	1.02217280	0.15255500
n	1.69971084	3.59846111	0.21201183
c	-0.58443551	4.79573634	0.31551514
c	-2.50052786	3.00853752	0.32562212
c	-1.31435759	0.57208874	0.22194654
c	-2.22160471	-1.91714301	0.18144851
h	-1.13476242	-5.80949670	0.04065728
h	3.44576512	-4.96844720	-0.07775805
h	5.09678815	-0.57182061	-0.00784941
h	-0.71728792	6.82670652	0.37547158
c	-5.12452540	3.49863411	0.42016400
h	-4.23181739	-2.29308781	0.23321821
h	3.42100321	4.45045330	0.18188580
n	-7.32991749	3.85344698	0.49800662
o	6.81743382	5.48895961	0.09797955
h	7.94861904	5.19472297	1.49056459
h	7.84950172	5.26590611	-1.38207855

TABLE S8. CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 1a (in bohr).

c	-0.38105345	-3.83893075	0.07104077
c	2.23569351	-3.38570202	0.00336583
c	3.16355004	-0.85564384	0.04465052
c	1.35596294	1.08631767	0.15327724
n	1.66868498	3.62903100	0.21518646
c	-0.67651928	4.94764299	0.32548900
c	-2.55322145	3.07127666	0.32836306
c	-1.34698477	0.63452648	0.22340654
c	-2.22961258	-1.85074071	0.18249469
h	-1.05120922	-5.77198341	0.03841591
h	3.53469908	-4.95765835	-0.07957431
h	5.16234083	-0.43306498	-0.00437962
h	-0.76963448	6.97457317	0.37563546
c	-5.18266883	3.44816550	0.41781414
h	-4.22694121	-2.28093242	0.23260354
h	3.40444914	4.47083358	0.18623731
n	-7.40784925	3.69929659	0.49144544
o	6.81898056	5.36715589	0.09607916
h	7.89057050	4.89104121	1.48663756
h	7.79128496	4.95653074	-1.38537371

TABLE S9. CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 1b (in bohr).

c	14.01062475	-3.02670173	2.32387528
c	16.35968064	-4.27112174	2.13769368
c	18.45811401	-3.08710787	1.09481879
c	18.13699180	-0.60954591	0.23926933
n	19.84927211	1.01399071	-0.86275675
c	18.69043472	3.25821062	-1.39327318
c	16.18309502	3.13847019	-0.64165215
c	15.78740553	0.67087326	0.41189409
c	13.69687053	-0.56490369	1.47226207
h	12.42363855	-4.01694839	3.14870986
h	16.53081291	-6.19006173	2.82217356
h	20.26474338	-4.03379350	0.94755928
h	19.69953830	4.79712735	-2.26497305
c	14.36682978	5.08313456	-0.87274371
h	11.89037178	0.38384441	1.61859348
h	21.68617777	0.58077377	-1.21395540
n	12.81079422	6.67861017	-1.04382922
o	24.87580944	-0.95216566	-1.51606613
h	26.30957139	-0.58045430	-0.46235115
h	25.59524736	-1.56900952	-3.06720467

TABLE S10. CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 1b (in bohr).

c	14.04829139	-3.07604036	2.29115137
c	16.36687216	-4.30373337	2.23705212
c	18.52563161	-3.03732767	1.23623811
c	18.19152211	-0.57244521	0.34596300
n	19.86977778	1.01991601	-0.75772613
c	18.72950249	3.34039392	-1.61148123
c	16.18204293	3.16814479	-0.72891891
c	15.79052063	0.72167956	0.39300839
c	13.70886291	-0.53793050	1.35318907
h	12.41603207	-4.04211340	3.05864661
h	16.53995039	-6.20772237	2.95244732
h	20.36409198	-3.93123774	1.16781678
h	19.88406395	5.02385296	-1.74552548
c	14.31367591	5.03121955	-0.93555793
h	11.86275005	0.34182902	1.40041567
h	21.69639660	0.51836717	-1.12472716
n	12.69088375	6.57886350	-1.06790683
o	24.79929644	-1.09732172	-1.57051895
h	26.35331439	-0.56466837	-0.79108352
h	25.29254446	-1.67050475	-3.22443831

TABLE S11. CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 2 (in bohr).

c	-0.84541036	-4.05462108	-0.35397617
c	1.78917761	-4.11797589	0.03520499
c	3.19216254	-1.91364697	0.29571365
c	1.86921612	0.36547366	0.15344416
n	2.71811115	2.82789755	0.33317146
c	0.73731690	4.46820079	0.07532844
c	-1.45653751	3.08741648	-0.27862750
c	-0.77896997	0.45743610	-0.23520503
c	-2.16254454	-1.78905516	-0.49415684
h	-1.86139052	-5.81750383	-0.55051332
h	2.74371388	-5.92318022	0.13218439
h	5.21505408	-1.96856043	0.59269460
h	1.00398758	6.48467620	0.15680589
c	-3.91606049	4.05812062	-0.62329953
h	-4.18871000	-1.73949508	-0.79324121
h	4.52629472	3.35109982	0.60850050
n	-6.01821145	4.75698423	-0.92285527
o	-8.49505060	-0.42383422	-1.27327369
h	-9.21293345	-0.42583235	0.39645736
h	-8.10254071	1.34110780	-1.53595888

TABLE S12. CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 2 (in bohr).

c	-0.85238860	-4.03429696	-0.27104076
c	1.74859696	-4.18103609	0.06637571
c	3.17728715	-1.92327143	0.28842820
c	1.88485906	0.38726382	0.14958286
n	2.76627081	2.78552086	0.22825943
c	0.80263155	4.67033001	-0.20965245
c	-1.46076161	3.19209420	-0.31895676
c	-0.81596857	0.55018545	-0.20455033
c	-2.18730674	-1.65386230	-0.42885748
h	-1.94771861	-5.75441708	-0.43619701
h	2.67980995	-5.99427114	0.16726094
h	5.20386399	-1.97576726	0.57006295
h	1.01889541	6.50329632	0.67969363
c	-3.94027466	4.05455677	-0.57407178
h	-4.21610082	-1.62222397	-0.73205982
h	4.62425277	3.22465122	0.24740370
n	-6.10208585	4.64387249	-0.78337105
o	-8.33207265	-0.52573725	-1.35650999
h	-9.33890264	-0.58121395	0.15576581
h	-7.95621189	1.25903429	-1.51916779

TABLE S13. CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 3 (in bohr).

c	-0.69382954	-4.02381608	0.03258585
c	1.93148558	-3.57906734	0.07686186
c	2.90589648	-1.14350127	0.19504916
c	1.16943838	0.84205423	0.26807445
n	1.55376232	3.42020682	0.38776307
c	-0.71375070	4.65753136	0.42253177
c	-2.63518159	2.88123492	0.32332175
c	-1.47912773	0.42987777	0.22453607
c	-2.41549430	-2.04543367	0.10503377
h	-1.37463060	-5.94895124	-0.05932216
h	3.21711682	-5.16710559	0.01815495
h	4.92328095	-0.80809589	0.22951186
h	-0.87583594	6.68658895	0.51480693
c	-5.24063488	3.45515022	0.33768254
h	-4.43048304	-2.39575248	0.07152071
h	3.25108452	4.27709932	0.45186277
n	-7.41400679	3.98174636	0.36156347
o	-4.57804958	9.35764669	0.41149673
h	-5.84394736	8.12982252	0.88021074
h	-5.03829997	9.76476340	-1.29951927

TABLE S14. CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 3 (in bohr).

c	-0.67572528	-4.00970142	0.10850208
c	1.93039793	-3.65753954	0.19671344
c	2.92963595	-1.16261155	0.26817577
c	1.21315870	0.85148859	0.24266643
n	1.61840115	3.37993848	0.22551951
c	-0.67799789	4.84621184	-0.00090087
c	-2.62158950	2.97834453	0.09710405
c	-1.49971657	0.50697311	0.15033260
c	-2.44036503	-1.93190668	0.06843265
h	-1.43117603	-5.91046612	0.06337441
h	3.18701810	-5.26511616	0.21776621
h	4.94593761	-0.82705998	0.35536141
h	-0.76425516	6.75665039	0.71613484
c	-5.21975375	3.46722924	0.13123072
h	-4.45120333	-2.29196107	-0.03229937
h	3.35665520	4.16909791	0.16069278
n	-7.42261326	3.91066335	0.18450785
o	-4.78863885	9.37038303	0.73448502
h	-6.01877638	8.08545390	1.13752922
h	-4.95060059	9.50592716	-1.07160176

TABLE S15. SCS CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 1a (in bohr).

c	-0.50943508	-3.90443260	0.07320923
c	2.11849563	-3.43424635	0.00586308
c	3.07027473	-0.98860819	0.04461428
c	1.31509552	0.99040069	0.15317802
n	1.70251905	3.57009586	0.21286945
c	-0.58142877	4.77677615	0.31610840
c	-2.50309642	3.00164567	0.32567182
c	-1.32384398	0.55233671	0.22172815
c	-2.24356123	-1.93918462	0.18081130
h	-1.17503783	-5.83761571	0.03988463
h	3.41472599	-5.01395943	-0.07766346
h	5.08181446	-0.62214869	-0.00671240
h	-0.70437275	6.80847168	0.37609827
c	-5.13561258	3.51485475	0.42034122
h	-4.25518008	-2.30755291	0.23226457
h	3.41839590	4.41933230	0.18365533
n	-7.32670823	3.89190795	0.49772843
o	6.87863147	5.54238500	0.09530881
h	8.02878180	5.35704486	1.49019913
h	7.93006440	5.42423187	-1.38234324

TABLE S16. SCS CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 1a (in bohr).

c	-0.45796106	-3.89295986	0.07624751
c	2.20165044	-3.43699398	0.00103662
c	3.16856639	-0.92003646	0.03568034
c	1.36419282	1.04382456	0.14642949
n	1.68734228	3.59423192	0.20239687
c	-0.64750612	4.86778804	0.31271328
c	-2.54048039	3.04093719	0.32672774
c	-1.36844775	0.59685976	0.22402020
c	-2.29267290	-1.89654728	0.18882912
h	-1.11993158	-5.82795253	0.04718166
h	3.48108436	-5.02609680	-0.08297634
h	5.17138894	-0.52554053	-0.01981592
h	-0.75309503	6.89647847	0.36981764
c	-5.18106380	3.49460249	0.42524408
h	-4.29334924	-2.30304254	0.24379359
h	3.40396714	4.45128104	0.16905854
n	-7.38176752	3.81664090	0.50591543
o	6.88094157	5.50691401	0.10350224
h	7.97739931	5.11265909	1.49906503
h	7.90026414	5.20868751	-1.37205212

TABLE S17. SCS CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 1b (in bohr).

c	13.97494317	-3.03152503	2.33306627
c	16.32696199	-4.28401126	2.15294129
c	18.42876387	-3.10453451	1.11402893
c	18.11487672	-0.62068436	0.25319264
n	19.84051137	0.99821880	-0.84804944
c	18.68418591	3.24752250	-1.38295913
c	16.17856996	3.13606222	-0.63872660
c	15.77283631	0.66269304	0.41925873
c	13.67176818	-0.57033442	1.47818881
h	12.38332878	-4.01784286	3.15497854
h	16.49179270	-6.20330412	2.83984352
h	20.23368617	-4.05565580	0.97233750
h	19.70057740	4.78242017	-2.25353223
c	14.36547903	5.09983480	-0.88080912
h	11.86688357	0.38226970	1.61933238
h	21.67295292	0.56951335	-1.19750718
n	12.83062784	6.70003094	-1.06202630
o	24.98024636	-0.89708539	-1.56751792
h	26.42022204	-0.54930847	-0.51514425
h	25.68680970	-1.54105830	-3.11285244

TABLE S18. SCS CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 1b (in bohr).

c	14.08777992	-3.05789027	2.33457602
c	16.46947179	-4.31405722	2.14541063
c	18.60080004	-3.06810047	1.06093088
c	18.20821441	-0.56971226	0.20730805
n	19.84043708	1.08459180	-0.89325833
c	18.65047525	3.39976636	-1.44982740
c	16.14663465	3.20580464	-0.66640587
c	15.77259678	0.73663851	0.39243065
c	13.68823946	-0.51777225	1.46683517
h	12.51429575	-4.06387999	3.16851119
h	16.64212833	-6.22798077	2.83561654
h	20.42206839	-3.97680454	0.89612163
h	19.65838463	4.93131495	-2.32644908
c	14.26923525	5.10917029	-0.86966686
h	11.86201344	0.38046405	1.63694665
h	21.68075925	0.68125391	-1.25776423
n	12.67439027	6.65472471	-1.01480411
o	25.03873553	-0.63928710	-1.69897144
h	26.06582575	-1.02218262	-0.24853123
h	25.33353805	-2.02284074	-2.84096487

TABLE S19. SCS CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 2 (in bohr).

c	-0.82454230	-4.06523776	-0.35142410
c	1.81644522	-4.12520094	0.03610277
c	3.21476140	-1.91880762	0.29458516
c	1.88567929	0.36465736	0.15304890
n	2.74074952	2.83104445	0.33381389
c	0.75290801	4.46986096	0.07736585
c	-1.43850146	3.09205667	-0.27441561
c	-0.75744217	0.45443678	-0.23227542
c	-2.14071818	-1.79991012	-0.49001110
h	-1.83911941	-5.82958418	-0.54661934
h	2.77254978	-5.93030834	0.13234957
h	5.23822618	-1.96919329	0.58985604
h	1.01879978	6.48660595	0.15932707
c	-3.90609513	4.08043035	-0.61623422
h	-4.16591661	-1.75602545	-0.78796504
h	4.54672888	3.35422851	0.60659820
n	-5.99000458	4.80180461	-0.90900485
o	-8.62049107	-0.42886496	-1.28284493
h	-9.32442874	-0.41629308	0.39243870
h	-8.22291342	1.32900808	-1.56629355

TABLE S20. SCS CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 2 (in bohr).

c	-0.82211776	-4.07223455	-0.34752152
c	1.84556001	-4.18733937	0.03845709
c	3.28750236	-1.92896104	0.30372312
c	1.94130768	0.36846504	0.16175154
n	2.75933413	2.80508758	0.33385206
c	0.75158465	4.55066774	0.07786400
c	-1.44476557	3.13410582	-0.27174068
c	-0.79979186	0.50359473	-0.23229323
c	-2.20103649	-1.73570916	-0.48751083
h	-1.85962494	-5.82325871	-0.54766482
h	2.76759645	-6.00648213	0.12557564
h	5.30921917	-1.97021823	0.59525743
h	1.06063339	6.55666592	0.16309449
c	-3.92312997	4.08171740	-0.61662459
h	-4.22514144	-1.71316897	-0.78070498
h	4.57317534	3.31333701	0.60279305
n	-6.02190751	4.76319006	-0.91401815
o	-8.63272107	-0.46771840	-1.28226071
h	-9.36961245	-0.43567081	0.37860957
h	-8.23938912	1.28863808	-1.58224049

TABLE S21. SCS CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 3-Cyanoindole water 3 (in bohr).

c	-0.68087267	-4.05140866	0.03714122
c	1.94923204	-3.59986200	0.08287741
c	2.91655941	-1.16210256	0.19771274
c	1.17144271	0.82488749	0.26617574
n	1.55768322	3.40873503	0.38184650
c	-0.71819819	4.64046989	0.41308312
c	-2.63513386	2.86558992	0.31570308
c	-1.47054895	0.40801691	0.22142618
c	-2.40434097	-2.07499680	0.10503928
h	-1.35763426	-5.97864895	-0.05217401
h	3.23784673	-5.18644095	0.02772779
h	4.93309441	-0.82047003	0.23313910
h	-0.87466506	6.66951374	0.50157219
c	-5.25457300	3.43769151	0.32618161
h	-4.41857602	-2.42987873	0.07045338
h	3.25118644	4.26772220	0.44594665
n	-7.41997551	3.95108338	0.34551774
o	-4.60259498	9.46197226	0.41531202
h	-5.87899949	8.25645895	0.90552799
h	-5.08213900	9.88366641	-1.28648273

TABLE S22. SCS CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 3-Cyanoindole water 3 (in bohr).

c	-0.68143478	-4.06540726	0.02006554
c	1.99000330	-3.65312386	0.06821297
c	3.00195346	-1.15817371	0.19848949
c	1.22985863	0.83534880	0.27439412
n	1.58151661	3.38884997	0.40076745
c	-0.72706349	4.70259448	0.43758414
c	-2.64071327	2.89919505	0.33028904
c	-1.51569456	0.43992376	0.22496380
c	-2.48165266	-2.03660361	0.09724981
h	-1.37290899	-5.98719592	-0.07833854
h	3.24555321	-5.26175500	0.00521494
h	5.01457465	-0.81291224	0.23823755
h	-0.84763253	6.72990725	0.54117168
c	-5.26399879	3.44599745	0.34140007
h	-4.48978637	-2.40563919	0.05982002
h	3.28211519	4.23954465	0.46851401
n	-7.43725664	3.92842559	0.36011666
o	-4.64880958	9.49948993	0.36831143
h	-5.91870386	8.34408117	0.97828434
h	-5.10112652	9.69945169	-1.38102153