SUPPORTING INFORMATION

Experimental and Theoretical Comprehension of ESIPT Fluorophores Based on a 2-(2'-Hydroxyphenyl)-3,3'-Dimethylindole (HDMI) Scaffold

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S1. Materials and methods

All commercially available chemicals were received from Sigma Aldrich or Fluorochem. Thin layer chromatographies (TLC) were performed on silica gel coated with a fluorescent indicator. Purifications by column chromatography were conducted using 40-63 μm silica gel.

^{1}H NMR (400 or 500 MHz) and ^{13}C NMR (100 or 126 MHz) spectra were recorded on a Bruker Advance spectrometer with deuterated solvents. Mass spectrometry analysis was performed by direct sample injection on a electrospray ionization time-of-flight (ESI-TOF) micrOTOF II mass spectrometer. Absorption spectra were recorded using a dual-beam grating Schimadzu UV-3000 absorption spectrometer with a quartz cuvette of 1 cm of optical path length. The steady-state fluorescence emission and excitation spectra were recorded by using a Horiba S2 Jobin Yvon Fluoromax 4. All fluorescence were corrected. Solvents for spectroscopy were spectroscopic grade. Potassium bromide was stored in a drying cabinet.

S2. ^{1}H and ^{13}C NMR spectra

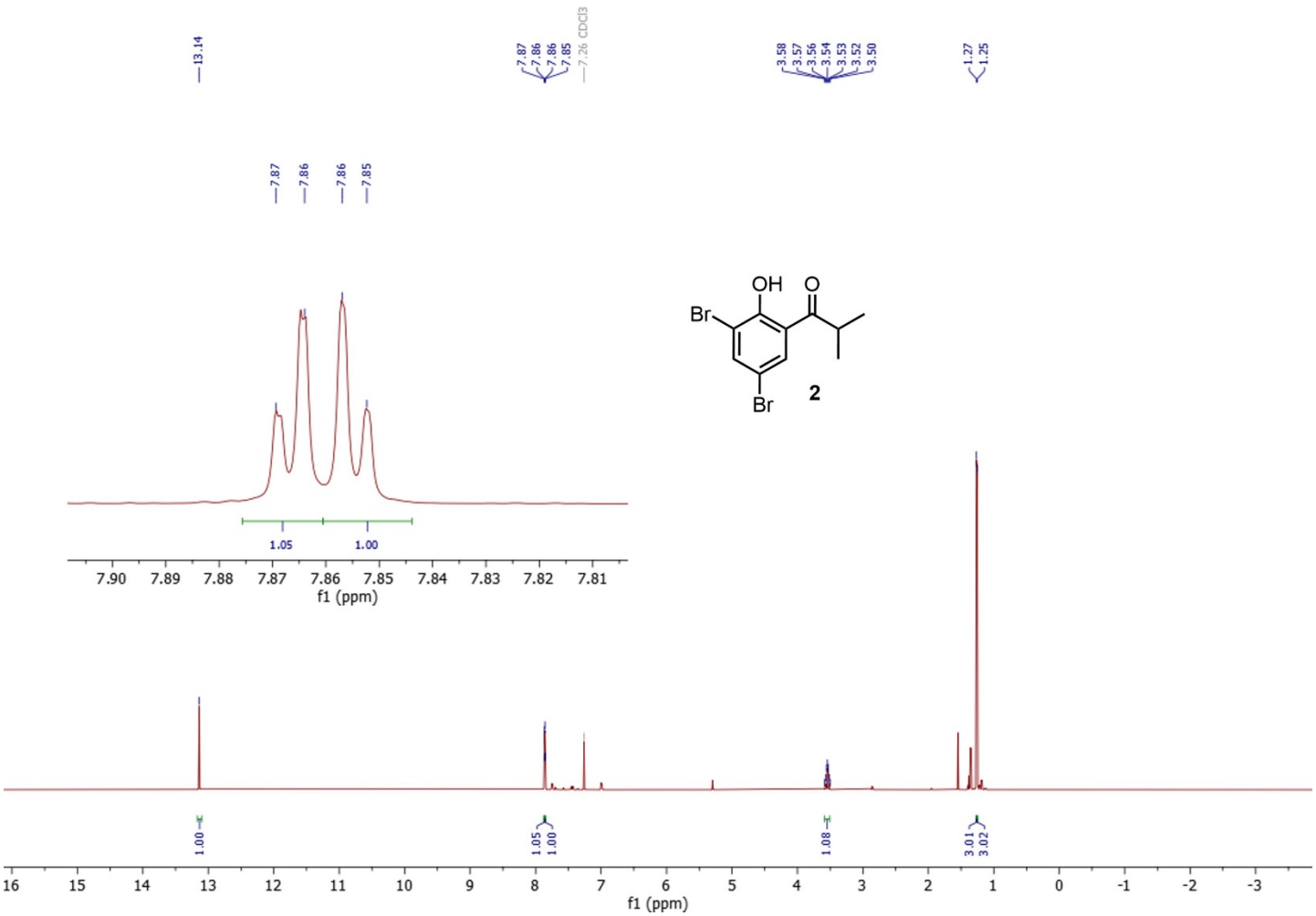


Figure S1. ^{1}H NMR spectrum of **2**

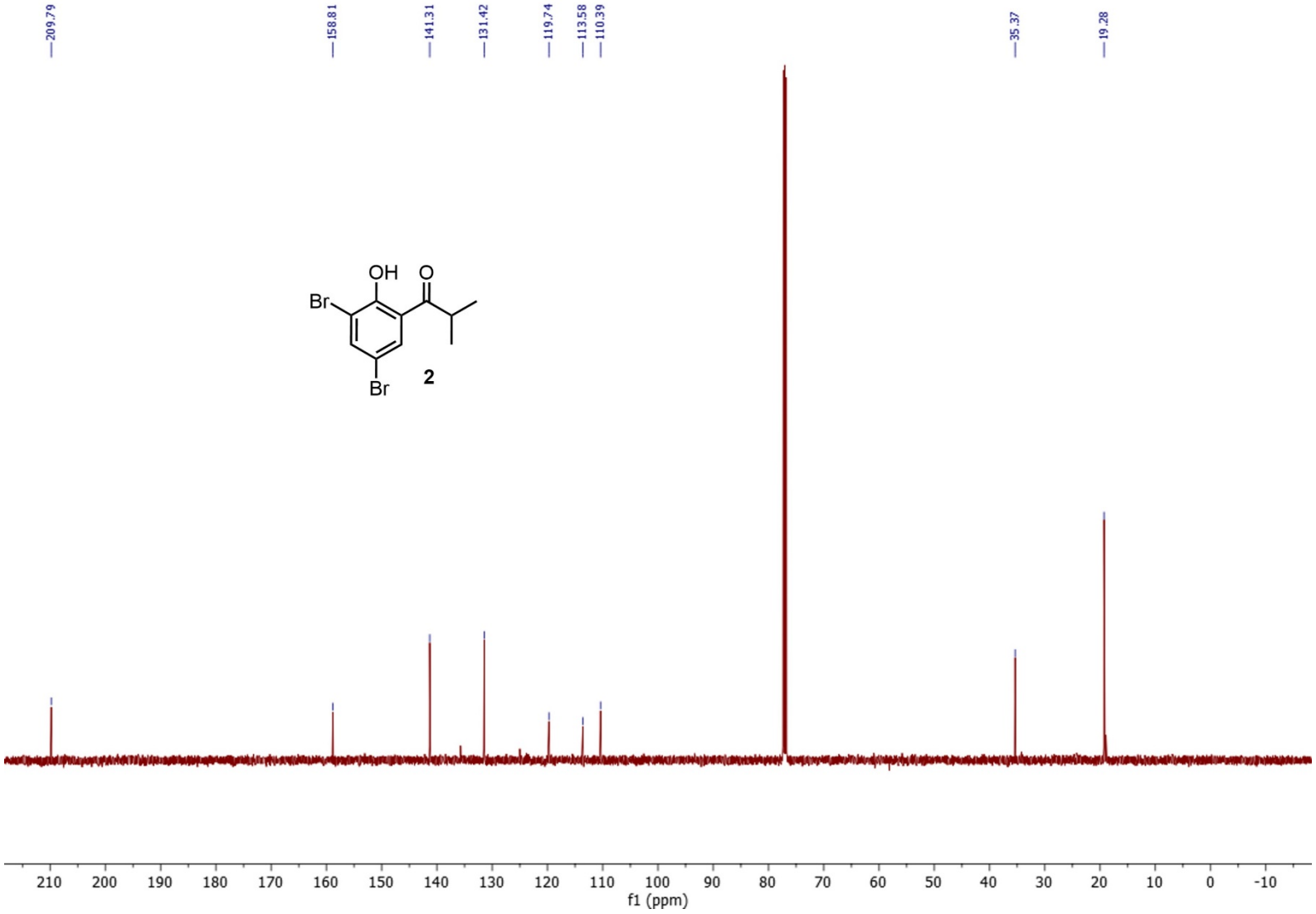


Figure S2. ^{13}C NMR spectrum of **2**

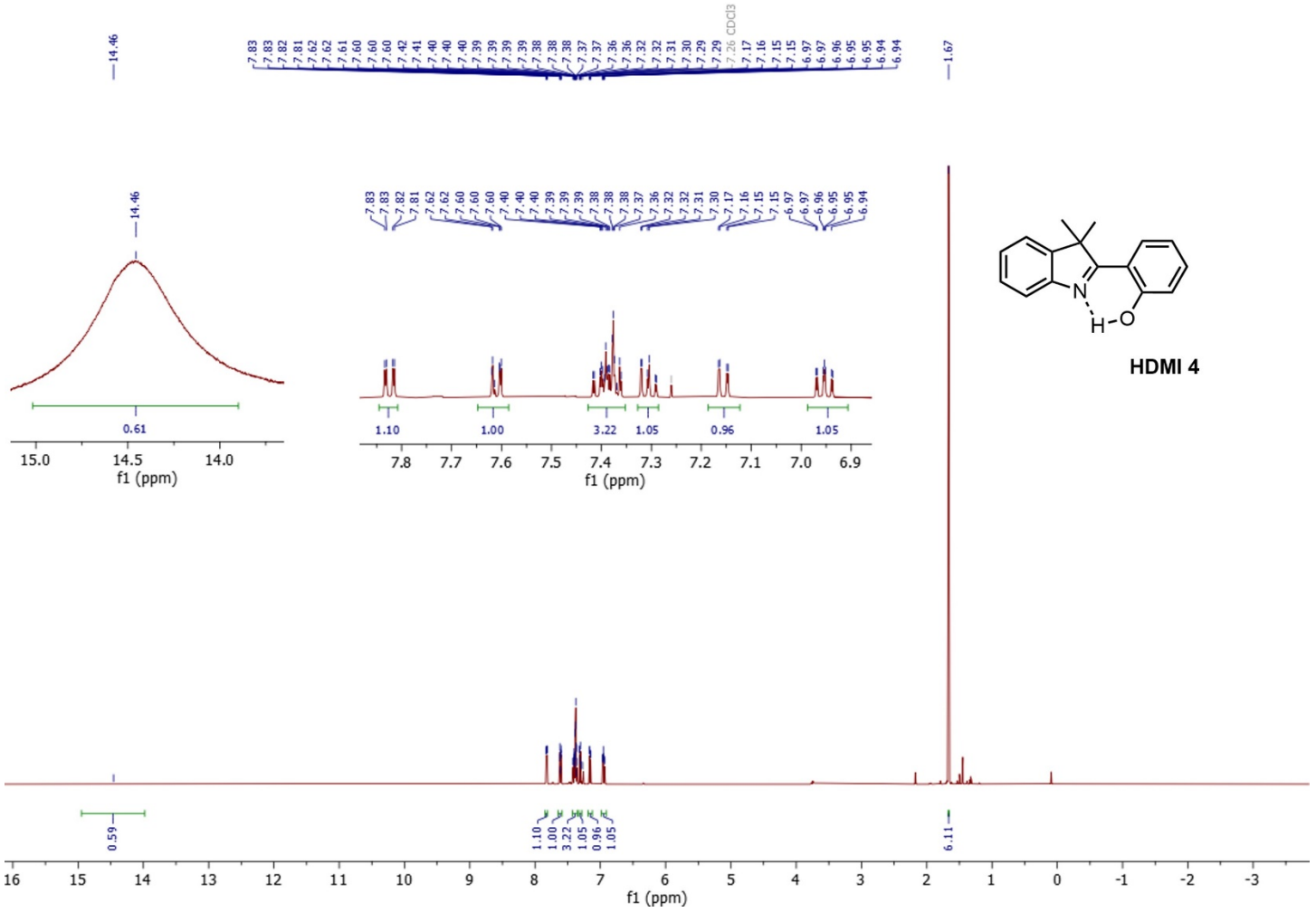


Figure S3. ^{1}H NMR spectrum of **HDMI 2**

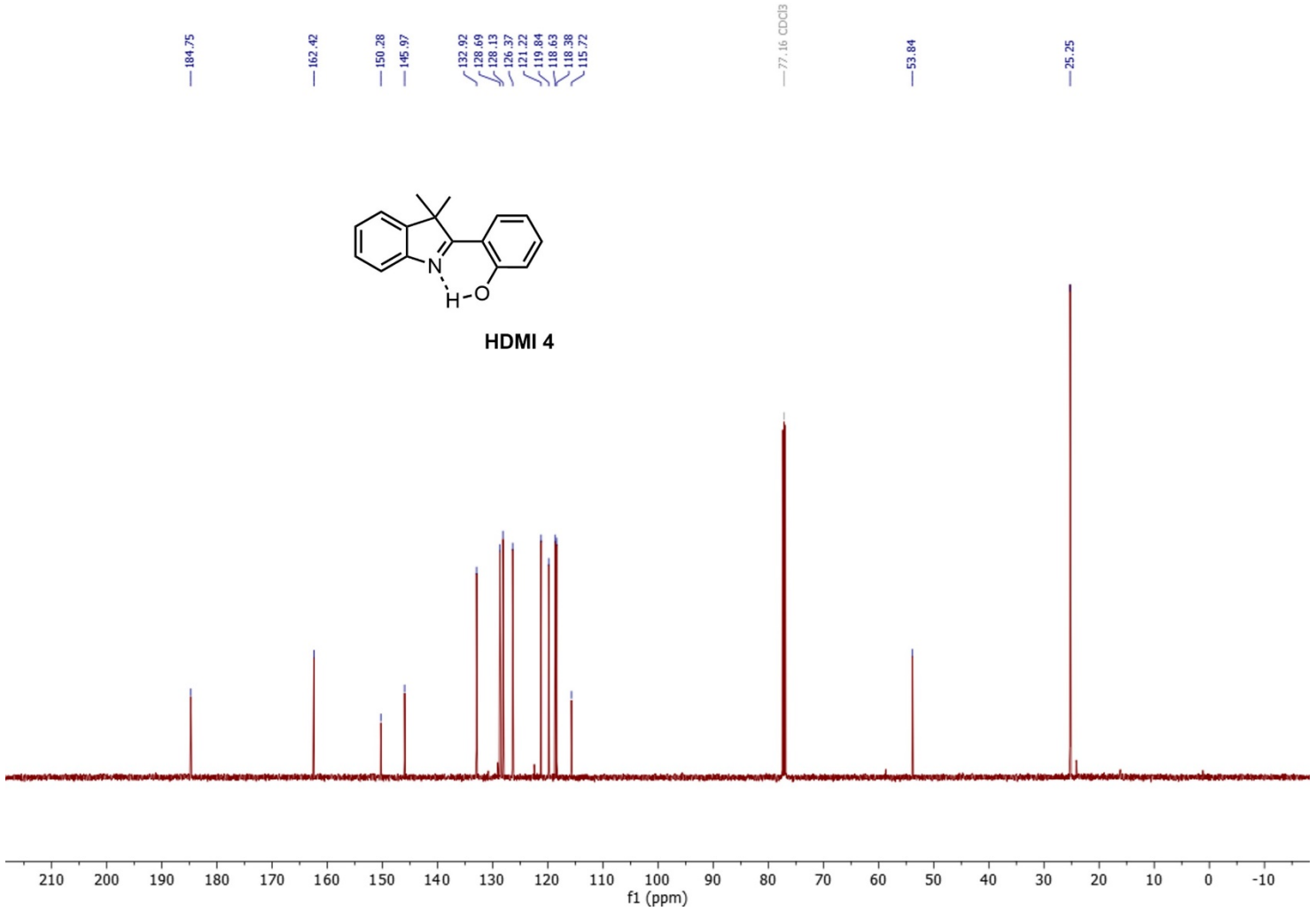


Figure S4. ^{13}C NMR spectrum of **HDMI 2**

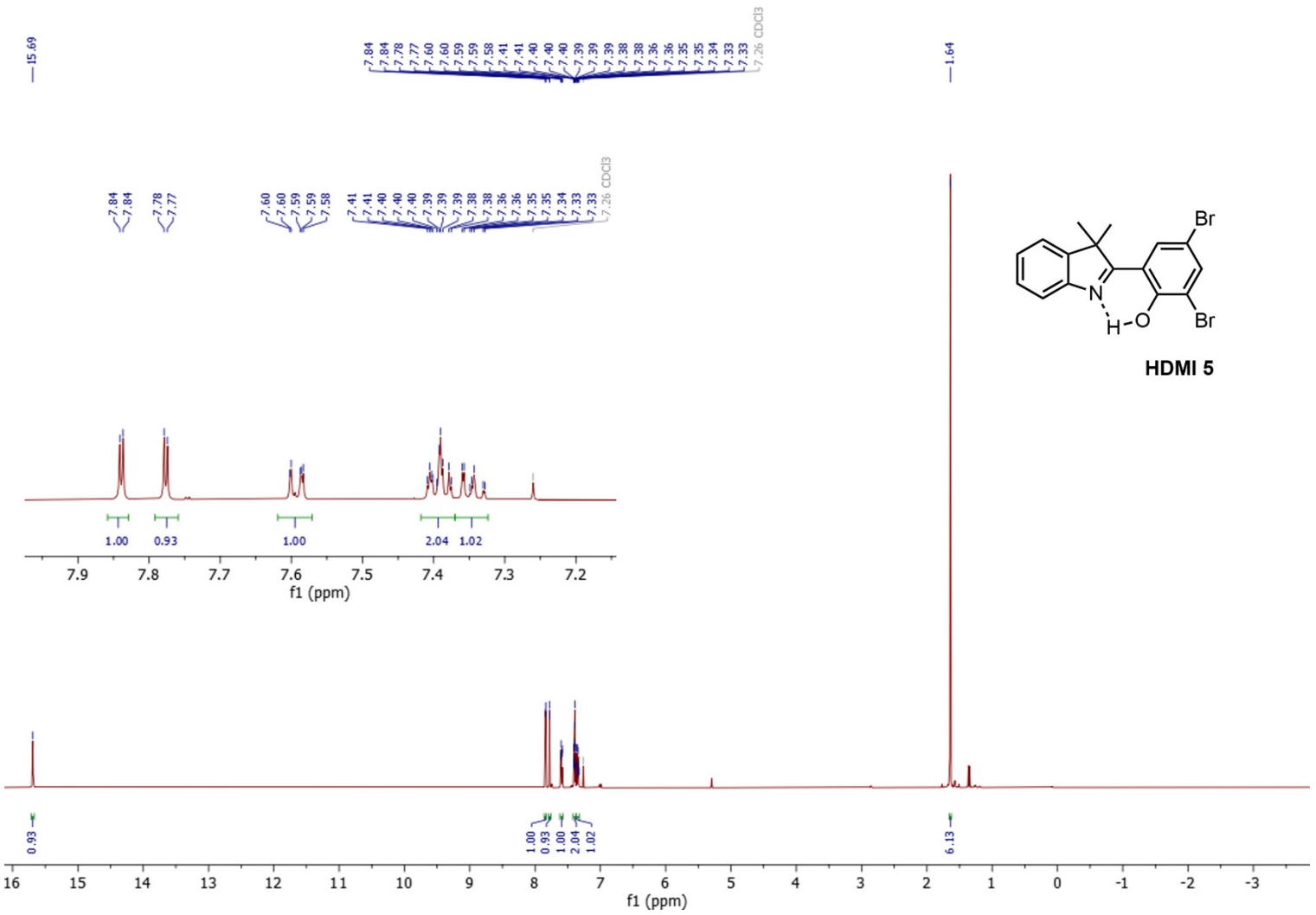


Figure S5. ^{1}H NMR spectrum of **HDMI 5**

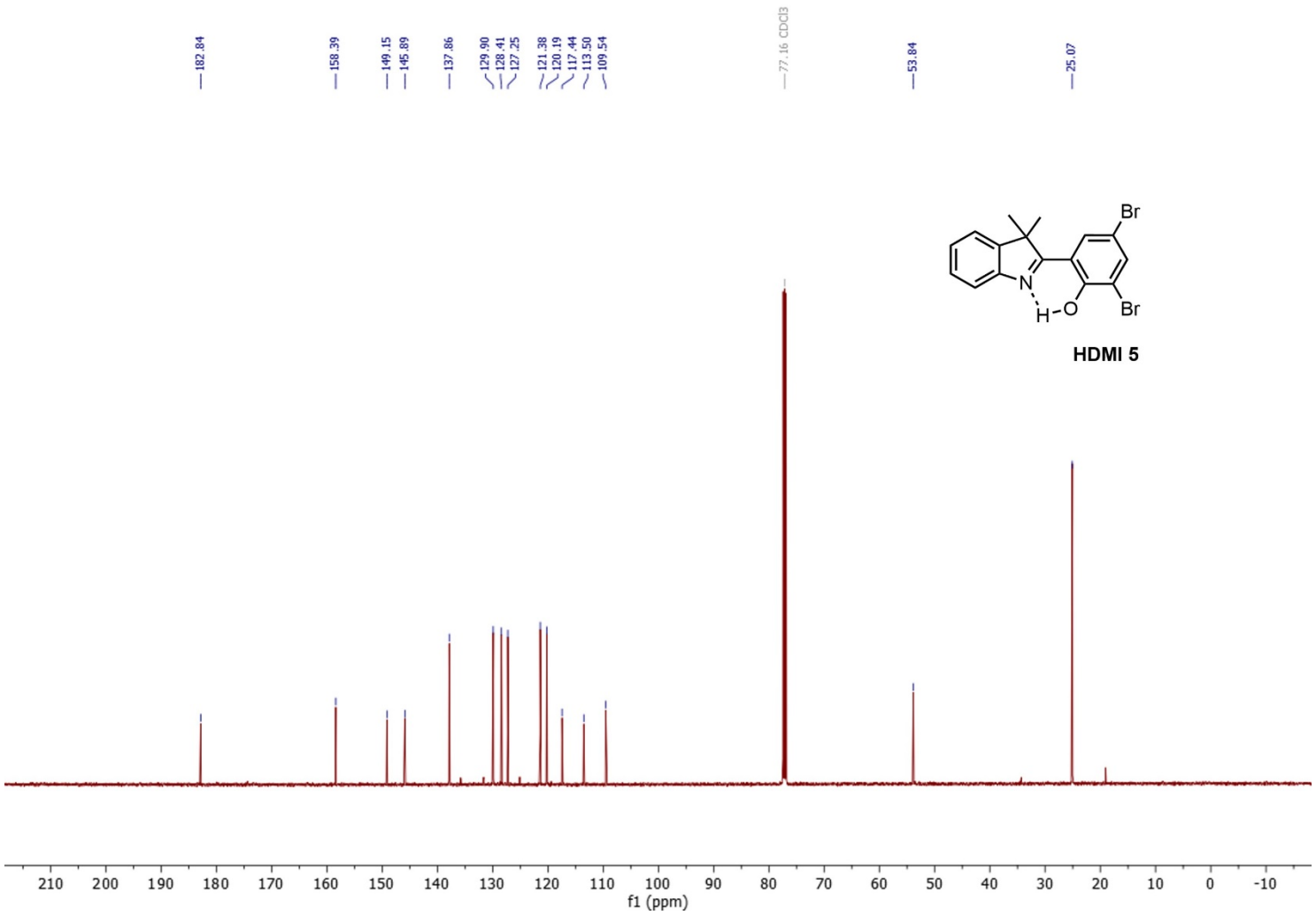


Figure S6. ^{13}C NMR spectrum of **HDMI 5**

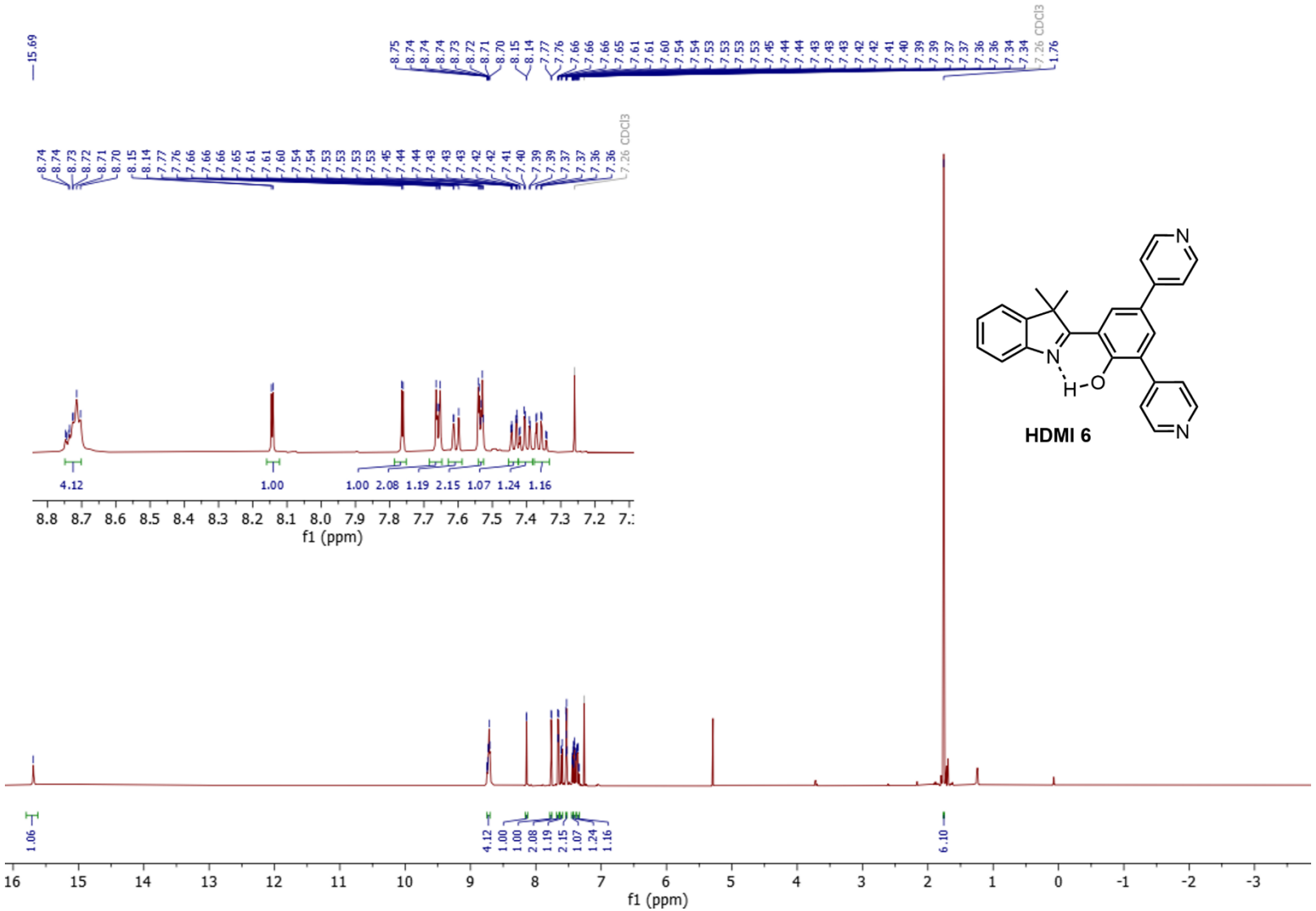


Figure S7. ^{1}H NMR spectrum of **HDMI 6**

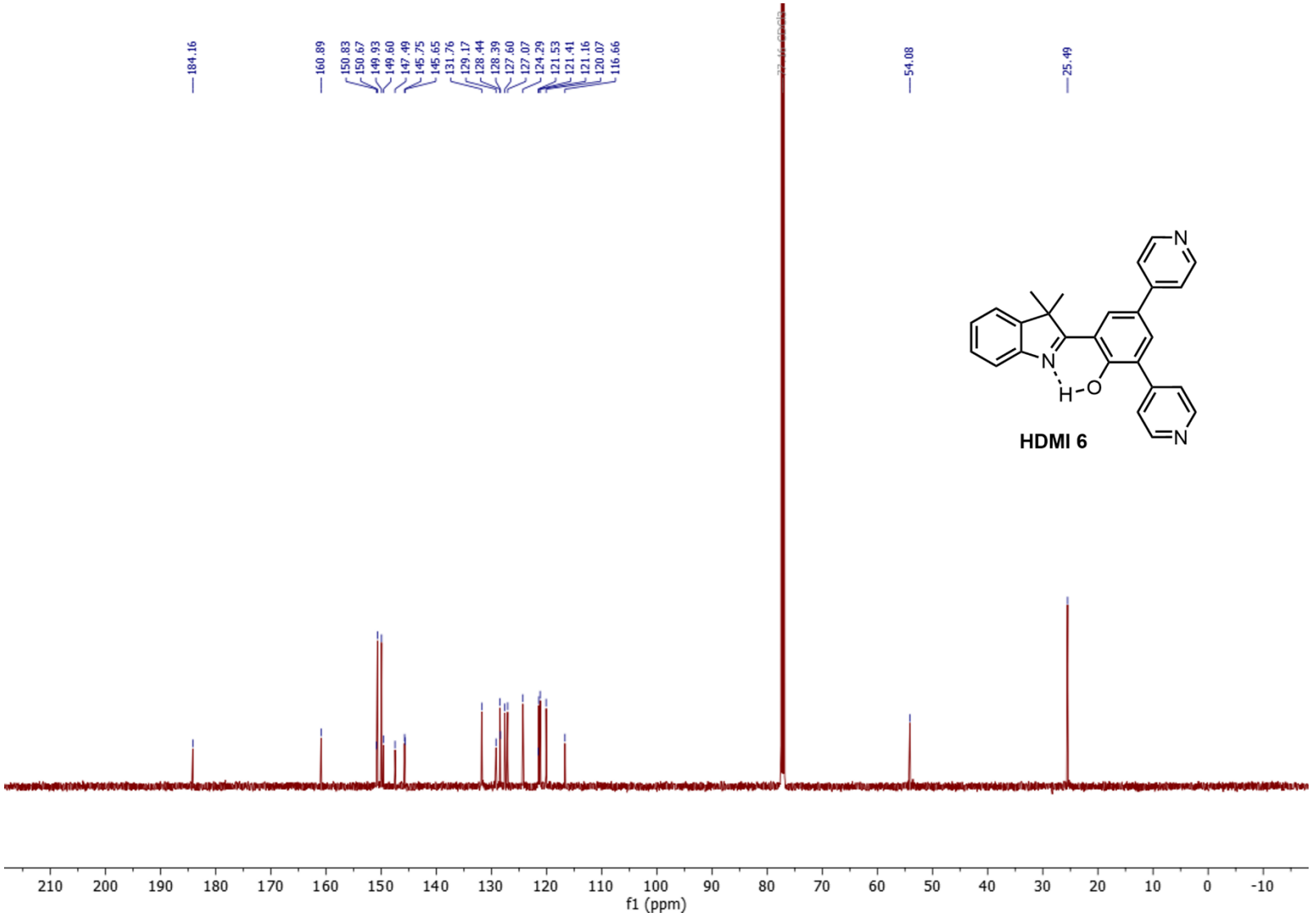


Figure S8. ^{13}C NMR spectrum of **HDMI 6**

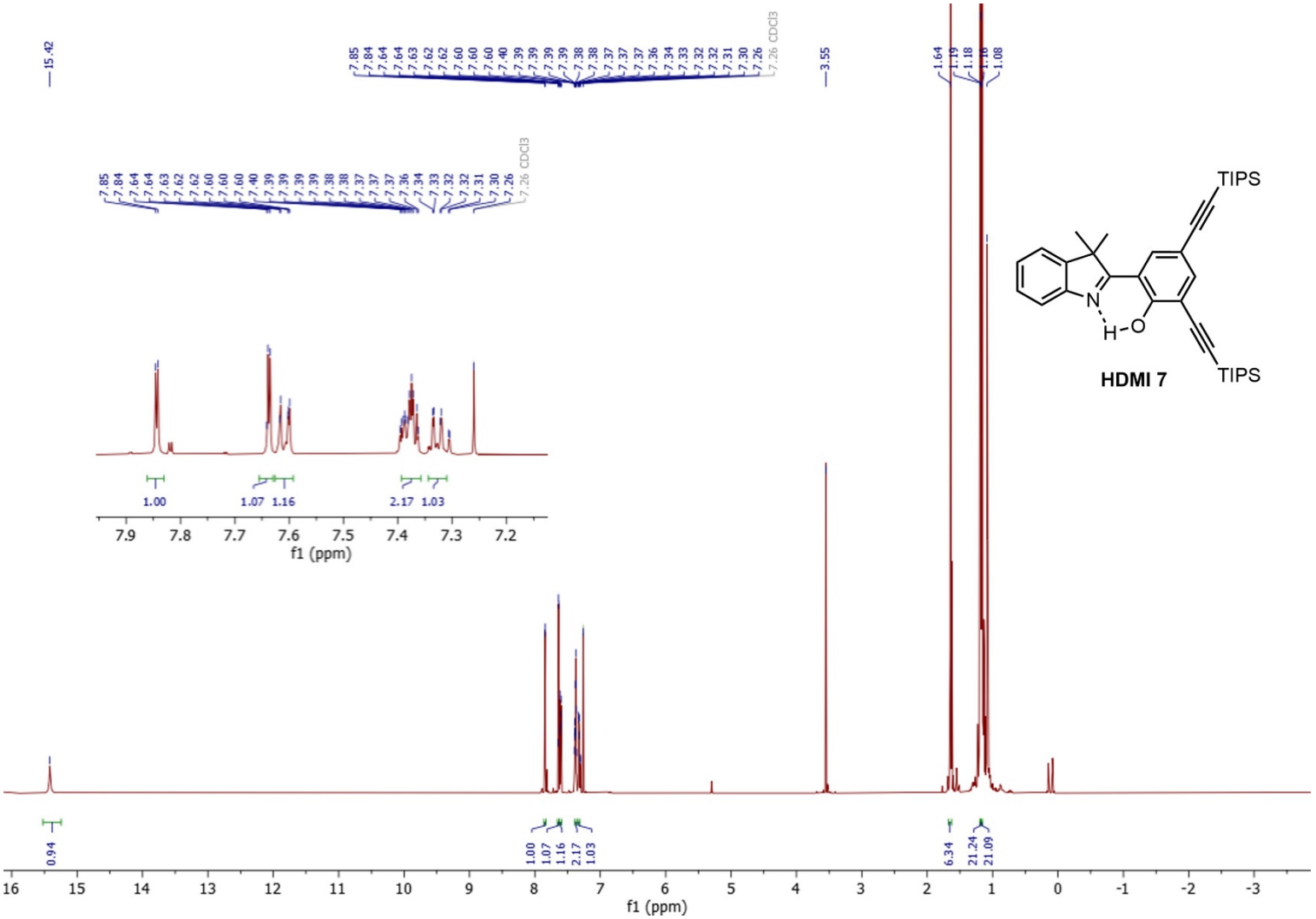


Figure S9. ^{1}H NMR spectrum of **HDMI 7**

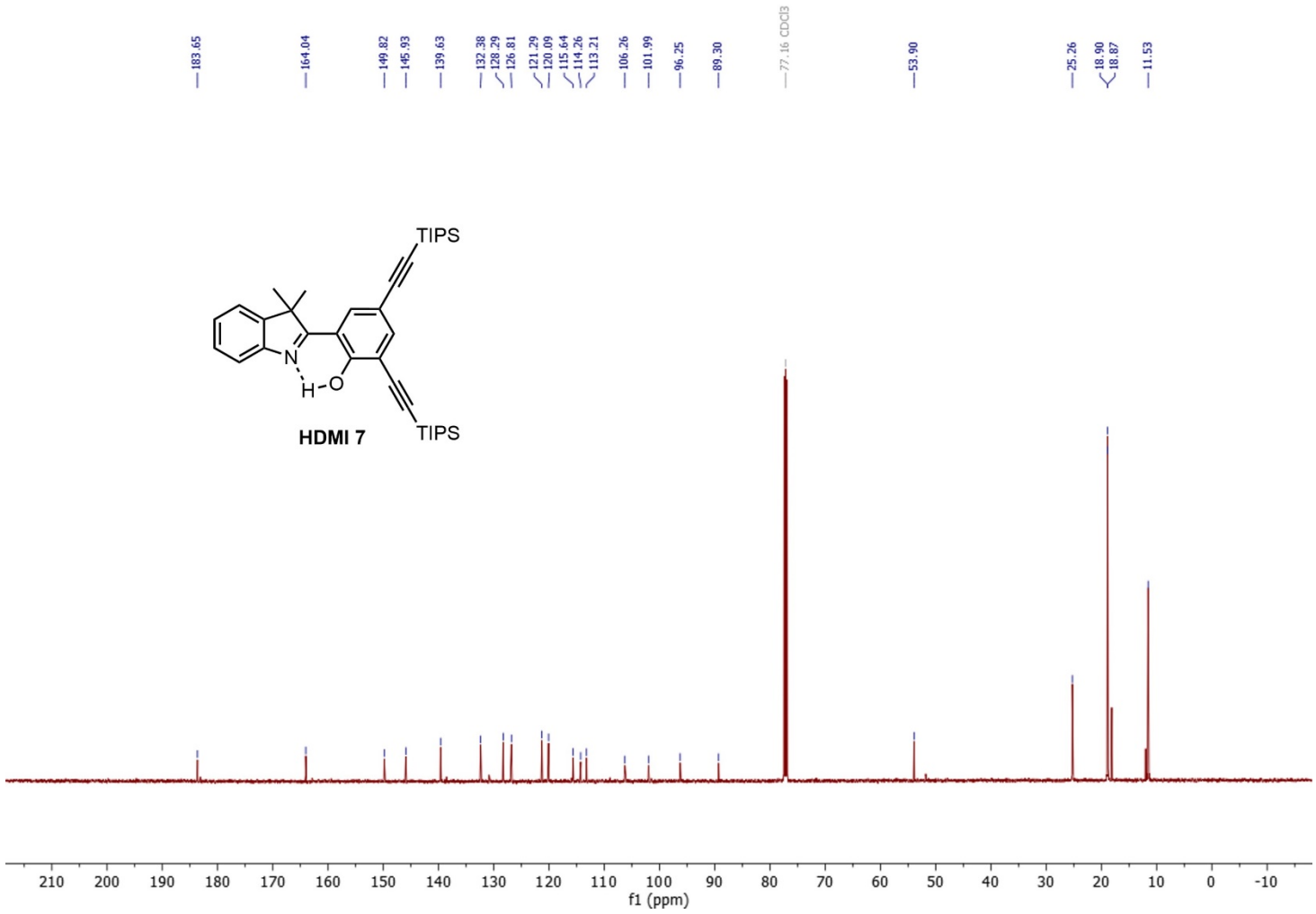


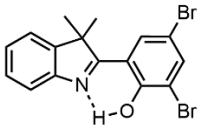
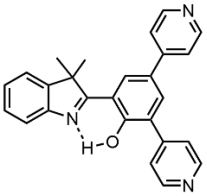
Figure S10. ^{13}C NMR spectrum of **HDMI 7**

S3. X-Ray diffraction data

Crystals suitable to Single Crystal X-ray Diffraction analyses were obtained for HDMI **5** and **6** by slow evaporation from dichloromethane/methanol solutions. Shortlisted samples cleaned and isolated in Paratone® oil were transferred upon an appropriate nylon loop for X-ray Mo(*Kα*) irradiation under a liquid nitrogen flow at 173K. The diffractometer used was a RIGAKU XtaLABPro equipped with a microfocus sealed tube generator coupled to a double-bounce confocal Max-Flux® multilayer optic and a HPAD PILATUS3R 200K detector *CrysAlisPro 1.171.42.90a* [1] was employed for the data strategy collection and data reduction applying an empirical absorption correction using spherical harmonics, implemented in the SCALE3 ABSPACK[1] scaling algorithm, combined with a numerical absorption correction based on Gaussian integration over a multifaceted crystal model. Both structures were readily solved by intrinsic phasing methods (*SHELXT* program),[2] then refined according to the canonical Independent-atom model (IAM) by full-matrix least-squares methods on F^2 using *SHELX-L.*[3] Thermal parameters for all non-hydrogen atoms were refined anisotropically and all the hydrogen atoms could be located in the difference Fourier maps. The final structure refinements for HDMI **5** and **6** were carried out by Hirshfeld Atom Refinement (HAR) with non-spherical atomic form factors using *NoSpherA2*[4] partitioning in *OLEX2*[5] based on electron density from iterative single-determinant SCF single-point DFT calculations using *ORCA* (version 5.0)[6] with a *R2SCAN* functional[7] and a *def2-TZVPP*[8] or cc-pVTZ basis set,[9] for **5** and **6** respectively. ISOR instruction was applied to restrain few hydrogen anisotropic displacement parameters in **5**. However, HAR refinement allowed the hydrogen atoms to be anisotropically refined in position, with also some similarity restraints on distances (concerning the aromatic H in **5**) comparable to those obtained by neutron diffraction. In addition, enhanced rigid-bond restraints (RIGU command) were also applied to the atoms of the two pyridine groups in **6**.

Crystal data, data collection and structure refinement details are summarized in Table S1. CCDC 2260125- 2260126 (for **5** and **6**, respectively) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement for HDMI dyes **5** and **6**.

Identification code		**HDMI 5**	**HDMI 6**
			
Empirical formula		$C_{16}H_{13}Br_2NO$	$C_{26}H_{21}N_3O$
Formula weight		395.09	391.48
Temperature	(K)	173.0 (2)	
Diffractometer	Rigaku®	XtaLABPro mm003 Pilatus 200 K	
Wavelength	(Å)	0.71073	
Crystal system, Space group		Monoclinic, P 2_1/m	Triclinic, P -1
Unit cell dimensions	(Å) (°)	8.6747(5) 6.9706(5) 12.3186(6) 90 107.234(6) 90	8.50238(18) 10.0282(2) 12.6916(3) 70.6975(19) 89.7069(17) 85.8279(17)
Volume	($Å^3$)	711.44(8)	1018.39
Z, Calculated density	 (Mg/m^3)	2, 1.844	2, 1.277
Absorption coefficient	(mm^{-1})	5.690	0.079
F(000)		388	412
Crystal size	(mm)	0.12 x 0.07 x 0.05	0.27 x 0.19 x 0.17
θ range for data collection	(°)	2.55 to 28.68	3.11 to 28.70
Limiting indices		$-12 \le h \le 13$, $-10 \le k \le 10$, $-18 \le l \le 18$	$-12 \le h \le 12$, $-15 \le k \le 13$, $-19 \le l \le 17$
Reflections collected / unique Rint		17279 / 1983 0.048	39300 / 5266 0.028
Completeness to θ_{max}=25.2°	(%)	99.9	99.8
Absorption correction		Semi-empirical from equivalents & Gaussian	
Max. and min. transmission		1.000 and 0.138	1.000 and 0.554
Refinement method		Full-matrix least-squares on F^2	
Data / restraints / parameters		1983 / 18 / 187	5266 / 72 / 461
Goodness-of-fit on F^2		1.035	1.071
Final R indices [I>2σ(I)]	R1, wR2	0.0199, 0.0326	0.0153, 0.0325
R indices (all data)	R1, wR2	0.0331, 0.0347	0.0200, 0.0336
Extinction coefficient		-	0.008(7)
Largest diff. peak and hole	e.$Å^{-3}$	0.411 and -0.587	0.111 and -0.125
CCDC deposit number		2260125	2260126

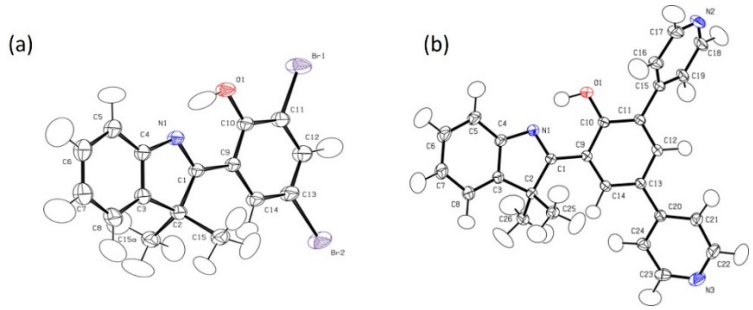


Figure S11. ORTEP drawings of (a) HDMI **5** and (b) HDMI **6**. Intramolecular hydrogen bond characteristics, for **5**: d(O_1–H_1) = 1.01(3)Å; d(O_1… N_1) = 2.563(2)Å; d (H_1… N_1) = 1.63(3) Å; ∠O_1-H_1…N_1=152(3)° and for **6**: d(O_1–H_1) = 1.009(7)Å; d (O_1… N_1) = 2.5363(3) Å; d (H_1… N_1) = 1.621(6) Å; ∠O_1-H_1…N_1=148.4(6)°.

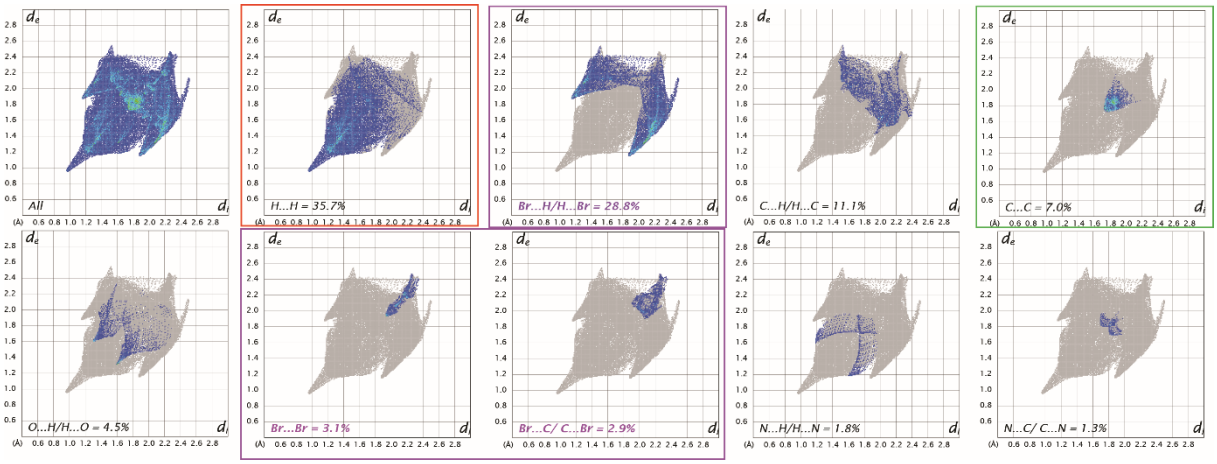


Figure S12. Full two-dimensional fingerprint plot for **5**, and those delineated into H···H, Br···H/H···Br, C···H/H···C, C···C, Br···Br, Br···C/C···Br, N···H/H···N, and N···C/C···N contacts.

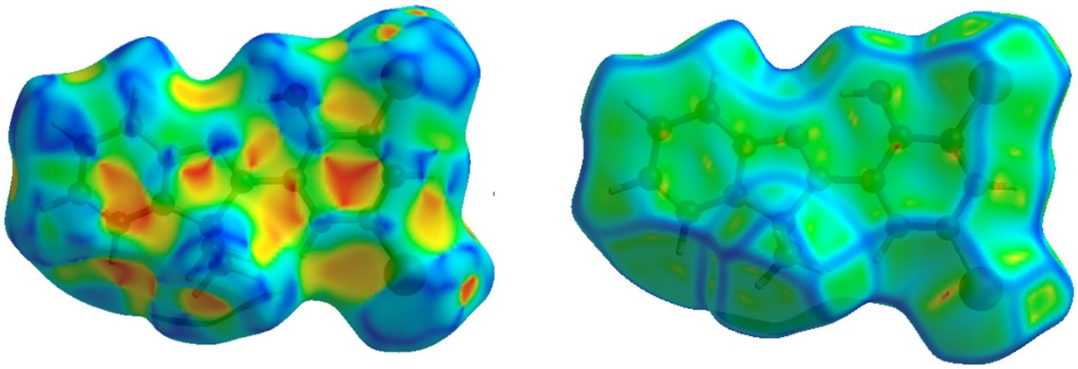


Figure S13. Two views of the Hirshfeld surface for **5** mapped over the shape-index property (left). The π-π stacking between the rings is indicated by the appearance of blue regions surrounding bright-red spots within the indol and phenol rings-, and over curvedness (right) - evident as the flat region outlined in blue that encompasses the indol-phenol platform.

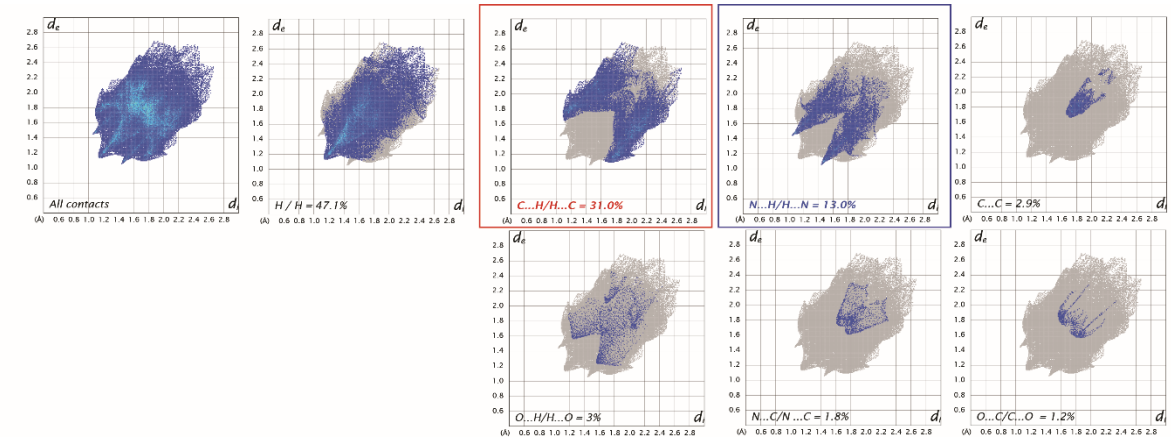


Figure S14. Full two-dimensional fingerprint plot for **6**, and those delineated into H···H, C···H/H···C, N···H/H···N, C···C, O···H/H···O, N···C/C···N, and O···C/C···O contacts.

S4. Photophysical data

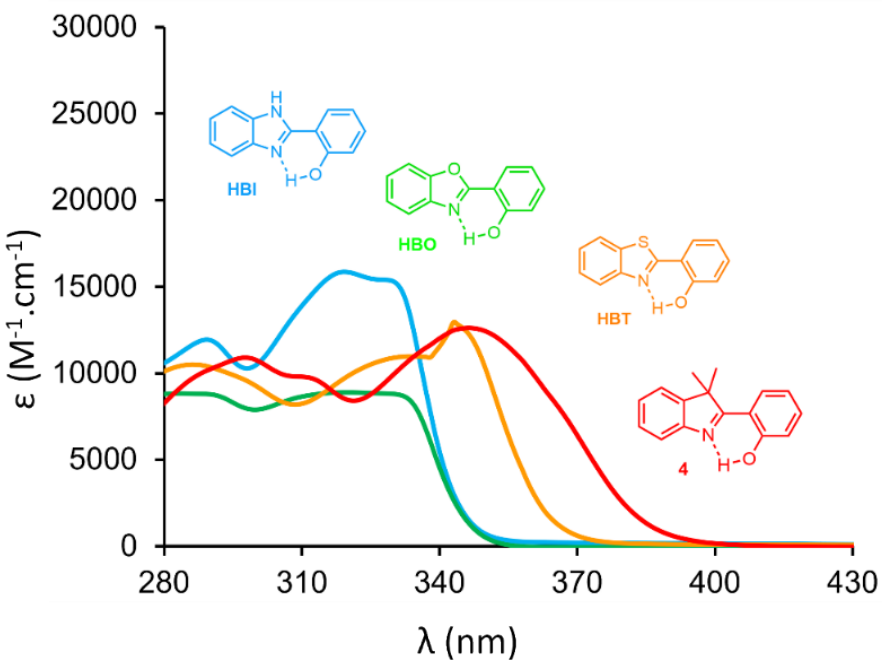


Figure S15. Absorption spectra of HBX dyes and HDMI **4** in dichloromethane.

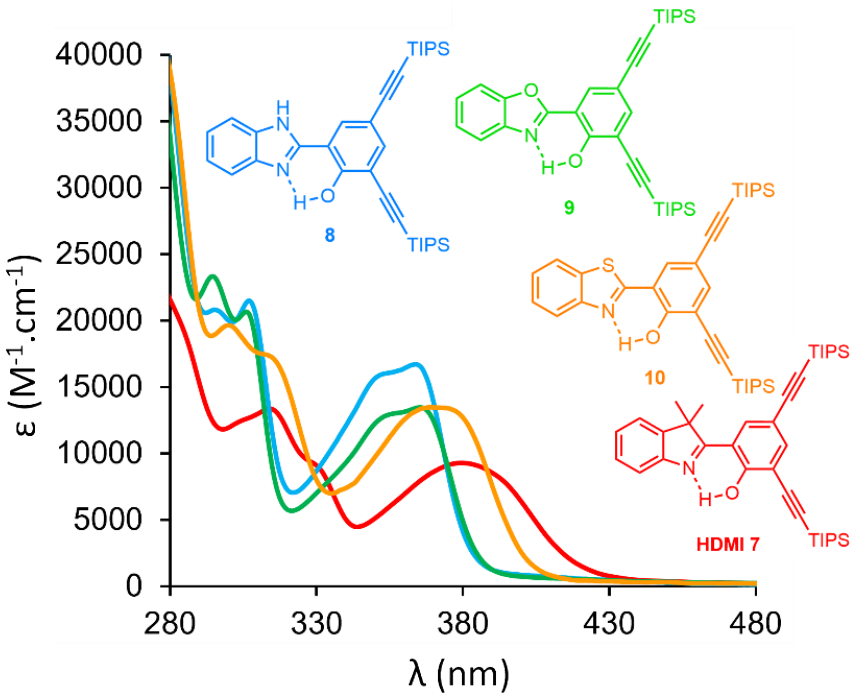


Figure S16. Absorption spectra of HBX dyes **7-10** in dichloromethane.

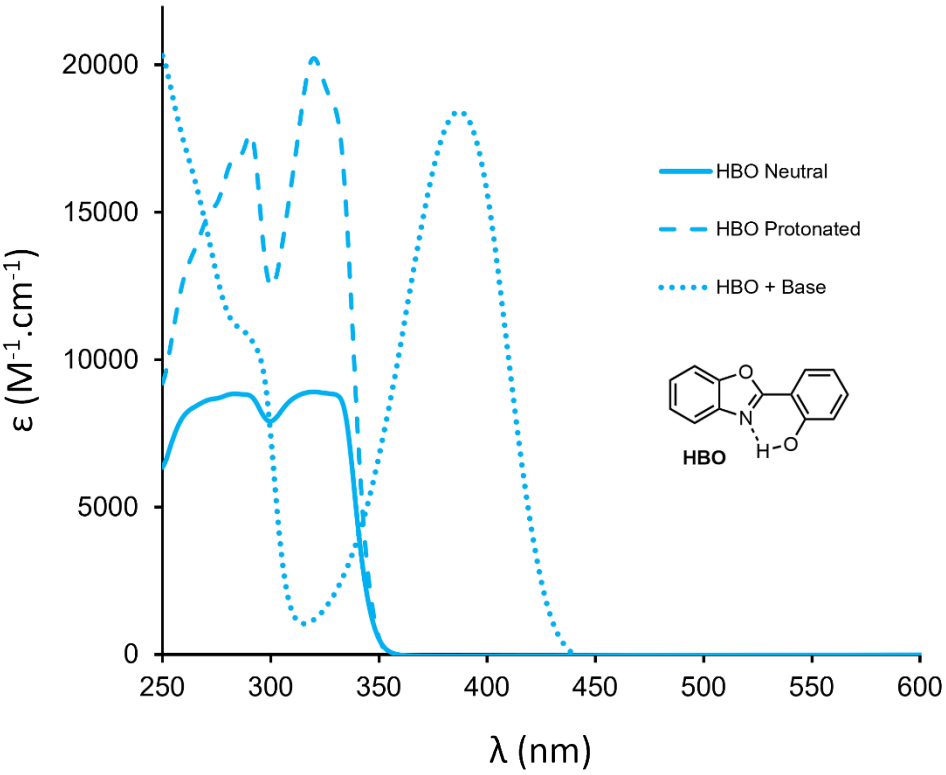


Figure S17. Absorption spectra of **HBO** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

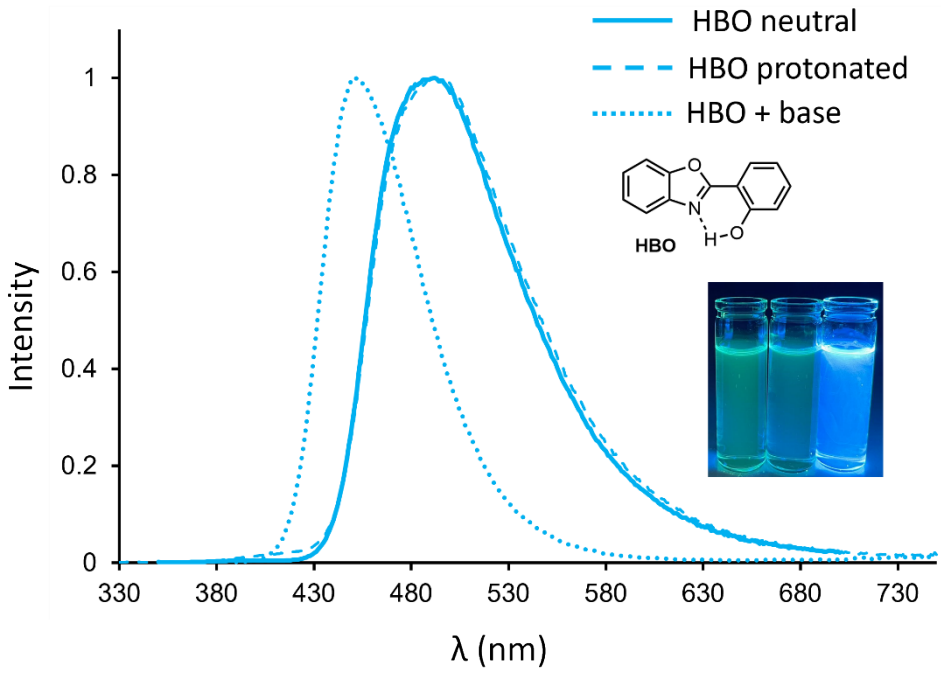


Figure S18. Emission spectra of **HBO** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

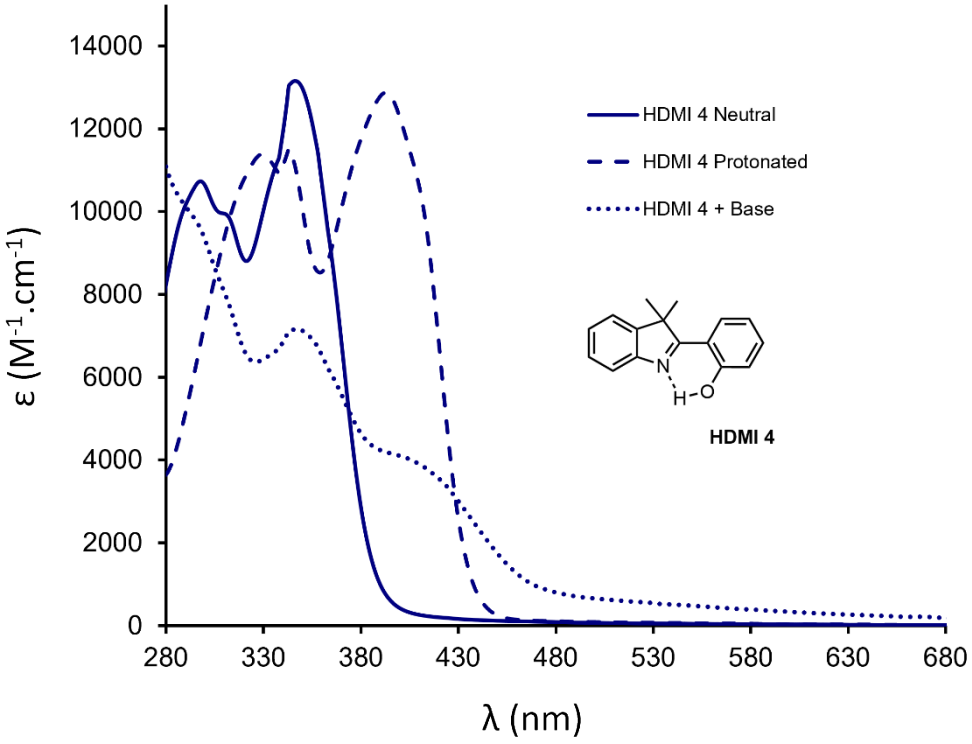


Figure S19. Absorption spectra of HDMI **4** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

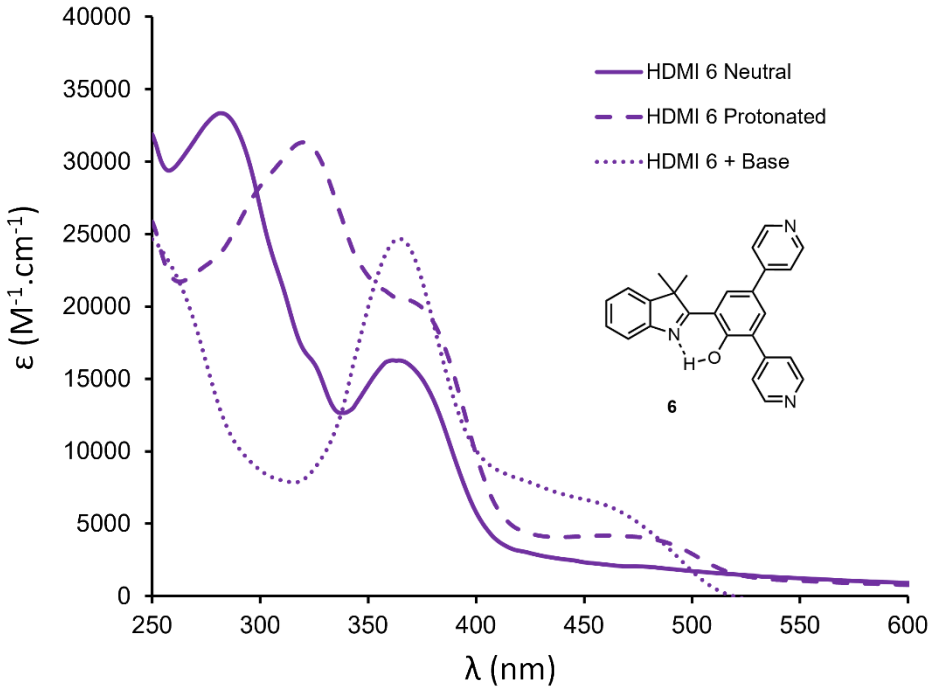


Figure S20. Absorption spectra of HDMI **6** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

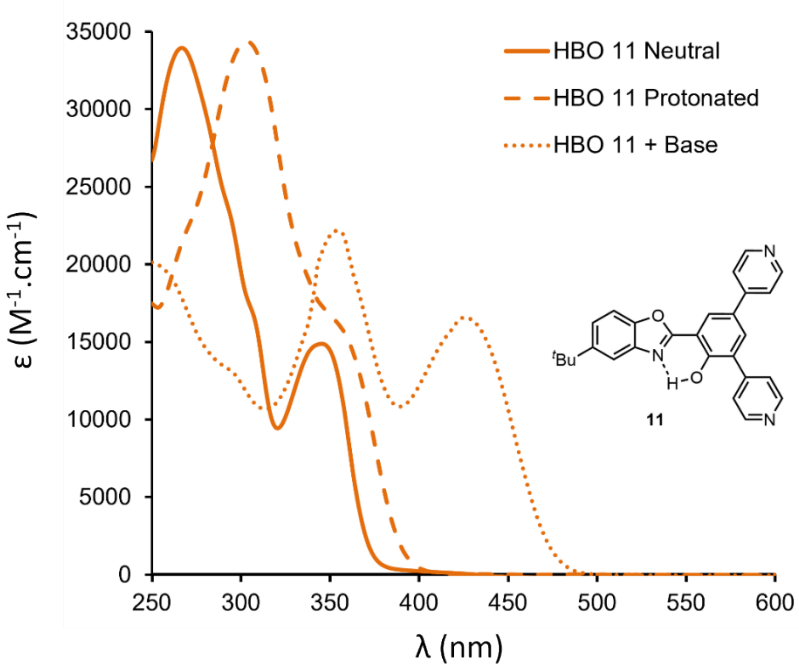


Figure S21. Absorption spectra of HBO **11** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

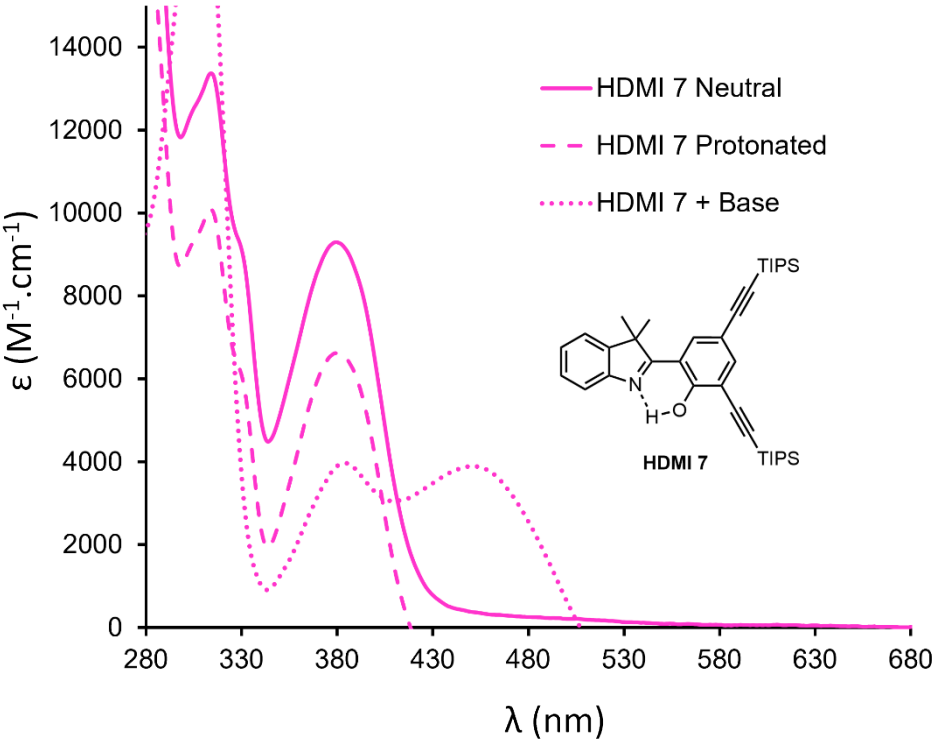


Figure S22. Absorption spectra of HDMI **7** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

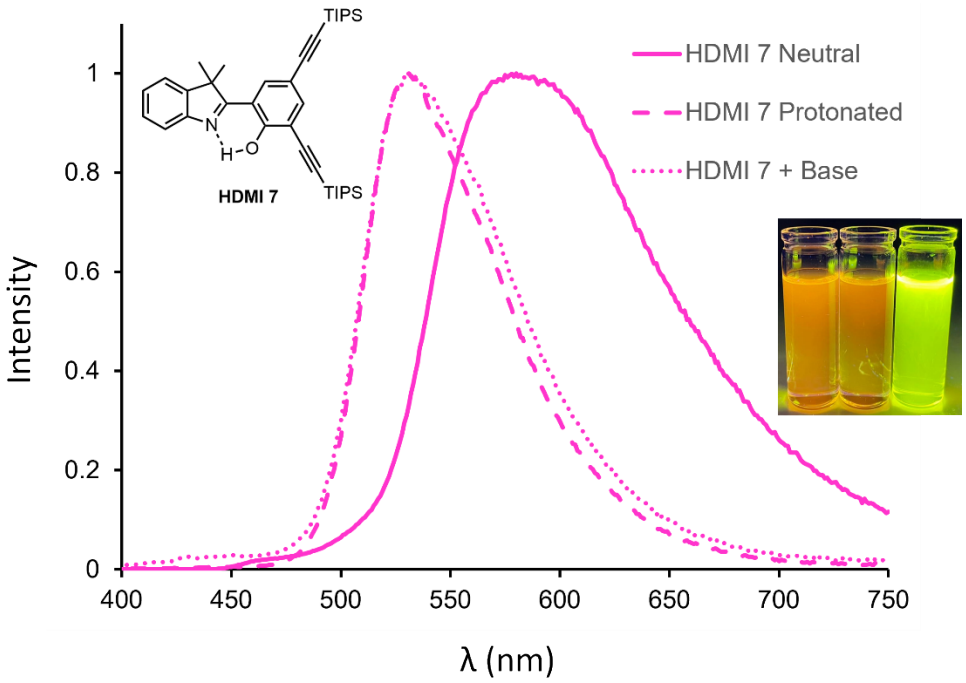


Figure S23. Emission spectra of HDMI **7** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

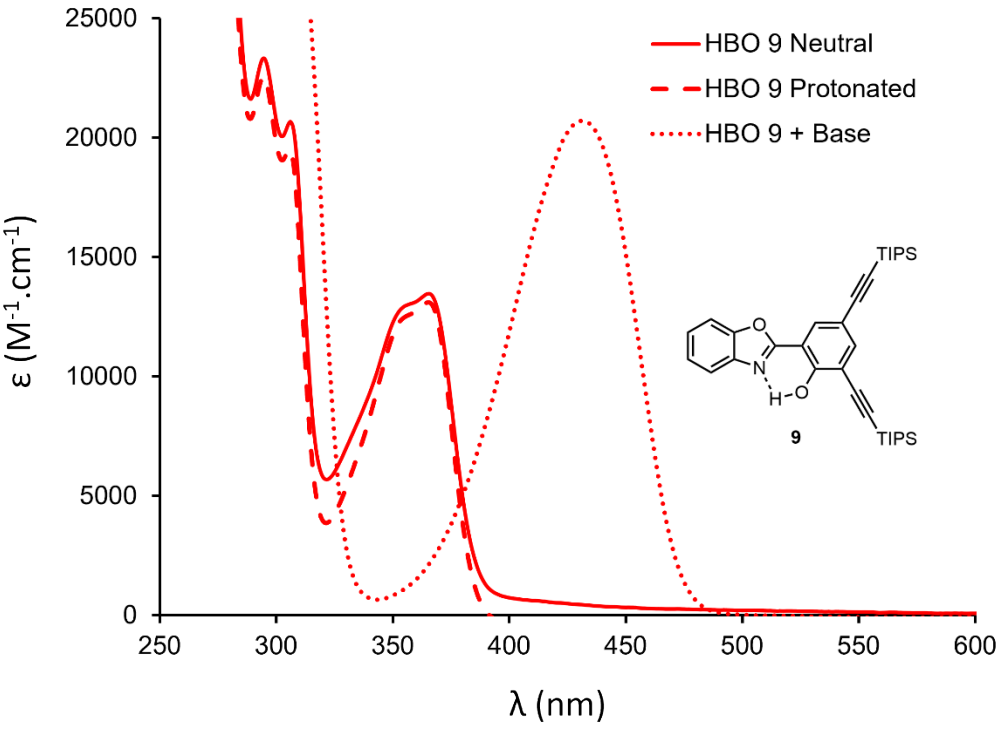


Figure S24. Absorption spectra of HBO **9** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

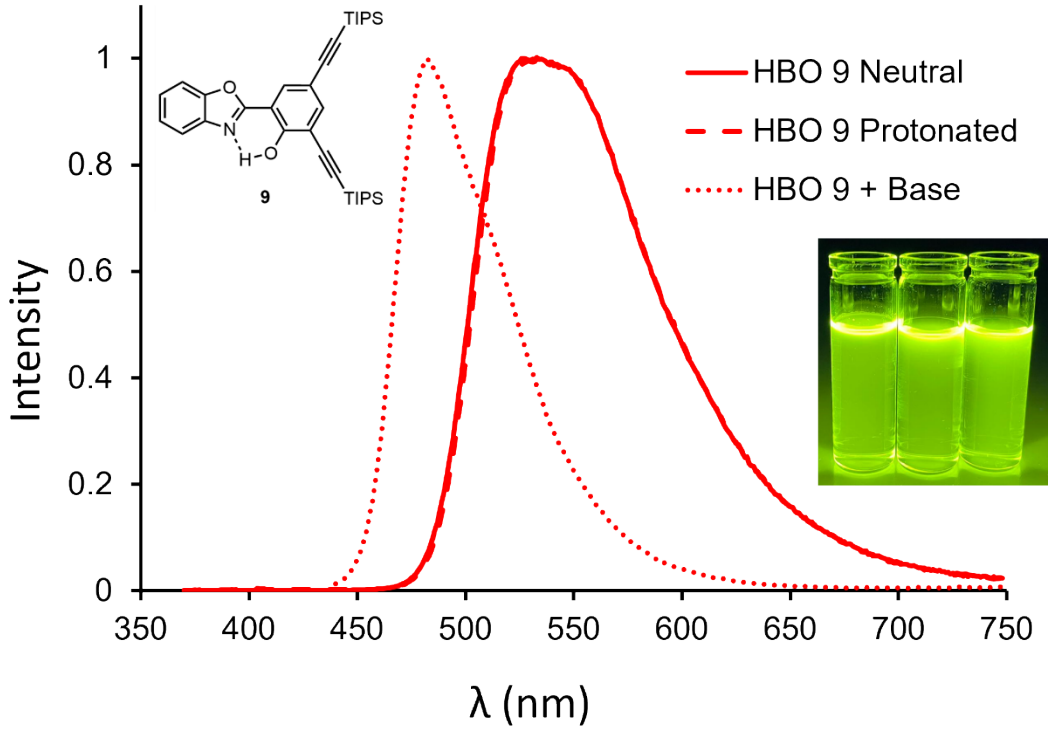


Figure S25. Emission spectra of HBO **9** in dichloromethane (neutral, plain; protonated with HCl_g, dashed and deprotonated with Bu_4NOH, dotted).

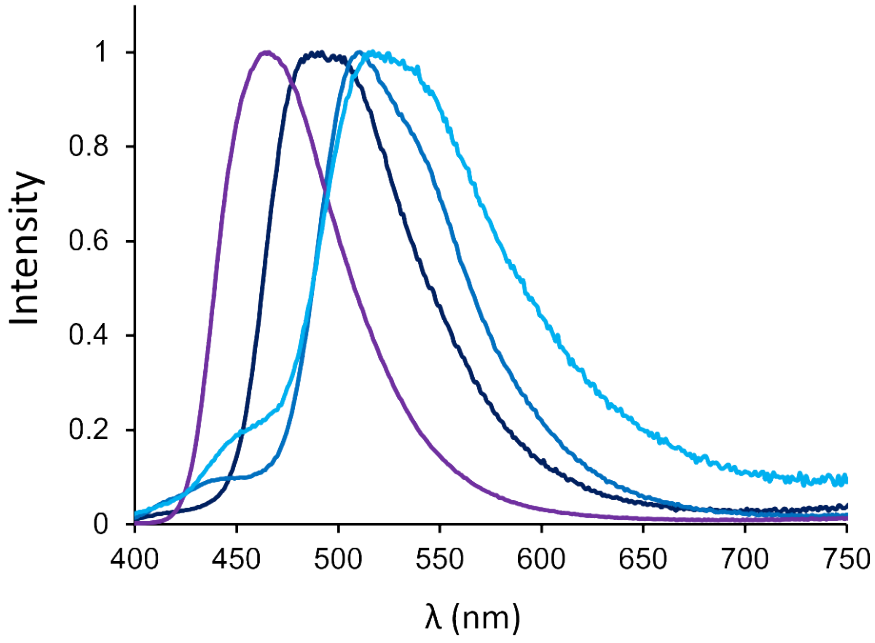


Figure S26. Emission spectra of HBX dyes (HBI = purple, HBO = navy blue, HBT = blue) and HDMI **4** (light blue) in the solid-state.

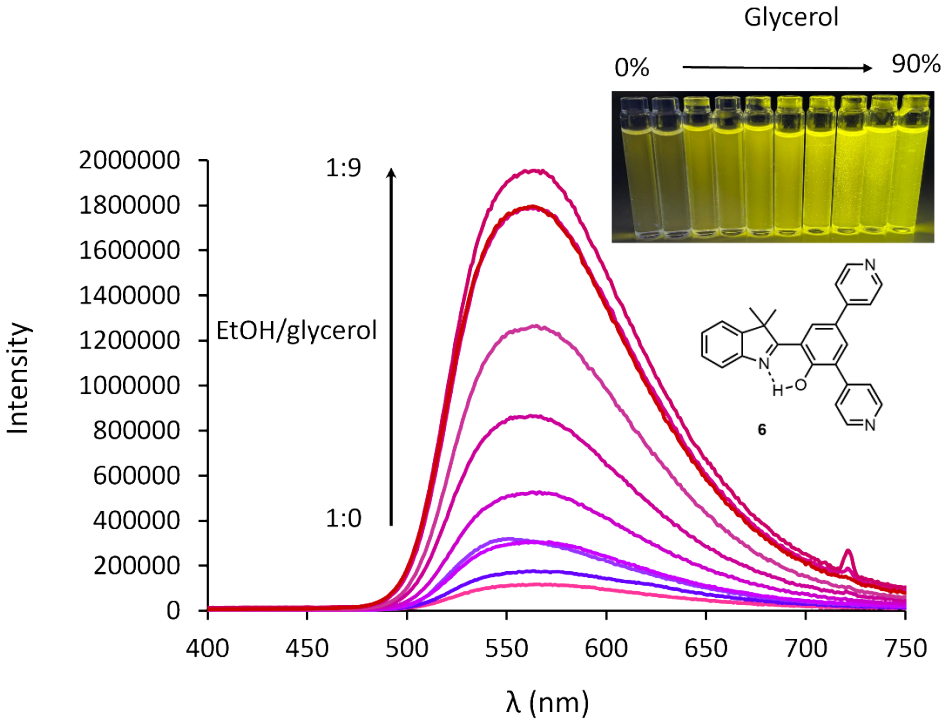


Figure S27. Emission spectra of HDMI **6** in ethanol/glycerol mixtures from EtOH (100%) to EtOH/glycerol (90/10). (Inset) Photographs of solutions of **6** in ethanol/glycerol mixtures under irradiation from a UV bench lamp (λ_{exc} = 365 nm).

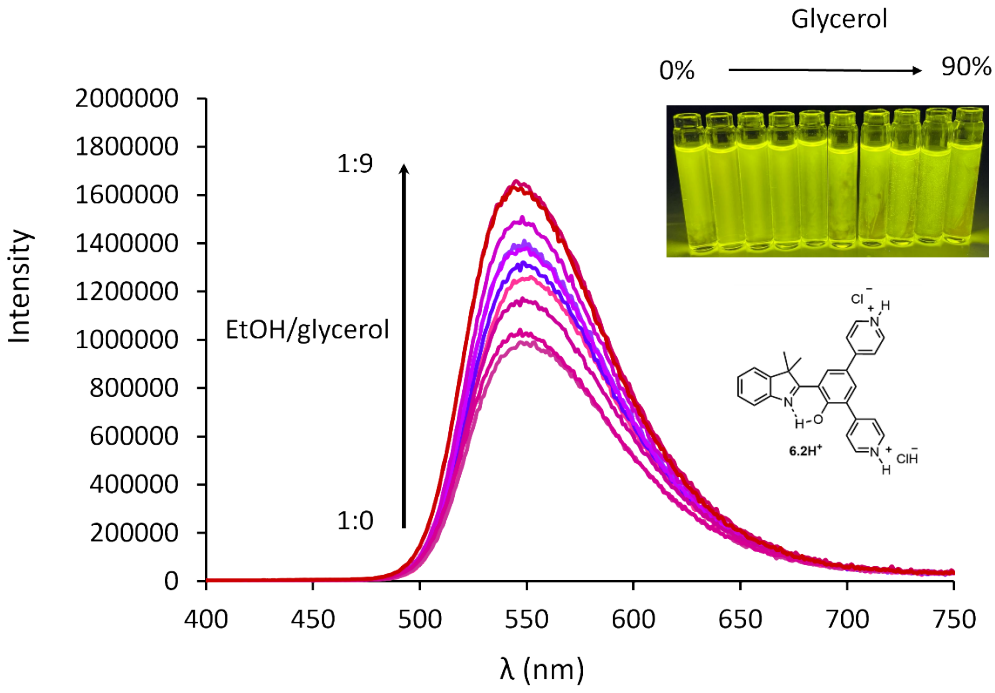


Figure S28. Emission spectra of HDMI **6.2H**$^+$ in ethanol/glycerol mixtures from EtOH (100%) to EtOH/glycerol (90/10). (Inset) Photographs of solutions of **6.2H**$^+$ in ethanol/glycerol mixtures under irradiation from a UV bench lamp (λ_{exc} = 365 nm).

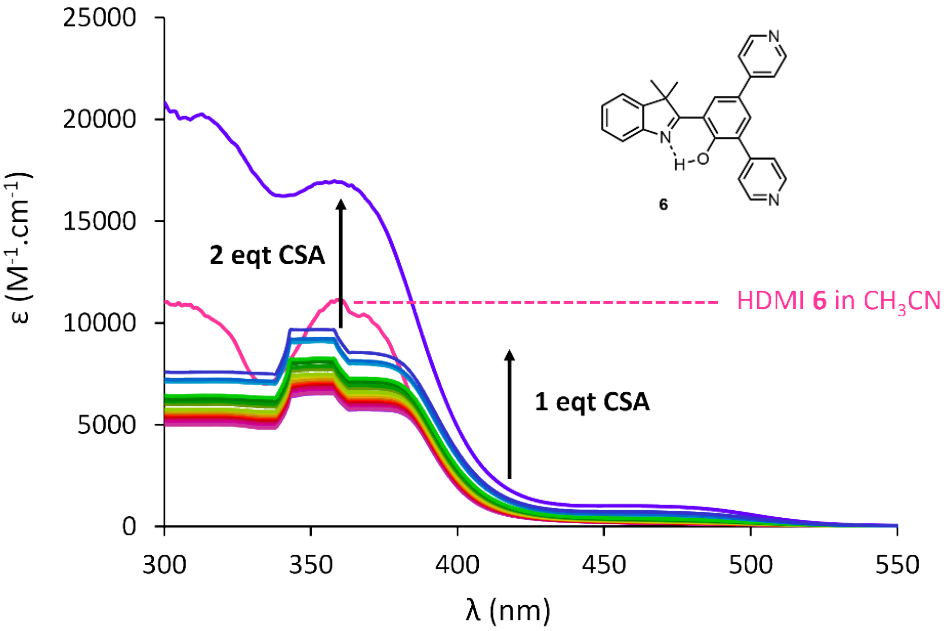


Figure S29. UV-Vis titration of HDMI **6** with 0 to 2 equivalents of Camphorsulfonic acid (CSA) in CH_3CN.

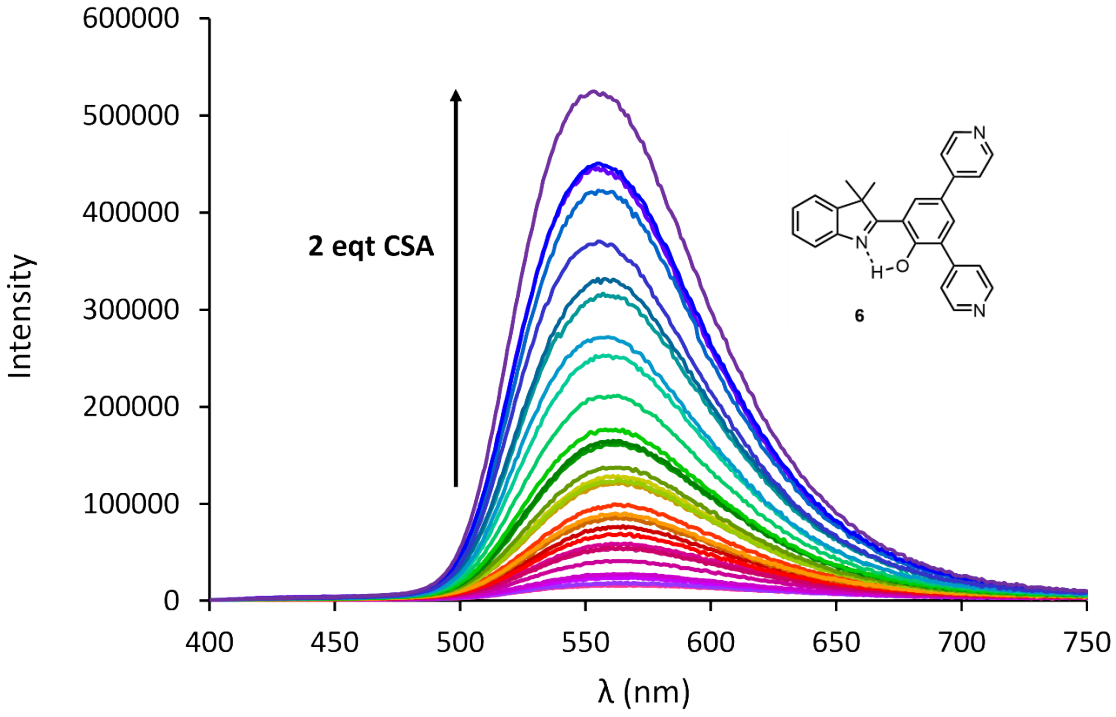


Figure S30. Fluorescence titration of HDMI **6** with 0 to 2 equivalents of with Camphorsulfonic acid (CSA) in CH_3CN (λ_{exc} = 360 nm).

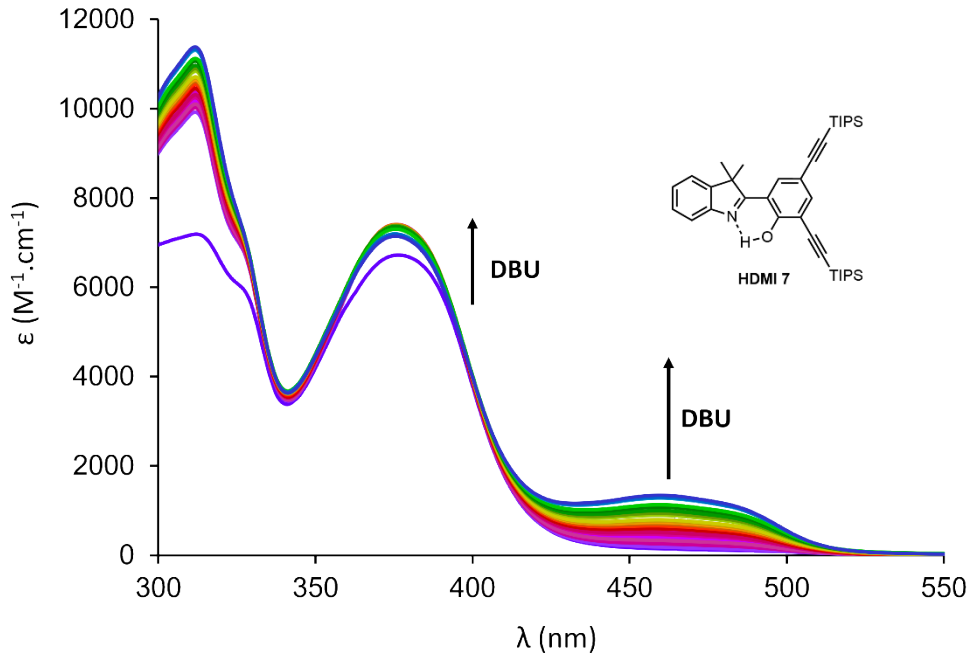


Figure S31. UV-Vis titration of HDMI **7** with 1,8-Diazabicyclo(5.4.0)undec-7-ene (DBU) in CH_3CN.

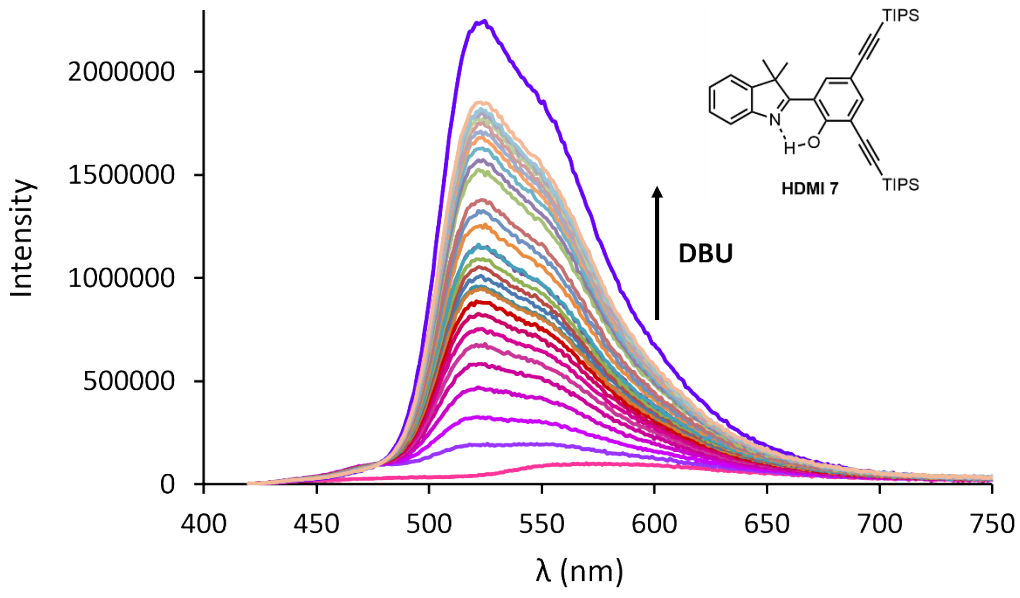


Figure S32. Fluorescence titration of HDMI **7** with 1,8-Diazabicyclo(5.4.0)undec-7-ene (DBU) in CH_3CN (λ_{exc} = 400 nm).

S5. Theoretical methods and data

Methods

To model ESIPT, we have relied on both Time-Dependent Density Functional Theory (TD-DFT) and a wavefunction coupled-cluster-based approach. We have used exact dye structures but for the replacement of the TIPS by TMS moieties for obvious computational reasons. We have optimized and computed the vibrational frequencies of the enol tautomer in its ground electronic state, and both enol and keto tautomers in their first excited state with TD-DFT. Depending on the considered structures, protonated or deprotonated structures were also computed. The comparison between E^* and K^* allowed computing the relative energies of the two species, and hence to determine if a driving force and a small barrier allow for ESIPT to take place (see below). The optimization and vibrational calculations were performed with the M06-2X functional[9] and the 6-31G(d) atomic basis set, including solvent effects (DCM as in the experiment) using the Polarizable Continuum Model (PCM), using the standard linear-response (LR) version of PCM for the TD-DFT part.[10] Next the vertical absorption and emission wavelengths have been respectively computed on both the optimal ground and excited state geometries. These calculations were done both in gas phase and in solution at the TD-M06-2X/6-311+G(2d,p) level, using the cLR^2 model[11,12] for the solution calculation, so as to simulatenously accounts for *linear-response* and *state-specific* solvent effects. All DFT and TD-DFT calculations were performed with Gaussian 16, using default algorithms but improved convergence thresholds for both ground state energies and residual forces.[13]

Secondly, we computed the vertical transition energies in gas-phase at the second-order coupled-cluster level, CC2,[14] with the *aug*-cc-pVDZ atomic basis set. These latter calculations were performed with the Turbomole package,[15] applying the RI approximation and freezing the core electrons. It was then possible to obtain theoretical best estimates of the vertical fluorescence energies using a combinatory approach

$$\Delta E^{\text{fluo}} = \Delta E^{\text{CC2}}_{\text{Gas}} + \left(\Delta E^{\text{TD-DFT}}_{\text{cLR}^2\text{-PCM}} - \Delta E^{\text{TD-DFT}}_{\text{Gas}}\right) \qquad \text{(S1)}$$

Therefore, the reported vertical transition wavelengths in the main text are CC2 values computed on TD-DFT geometries and corrected for solvation thanks to cLR^2-TD-M06-2X calculations. Such combination allows to obtain accurate estimates at a reasonable computational cost.

For the molecules for which both E^* and K^* minima could be identified, we have also determined the ESIPT transition state, performing a true TS^* search (not a scan) thanks to analytical TD-DFT Hessian implemented in Gaussian. It was checked that the final TS^* had a single imaginary frequency corresponding to the ESIPT.

Electron density difference (EDD) Plots

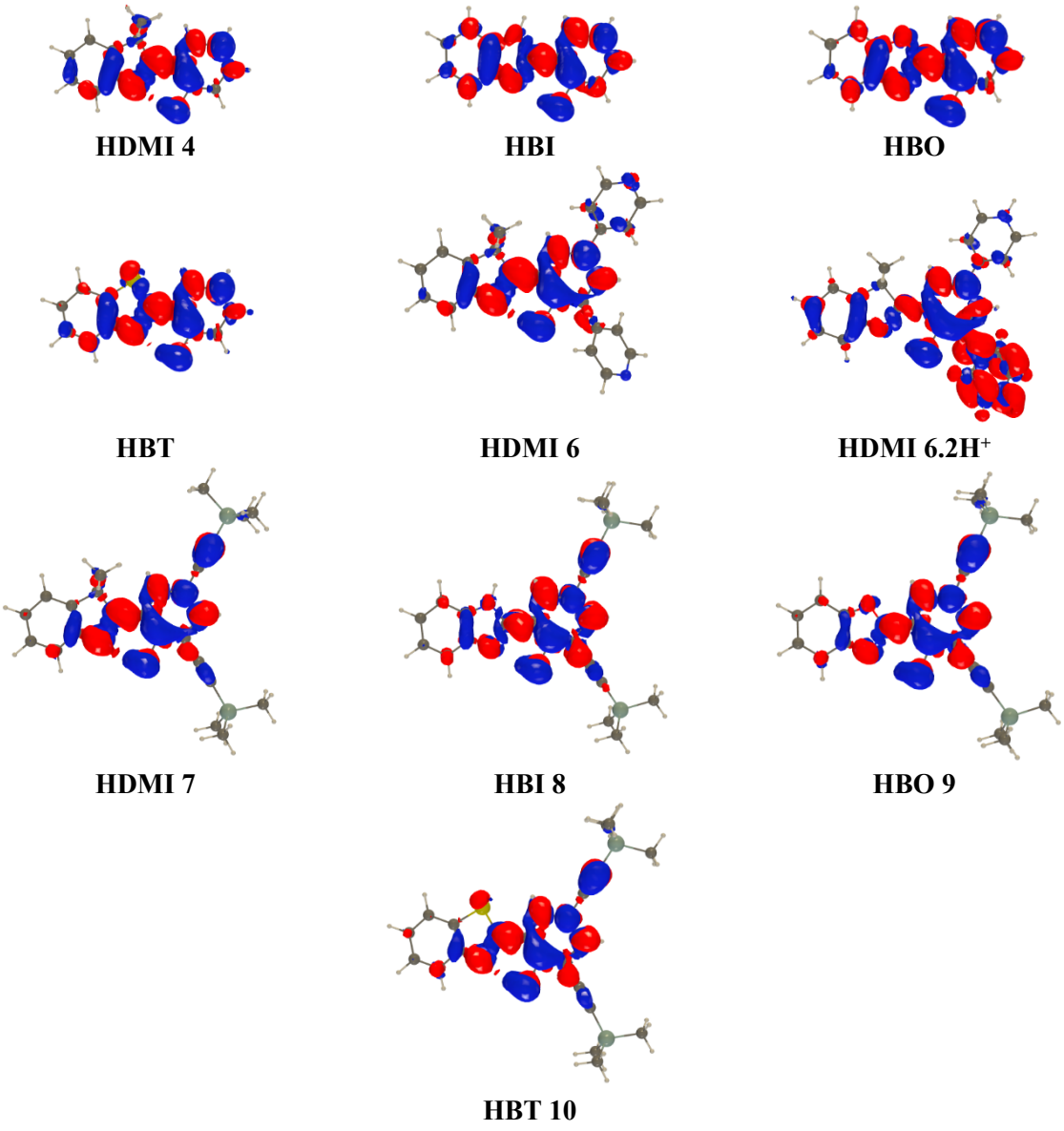


Figure S33. Electron density difference (EDD) plots showing changes of density upon absorption from the ground-state. Blue and red lobes correspond to regions of decrease and increase of electron density upon absorption. Contour threshold: 0.001 au.

PES scans around the central ring

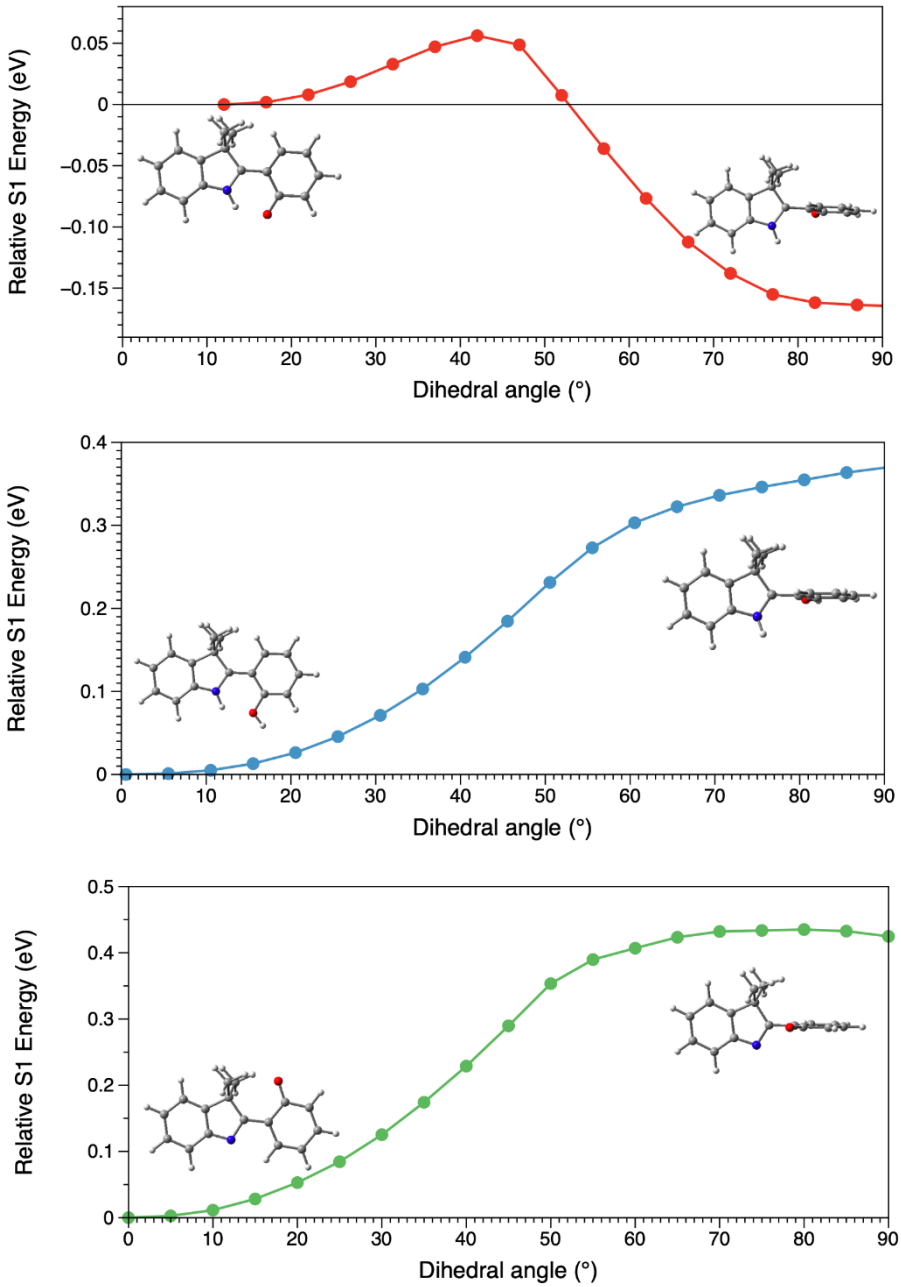


Figure S34. Potential energy surfaces of the S_1 state obtained by a relaxed (LR-PCM)-TD-DFT scan around the inter-ring dihedral angle for HDMI **4**, under its keto (top), protonated (center) and deprotonated (bottom) forms.

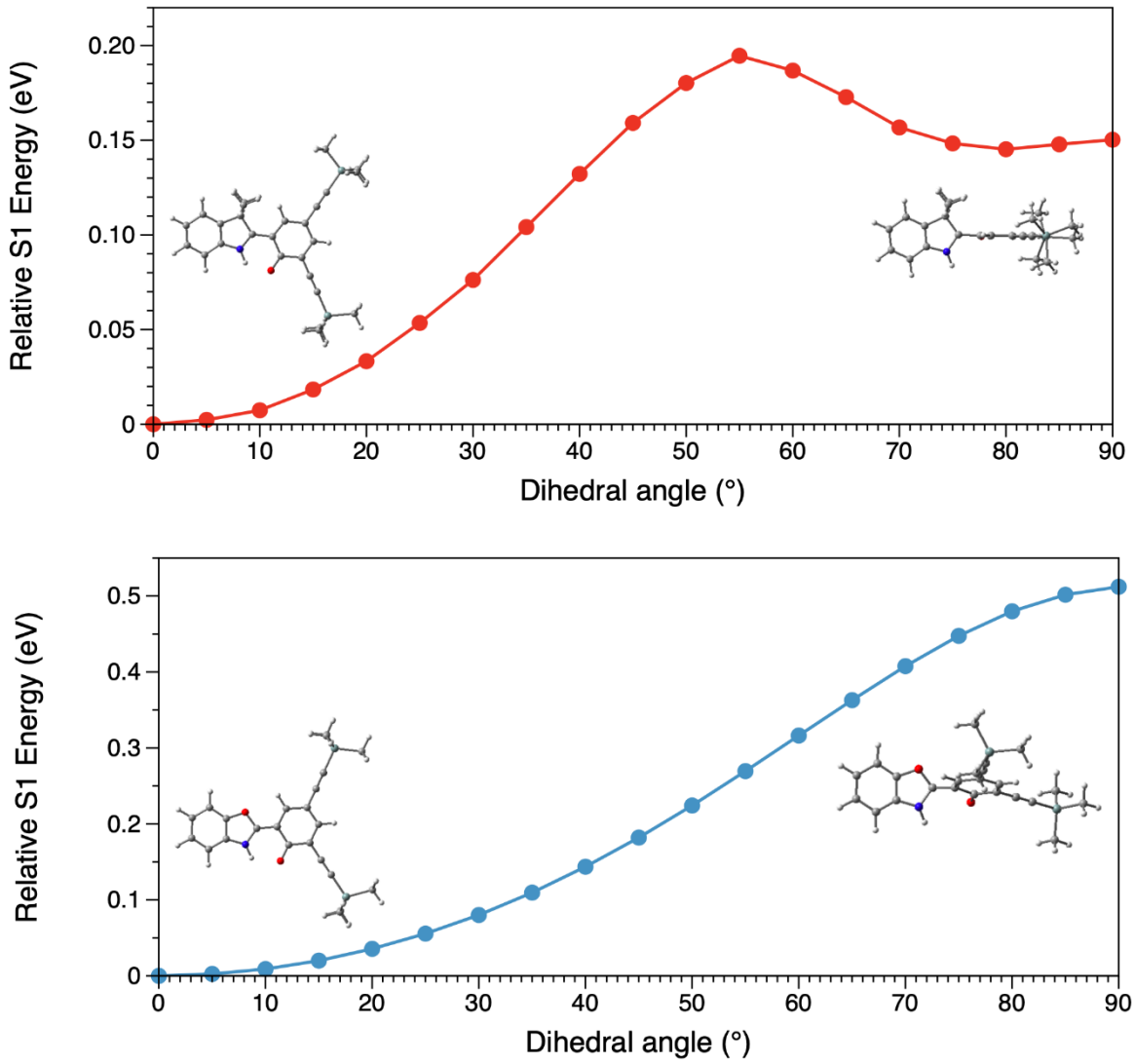


Figure S35. Potential energy surfaces of the S_1 state obtained by a relaxed (LR-PCM)-TD-DFT scan around the inter-ring dihedral angle of the keto forms of HDMI **7** (top) and HBO **9** (bottom).

Comparisons of HBO and 4 emissive K* geometries

HBO (K*) **4 (K*)**

Figure S36. Top views of the optimal excited-state geometries of the keto forms of **HBO** (left) and HDMI **4** (right).

H-bond strength in the E* form

To estimate the H-bond strength in the excited-state (enol form), we have taken the optimal E* structures of HDMI **4**, **HBI**, **HBO** and **HBT** and simply "flipped" the hydroxyl group (see Figure S31) without reoptimizing the structure. We have next compared the cLR[2]-TD-M06-2X energies of the two structures to estimate the H-bond strength. While this approach is obviously approximated, what is of interest for our purposes are the trends in the series. We obtain the following estimates: 17.9 kcal.mol^{-1} for HDMI **4**, 15.5 kcal.mol^{-1} for **HBI,** 13.2 kcal.mol^{-1} for **HBO**, and 16.7 kcal.mol^{-1} for **HBT.**

4 (E*) **4 (E* flipped)**

Figure S37. Illustration for HDMI **4** of the optimal E* structure (left) and the "flipped OH" one (right) used for estimating the H-bond strength. Similar structures are used for the other compounds.

Computed wavelengths and oscillator strengths

In Table S2, we compare theoretical vertical absorption energies to experimental wavelengths of maximal absorption. In all cases, the transition reported corresponds to a S_0-S_1 excitation, and all transitions are bright, as indicated by the large oscillator strengths.

It should be recalled that, the former values do not account for vibronic couplings, hence, one cannot expect a perfect match with the experimental wavelengths, yet similar trends are often observed. In Table S2, one observes that the theoretical wavelengths are nearly systematically (one exception only) smaller than their experimental counterparts, which is the expected trend for absorption since the account of vibronic effects typically tends to redshift the experimental estimates. The mean absolute deviation between experiment and theory attains 28 nm (or 0.28 eV). In addition, the linear correlation coefficient (R) between experimental and theoretical energies attains 0.94, indicating that theory provides ca. 89% of the experimental variability.

Table S2. Comparison between the computed vertical absorption wavelengths and the experimentally measured λ_{max} (in nm). We also provide the computed oscillator strengths (f). The theoretical wavelengths are the ones obtained using Eq. (S1), whereas the oscillator strengths are the LR(neq)-PCM-TD-DFT ones. In all case, the reported (bright) state corresponds to a S_0-S_1 transition.

Dye	$\lambda_{abs}^{vert-theo}$ (nm)	f^{theo}	λ_{max}^{exp} (nm)
HDMI **4**	327	*0.609*	349
Protonated	353	*0.602*	393
Deprotonated	444	*0.478*	411
HBI	300	*0.733*	320
HBO	300	*0.687*	321
HBT	316	*0.628*	343
HDMI **6**	345	*0.580*	367
(di)Protonated	356	*0.487*	
Deprotonated	469	*0.533*	460
HDMI **7**	351	*0.505*	382
HBI **8**	327	*0.554*	362
HBO **9**	327	*0.474*	367
HBT **10**	341	*0.491*	373

Table S3 does provide the equivalent of Table S2 for emission. First, it should be noted that irrespective of the considered molecule (and form), all states are bright (large *f*) compatible with emission. There is no reason to expect an anti-Kasha emission here, and the lowest excited state was considered. As above, one has to be cautious in assessing the theoretical accuracy using such *vertical versus maximum* comparison. Yet, from the values listed in Table S3, we obtain MAE of 26 nm or 0.13 eV, which are very satisfying for this level of theory. The *R* determined on the basis of excitation energies remains very large, 0.87, though slightly below its value for absorption.

Table S3. Comparison between the computed vertical emission wavelengths and the experimentally measured λ_{fl} (in nm). We also provide the computed oscillator strengths (*f*) in parenthesis. The theoretical wavelengths are the ones obtained using Eq. (S1), whereas the oscillator strengths are the LR(neq)-PCM-TD-DFT ones. In all case, the reported (bright) state corresponds to a S_1-S_0 transition.

Dye	$\lambda_{\mathrm{fl}}^{\mathrm{vert-theo}}$ (E*/D*) (nm)	$\lambda_{\mathrm{fl}}^{\mathrm{vert-theo}}$ (K*) (nm)	$\lambda_{l\mathrm{fl}}^{\mathrm{exp}}$ (E*/D*) (nm)	$\lambda_{l\mathrm{fl}}^{\mathrm{exp}}$(K*) (nm)
HDMI **4**	399 *(0.695)*	505 *(0.380)*		519
Protonated	442*(0.667)*		476	
Deprotonated	517*(0.531)*		512	
HBI	345 (*0.875*)	440 (*0.506*)		467
HBO	348 (*0.853*)	448 (*0.437*)		495
HBT	371 *(0.730)*	479 (*0.462*)		528
HDMI **6**	[a]	529 (*0.624*)		537
(di)Protonated	[a]	524 (*0.667*)		535
Deprotonated	544(*0.616*)		532	
HDMI **7**	[a]	538 *(0.509)*		580
HBI **8**	376 *(0.624)*	481 *(0.589)*		504
HBO **9**	379 *(0.554)*	496 *(0.525)*		533
HBT **10**	412 *(0.556)*	532 *(0.546)*		566

[a] During the TD-DFT optimization, the E* form transforms into the K* spontaneously.

Cartesian coordinates

Below are the Cartesian coordinates (Å) for all compounds listed in Table 2 of the main text. We also provide the LR-PCM-TD-DFT free energies for all species. All structures are true minima of their respective PES (no imaginary frequency), but for the ESIPT TS for which one imaginary frequency is found.

HDMI 4 — E (S_0) — G= -748.183934 au.

C	-1.2085070	-1.5992110	0.0000000
C	0.0961370	-2.0970350	0.0000000
C	0.3247080	-3.4631990	0.0000000
C	-0.7804500	-4.3209420	0.0000000
C	-2.0819290	-3.8131020	0.0000000
C	-2.3160790	-2.4374110	0.0000000
C	0.0234570	0.2265930	0.0000000
H	1.3343150	-3.8665150	0.0000000
H	-0.6252610	-5.3951090	0.0000000
H	-2.9233990	-4.4986970	0.0000000
H	-3.3218930	-2.0302860	0.0000000
C	0.3169180	1.6610680	0.0000000
C	-0.7465360	2.6039840	0.0000000
C	1.6344900	2.1562180	0.0000000
C	-0.4621830	3.9759880	0.0000000
C	1.9075020	3.5132270	0.0000000
H	2.4635830	1.4603170	0.0000000
C	0.8471530	4.4249330	0.0000000
H	-1.2998220	4.6655030	0.0000000
H	2.9343970	3.8611490	0.0000000
H	1.0468060	5.4921450	0.0000000
N	-1.2089390	-0.1907470	0.0000000
O	-2.0386940	2.2483580	0.0000000
H	-2.0779910	1.2521550	0.0000000
C	1.0468690	-0.9211970	0.0000000
C	1.9075020	-0.9410440	1.2760360
H	2.5974400	-0.0958860	1.3231870
H	1.2751350	-0.9217460	2.1681920
H	2.4984550	-1.8619980	1.2947340
C	1.9075020	-0.9410440	-1.2760360
H	1.2751350	-0.9217460	-2.1681920
H	2.5974400	-0.0958860	-1.3231870
H	2.4984550	-1.8619980	-1.2947340

HDMI 4 — E* (S_1) — G= -748.058774 au.

C	-0.1673430	-1.9677100	0.0000000
C	1.2352840	-1.6714000	0.0000000
C	2.1680970	-2.6867440	0.0000000
C	1.7207720	-4.0148430	0.0000000
C	0.3402450	-4.3135200	0.0000000
C	-0.6134390	-3.3170980	0.0000000
C	-0.0663720	0.2425080	0.0000000
H	3.2333470	-2.4681330	0.0000000
H	2.4410110	-4.8264980	0.0000000
H	0.0277420	-5.3532500	0.0000000
H	-1.6754580	-3.5386560	0.0000000
C	-0.6137500	1.5362620	0.0000000
C	-2.0707620	1.7282960	0.0000000
C	0.1744870	2.7279770	0.0000000
C	-2.6204240	3.0177720	0.0000000
C	-0.3978730	3.9802980	0.0000000
H	1.2536010	2.6417650	0.0000000

C	-1.8037690	4.1355200	0.0000000
H	-3.7023670	3.0990900	0.0000000
H	0.2384200	4.8594350	0.0000000
H	-2.2410170	5.1283990	0.0000000
N	-0.9138540	-0.8572790	0.0000000
O	-2.9013610	0.7018700	0.0000000
H	-2.3335140	-0.1533500	0.0000000
C	1.4084390	-0.1686840	0.0000000
C	2.1680970	0.2778910	1.2668110
H	2.2980770	1.3625930	1.3015910
H	1.6332110	-0.0357520	2.1673430
H	3.1624010	-0.1814930	1.2777720
C	2.1680970	0.2778910	-1.2668110
H	1.6332110	-0.0357520	-2.1673430
H	2.2980770	1.3625930	-1.3015910
H	3.1624010	-0.1814930	-1.2777720

HDMI 4 — K* (S_1) — G= -748.069009 au.

C	1.8100970	-0.9066070	-0.1366080
C	2.0297450	0.4694580	0.0499070
C	3.3196710	0.9463490	0.1960320
C	4.3838510	0.0374980	0.1583080
C	4.1476820	-1.3298620	-0.0283850
C	2.8582200	-1.8290860	-0.1815610
C	-0.2656910	0.0280990	-0.1086930
H	3.5082090	2.0072180	0.3404060
H	5.4016160	0.3949590	0.2738280
H	4.9873100	-2.0173260	-0.0535120
H	2.6708950	-2.8879640	-0.3242050
C	-1.6936990	0.0167400	-0.0586900
C	-2.4211610	-1.2750210	0.0964870
C	-2.4555990	1.1812640	-0.1579210
C	-3.8517220	-1.2322490	0.1031210
C	-3.8637280	1.1658760	-0.1004380
H	-1.9632840	2.1360870	-0.2997080
C	-4.5611600	-0.0384440	0.0247580
H	-4.3576140	-2.1844040	0.2297580
H	-4.4011160	2.1061670	-0.1678280
H	-5.6456510	-0.0416370	0.0584350
N	0.4565090	-1.1181830	-0.2601670
O	-1.7976500	-2.3635690	0.2301910
C	0.6995660	1.2014890	0.0211040
C	0.4822980	2.0136640	1.3110230
H	-0.4916710	2.5099840	1.3085540
H	0.5398970	1.3659020	2.1896500
H	1.2572860	2.7824750	1.3942470
C	0.6668710	2.1311210	-1.2154760
H	0.7911950	1.5533170	-2.1352720
H	-0.2679170	2.6927240	-1.2796610
H	1.4896030	2.8500920	-1.1446730
H	-0.0445670	-2.0134830	-0.2481890

HDMI 4 — TS* (S_1) — G= -748.060859 au, ν=1090.3 i cm^{-1}

C	1.7304650	-0.9090390	-0.0898120
C	2.0180720	0.4810690	0.0289090
C	3.3242540	0.9179390	0.1252080
C	4.3567480	-0.0286210	0.1083480
C	4.0709550	-1.4012870	-0.0082770
C	2.7700270	-1.8631200	-0.1114740
C	-0.2617410	0.0891620	-0.0803800
H	3.5537060	1.9772920	0.2119850

H	5.3888750	0.2978560	0.1826630
H	4.8909960	-2.1127670	-0.0173530
H	2.5442620	-2.9205650	-0.1998840
C	-1.6700320	0.0738620	-0.0207860
C	-2.3548390	-1.2367570	0.0559940
C	-2.4940600	1.2247540	-0.0402090
C	-3.7656800	-1.2954110	0.0269440
C	-3.8760620	1.1235170	-0.0282330
H	-2.0354510	2.2055250	-0.0893240
C	-4.5194390	-0.1357930	0.0010910
H	-4.2235460	-2.2781630	0.0692180
H	-4.4749990	2.0282510	-0.0533530
H	-5.6028750	-0.1889640	0.0063250
N	0.3982230	-1.1163650	-0.1909710
O	-1.6619600	-2.3289400	0.1676680
H	-0.5529980	-2.0194420	0.0048450
C	0.7156450	1.2564040	-0.0040710
C	0.5501700	2.1079000	1.2686340
H	-0.3993100	2.6501090	1.2674710
H	0.5892530	1.4793350	2.1622810
H	1.3590100	2.8438860	1.3268390
C	0.6586270	2.1531800	-1.2596390
H	0.7818820	1.5551920	-2.1666500
H	-0.2934760	2.6877550	-1.3230490
H	1.4641240	2.8942350	-1.2200420

HDMI 4 — P (S_0) — G= -748.603466 au.

C	-1.8559250	-0.8895140	-0.0000050
C	-2.0518270	0.4847950	0.0000040
C	-3.3428800	0.9884710	0.0000090
C	-4.4042250	0.0799120	0.0000040
C	-4.1784930	-1.2997730	-0.0000050
C	-2.8842150	-1.8179550	-0.0000090
C	0.2469090	-0.0148910	-0.0000050
H	-3.5305530	2.0580190	0.0000160
H	-5.4231770	0.4516920	0.0000070
H	-5.0226090	-1.9805920	-0.0000090
H	-2.6938830	-2.8854810	-0.0000160
C	1.6940820	0.0048590	-0.0000050
C	2.4638770	-1.1864610	0.0000030
C	2.3926120	1.2323490	-0.0000080
C	3.8561680	-1.1344330	0.0000030
C	3.7723710	1.2820980	-0.0000080
H	1.8406650	2.1610690	-0.0000100
C	4.5038800	0.0910340	-0.0000030
H	4.4219800	-2.0613050	0.0000090
H	4.2798410	2.2391790	-0.0000120
H	5.5884090	0.1177870	-0.0000030
N	-0.4634120	-1.1199930	-0.0000080
O	1.8107290	-2.3690250	0.0000120
H	2.4336070	-3.1141160	0.0000150
C	-0.7082480	1.1832420	0.0000030
C	-0.5680700	2.0297900	-1.2823780
H	0.3784990	2.5700950	-1.3248220
H	-0.6545110	1.4021120	-2.1730410
H	-1.3788230	2.7630770	-1.2982560
C	-0.5680550	2.0297780	1.2823900
H	-0.6544620	1.4020890	2.1730490
H	0.3785060	2.5701000	1.3248150
H	-1.3788190	2.7630510	1.2982960
H	-0.0343890	-2.0444290	-0.0000090

HDMI 4 — P* (S_1) — G= -748.484366 au.

C	1.8274170	0.9259870	0.0062970
C	2.0348630	-0.4852680	-0.0026850
C	3.3206220	-0.9859640	-0.0056810
C	4.3871250	-0.0822100	0.0010090
C	4.1689250	1.3186780	0.0106180
C	2.8977380	1.8479650	0.0134490
C	-0.2568450	-0.0064030	-0.0019760
H	3.5071460	-2.0554590	-0.0124410
H	5.4054140	-0.4555680	-0.0006760
H	5.0259160	1.9831250	0.0158330
H	2.7156310	2.9164430	0.0208170
C	-1.6635070	-0.0145200	-0.0034330
C	-2.4742930	1.1936190	-0.0070760
C	-2.3934070	-1.2425960	0.0016790
C	-3.8630630	1.1389080	0.0062770
C	-3.7689180	-1.2781350	0.0113560
H	-1.8490150	-2.1759200	0.0000540
C	-4.5177590	-0.0838240	0.0158170
H	-4.4245830	2.0689530	0.0062290
H	-4.2794090	-2.2346870	0.0164810
H	-5.6015330	-0.1159840	0.0248950
N	0.5018200	1.1697820	0.0071230
O	-1.8288040	2.3719890	-0.0267290
H	-2.4553780	3.1155420	-0.0286310
C	0.7016440	-1.1992420	-0.0051790
C	0.5924030	-2.0668190	-1.2803250
H	-0.3526370	-2.6113190	-1.3244910
H	0.6802360	-1.4475580	-2.1764810
H	1.4038050	-2.8009090	-1.2835010
C	0.5942790	-2.0733750	1.2661100
H	0.6800400	-1.4582040	2.1652990
H	-0.3488510	-2.6212700	1.3076210
H	1.4081510	-2.8047380	1.2657660
H	0.0794110	2.0923610	0.0096570

HDMI 4 — D (S_0) — G= -747.696325 au.

C	-0.8930130	-1.9228710	0.0000000
C	0.5036460	-2.0126850	0.0000000
C	1.1359320	-3.2432080	0.0000000
C	0.3488330	-4.4030200	0.0000000
C	-1.0439310	-4.3113060	0.0000000
C	-1.6838160	-3.0690620	0.0000000
C	-0.2837140	0.1891960	0.0000000
H	2.2216840	-3.3157300	0.0000000
H	0.8246850	-5.3790910	0.0000000
H	-1.6399110	-5.2196080	0.0000000
H	-2.7668840	-2.9912130	0.0000000
C	-0.4528860	1.6454250	0.0000000
C	0.6307700	2.6150480	0.0000000
C	-1.7906500	2.1127740	0.0000000
C	0.2150630	4.0034220	0.0000000
C	-2.1338990	3.4471550	0.0000000
H	-2.5707940	1.3580190	0.0000000
C	-1.0960800	4.4039170	0.0000000
H	1.0234120	4.7309950	0.0000000
H	-3.1752850	3.7532870	0.0000000
H	-1.3366740	5.4657750	0.0000000
N	-1.3355020	-0.5934880	0.0000000
O	1.8675740	2.3452270	0.0000000

C	1.0433270	-0.6030440	0.0000000
C	1.8675740	-0.3563030	1.2740920
H	2.2011410	0.6807260	1.3002030
H	1.2698960	-0.5807070	2.1641370
H	2.7386150	-1.0223510	1.2760040
C	1.8675740	-0.3563030	-1.2740920
H	1.2698960	-0.5807070	-2.1641370
H	2.2011410	0.6807260	-1.3002030
H	2.7386150	-1.0223510	-1.2760040

HDMI 4 — D^* (S_1) — G= -747.592567 au.

C	-0.9834820	-1.8561650	0.0000000
C	0.4294140	-2.0173760	0.0000000
C	1.0049700	-3.2731030	0.0000000
C	0.1760500	-4.4056590	0.0000000
C	-1.2215560	-4.2535320	0.0000000
C	-1.8161570	-3.0006600	0.0000000
C	-0.2357550	0.2140800	0.0000000
H	2.0880440	-3.3881100	0.0000000
H	0.6118830	-5.4000530	0.0000000
H	-1.8500140	-5.1407890	0.0000000
H	-2.8964940	-2.8874960	0.0000000
C	-0.4129510	1.6354920	0.0000000
C	0.7016050	2.6194370	0.0000000
C	-1.7334810	2.1623870	0.0000000
C	0.3666360	4.0162710	0.0000000
C	-1.9939720	3.5271850	0.0000000
H	-2.5512920	1.4520680	0.0000000
C	-0.9414290	4.4660910	0.0000000
H	1.2069410	4.7048540	0.0000000
H	-3.0245460	3.8723570	0.0000000
H	-1.1596430	5.5305750	0.0000000
N	-1.3640890	-0.5564820	0.0000000
O	1.9053470	2.2529450	0.0000000
C	1.0492320	-0.6380020	0.0000000
C	1.9053470	-0.4589850	1.2682420
H	2.3206880	0.5497210	1.3001370
H	1.2977360	-0.6293410	2.1633910
H	2.7226150	-1.1916040	1.2706110
C	1.9053470	-0.4589850	-1.2682420
H	1.2977360	-0.6293410	-2.1633910
H	2.3206880	0.5497210	-1.3001370
H	2.7226150	-1.1916040	-1.2706110

HBI — E (S_0) — G= -685.724167 au.

C	1.1784210	1.5995870	0.0000000
C	2.0917470	0.5273730	0.0000000
C	3.4732740	0.7199770	0.0000000
C	3.9168470	2.0347050	0.0000000
C	3.0163940	3.1182030	0.0000000
C	1.6444740	2.9189130	0.0000000
C	-0.0000000	-0.2109390	0.0000000
H	4.1649490	-0.1155860	0.0000000
H	4.9836920	2.2331110	0.0000000
H	3.4091650	4.1297610	0.0000000
H	0.9464870	3.7494980	0.0000000
C	-1.1430810	-1.1224020	-0.0000000
C	-2.4524180	-0.5884420	-0.0000000
C	-0.9785250	-2.5154170	-0.0000000
C	-3.5487630	-1.4596590	-0.0000000
C	-2.0682470	-3.3702690	-0.0000000

H	0.0206160	-2.9413380	0.0000000
C	-3.3588420	-2.8319590	-0.0000000
H	-4.5424710	-1.0242420	-0.0000000
H	-1.9178220	-4.4439660	-0.0000000
H	-4.2218060	-3.4905590	-0.0000000
N	-0.1117810	1.1055800	-0.0000000
O	-2.7066960	0.7308460	-0.0000000
H	-1.8406820	1.2173390	-0.0000000
N	1.3082210	-0.6084020	0.0000000
H	1.6486740	-1.5590550	0.0000000

HBI — E^* (S_1) — G= -685.583031au.

C	1.0996030	1.6286280	-0.0000000
C	2.0806290	0.5705930	-0.0000000
C	3.4507160	0.8220050	-0.0000000
C	3.8421180	2.1614310	-0.0000000
C	2.8977600	3.2137610	-0.0000000
C	1.5337000	2.9763500	-0.0000000
C	0.0000000	-0.2585310	0.0000000
H	4.1742260	0.0146340	-0.0000000
H	4.9000350	2.4031230	-0.0000000
H	3.2597010	4.2371920	-0.0000000
H	0.8082810	3.7819560	-0.0000000
C	-1.0586020	-1.1610670	0.0000000
C	-2.4375370	-0.6482630	0.0000000
C	-0.8951180	-2.5855740	0.0000000
C	-3.5207960	-1.5268550	0.0000000
C	-1.9918870	-3.4194750	0.0000000
H	0.1030190	-3.0101860	0.0000000
C	-3.3106850	-2.9041220	0.0000000
H	-4.5173250	-1.0983560	0.0000000
H	-1.8424860	-4.4947250	0.0000000
H	-4.1569060	-3.5823200	0.0000000
N	-0.1372970	1.1122100	-0.0000000
O	-2.6731790	0.6530920	0.0000000
H	-1.7888780	1.1484840	0.0000000
N	1.3600790	-0.5863390	-0.0000000
H	1.7468810	-1.5189130	-0.0000000

HBI — K^* (S_1) — G= -685.596701au.

C	0.8855590	-1.8319140	-0.0000000
C	1.9527690	-0.9014220	-0.0000000
C	3.2805180	-1.3180460	-0.0000000
C	3.5126500	-2.6957320	-0.0000000
C	2.4582190	-3.6169070	-0.0000000
C	1.1245810	-3.2054520	-0.0000000
C	0.0000000	0.2459370	-0.0000000
H	4.0951360	-0.6026710	-0.0000000
H	4.5352300	-3.0580930	-0.0000000
H	2.6817080	-4.6786880	-0.0000000
H	0.3062470	-3.9161890	-0.0000000
C	-0.9257510	1.3171770	0.0000000
C	-2.3840180	1.0103740	0.0000000
C	-0.5223520	2.6589780	0.0000000
C	-3.2914500	2.1116140	0.0000000
C	-1.4693160	3.6996520	0.0000000
H	0.5317630	2.9192370	-0.0000000
C	-2.8448380	3.4330420	0.0000000
H	-4.3488950	1.8667230	0.0000000
H	-1.1161690	4.7260790	0.0000000
H	-3.5557700	4.2525310	0.0000000

N	-0.2720600	-1.1007940	0.0000000
O	-2.7710480	-0.1879820	0.0000000
N	1.3771660	0.3490410	-0.0000000
H	1.8861790	1.2211940	-0.0000000
H	-1.2422170	-1.4077930	0.0000000

HBI — TS* (S_1) — G= -685.584196 au, ν=1260.7 i cm^{-1}

C	1.2939280	-1.4482400	-0.0000000
C	2.1482030	-0.2987810	-0.0000000
C	3.5361520	-0.4093760	-0.0000000
C	4.0674440	-1.7007860	-0.0000000
C	3.2394950	-2.8382510	-0.0000000
C	1.8530120	-2.7379550	-0.0000000
C	-0.0000000	0.3393430	0.0000000
H	4.1719440	0.4690760	-0.0000000
H	5.1448920	-1.8291050	-0.0000000
H	3.6988880	-3.8217390	-0.0000000
H	1.2146380	-3.6141490	-0.0000000
C	-1.1866730	1.0770800	0.0000000
C	-2.4551190	0.3001560	0.0000000
C	-1.2795300	2.4917790	0.0000000
C	-3.6888750	0.9809390	0.0000000
C	-2.5217240	3.1130380	0.0000000
H	-0.3769840	3.0940900	0.0000000
C	-3.7273150	2.3714990	0.0000000
H	-4.5910640	0.3787580	0.0000000
H	-2.5678330	4.1977000	0.0000000
H	-4.6790360	2.8910830	0.0000000
N	0.0068360	-1.0327810	-0.0000000
O	-2.4088910	-0.9935580	0.0000000
H	-1.2705790	-1.3111950	0.0000000
N	1.3137710	0.7893600	-0.0000000
H	1.6080310	1.7552140	-0.0000000

HBO — E (S_0) — G= -705.586834 au.

C	0.5135320	1.9461380	0.0000000
C	1.6979840	1.2078430	0.0000000
C	2.9614020	1.7733790	0.0000000
C	2.9935780	3.1659910	0.0000000
C	1.8157640	3.9321640	0.0000000
C	0.5575850	3.3397990	0.0000000
C	-0.0000000	-0.1282030	-0.0000000
H	3.8613250	1.1698400	0.0000000
H	3.9536890	3.6709250	0.0000000
H	1.8929030	5.0143310	0.0000000
H	-0.3531540	3.9282060	0.0000000
C	-0.6893010	-1.4062280	-0.0000000
C	-2.1008760	-1.4308710	-0.0000000
C	0.0286920	-2.6117840	-0.0000000
C	-2.7586650	-2.6662080	-0.0000000
C	-0.6322450	-3.8275620	-0.0000000
H	1.1131480	-2.5724760	-0.0000000
C	-2.0319280	-3.8461050	-0.0000000
H	-3.8434050	-2.6671420	-0.0000000
H	-0.0700450	-4.7545100	-0.0000000
H	-2.5597980	-4.7946930	-0.0000000
N	-0.5524250	1.0498160	0.0000000
O	-2.8570430	-0.3194030	-0.0000000
H	-2.2711490	0.4732340	0.0000000
O	1.3583350	-0.1189160	-0.0000000

HBO — E* (S_1) — G= -705.446564 au.

C	0.7675480	1.8326530	0.0000000
C	1.8720820	0.9262950	0.0000000
C	3.1917280	1.3226960	0.0000000
C	3.4135940	2.7071290	0.0000000
C	2.3452990	3.6287800	0.0000000
C	1.0203000	3.2250080	0.0000000
C	-0.0000000	-0.1831660	-0.0000000
H	4.0031260	0.6046330	0.0000000
H	4.4327110	3.0787600	0.0000000
H	2.5756650	4.6894750	0.0000000
H	0.2004190	3.9337870	0.0000000
C	-0.8348560	-1.2915950	-0.0000000
C	-2.2915320	-1.0899930	-0.0000000
C	-0.3532330	-2.6359920	-0.0000000
C	-3.1535810	-2.1864510	-0.0000000
C	-1.2392800	-3.6918710	-0.0000000
H	0.7175480	-2.8032470	-0.0000000
C	-2.6411160	-3.4799920	-0.0000000
H	-4.2204700	-1.9913320	-0.0000000
H	-0.8574090	-4.7078540	-0.0000000
H	-3.3154110	-4.3292230	-0.0000000
N	-0.3761440	1.1278420	-0.0000000
O	-2.8064190	0.1282760	-0.0000000
H	-2.0677030	0.8083720	-0.0000000
O	1.3792710	-0.3381850	0.0000000

HBO — K* (S_1) — G= -705.454711au.

C	0.4844910	-1.9904720	-0.0000000
C	1.6727580	-1.2419850	-0.0000000
C	2.9261460	-1.8171760	-0.0000000
C	2.9584990	-3.2175710	-0.0000000
C	1.7822680	-3.9756620	-0.0000000
C	0.5183280	-3.3836880	-0.0000000
C	-0.0000000	0.1903220	0.0000000
H	3.8257740	-1.2135970	-0.0000000
H	3.9180680	-3.7226960	-0.0000000
H	1.8526630	-5.0583210	-0.0000000
H	-0.3912970	-3.9721720	0.0000000
C	-0.6575720	1.4401310	0.0000000
C	-2.1429210	1.4578640	0.0000000
C	0.0449220	2.6433120	-0.0000000
C	-2.7771160	2.7349270	0.0000000
C	-0.6449480	3.8768830	0.0000000
H	1.1299400	2.6327070	-0.0000000
C	-2.0416010	3.9240720	0.0000000
H	-3.8625860	2.7386070	0.0000000
H	-0.0691300	4.7967160	0.0000000
H	-2.5520650	4.8812340	0.0000000
N	-0.5274210	-1.0643680	0.0000000
O	-2.7802890	0.3705950	0.0000000
O	1.3606530	0.0912180	-0.0000000
H	-1.5418480	-1.1721500	0.0000000

HBO — TS* (S_1) — G= -705.445825au, ν=1269.2 *i* cm^{-1}

C	1.8543590	-0.6290160	-0.0001070
C	1.9557070	0.7847450	-0.0000040
C	3.1557870	1.4628020	0.0000080
C	4.3104160	0.6686010	-0.0000890
C	4.2350720	-0.7329190	-0.0001920

C	3.0193240	-1.4101330	-0.0002040
C	-0.1507520	0.2372470	0.0000220
H	3.1955040	2.5456890	0.0000880
H	5.2825450	1.1495410	-0.0000850
H	5.1562580	-1.3067650	-0.0002650
H	2.9649010	-2.4924360	-0.0002830
C	-1.5453300	0.3174930	0.0000740
C	-2.2715250	-0.9814120	-0.0000040
C	-2.2971160	1.5060210	0.0001910
C	-3.6831710	-0.9795890	0.0000450
C	-3.6917200	1.4495240	0.0002340
H	-1.7831450	2.4608030	0.0002490
C	-4.3881860	0.2197690	0.0001630
H	-4.1834000	-1.9420050	-0.0000140
H	-4.2546550	2.3775230	0.0003260
H	-5.4722760	0.2148960	0.0001990
N	0.5311690	-0.9365250	-0.0000880
O	-1.5988790	-2.0827490	-0.0001140
H	-0.4153980	-1.7991700	-0.0001270
O	0.6956670	1.3163490	0.0000770

HBT — E (S_0) — G= -1028.555265 au.

C	-0.5475250	1.8613250	0.0000000
C	-1.8479470	1.3244250	0.0000000
C	-2.9743330	2.1473300	0.0000000
C	-2.7751820	3.5212060	0.0000000
C	-1.4810280	4.0667560	0.0000000
C	-0.3629140	3.2487520	0.0000000
C	-0.0000000	-0.2989050	0.0000000
H	-3.9741390	1.7270530	0.0000000
H	-3.6352520	4.1826070	0.0000000
H	-1.3566230	5.1445170	0.0000000
H	0.6428290	3.6554410	0.0000000
C	0.8558310	-1.4834720	0.0000000
C	2.2634660	-1.3373330	0.0000000
C	0.3097280	-2.7775030	0.0000000
C	3.0728520	-2.4806730	0.0000000
C	1.1160250	-3.9015030	0.0000000
H	-0.7706820	-2.8980160	0.0000000
C	2.5067040	-3.7441480	0.0000000
H	4.1485140	-2.3399170	0.0000000
H	0.6727960	-4.8908190	0.0000000
H	3.1513440	-4.6175480	0.0000000
N	0.4638260	0.9171560	0.0000000
O	2.8804980	-0.1447020	0.0000000
H	2.1919380	0.5648200	0.0000000
S	-1.7609730	-0.4167590	0.0000000

HBT — E* (S_1) — G= -1028.423091 au.

C	-0.5941130	1.8175710	0.0000000
C	-1.9052940	1.2266790	0.0000000
C	-3.0549900	2.0054740	0.0000000
C	-2.9176930	3.3919390	0.0000000
C	-1.6392560	3.9914010	0.0000000
C	-0.4877640	3.2346930	0.0000000
C	-0.0000000	-0.3462020	0.0000000
H	-4.0373010	1.5447110	0.0000000
H	-3.8039320	4.0173980	0.0000000
H	-1.5653130	5.0744170	0.0000000
H	0.4969930	3.6892890	0.0000000
C	0.8684620	-1.4420070	0.0000000

C	2.3252980	-1.2139510	0.0000000
C	0.4291160	-2.7976630	0.0000000
C	3.2139880	-2.2952170	0.0000000
C	1.3355420	-3.8374530	0.0000000
H	-0.6364880	-3.0058260	0.0000000
C	2.7319820	-3.5958030	0.0000000
H	4.2757790	-2.0741460	0.0000000
H	0.9735870	-4.8604500	0.0000000
H	3.4237760	-4.4309600	0.0000000
N	0.4249710	0.9520570	0.0000000
O	2.8105030	0.0091170	0.0000000
H	2.0317680	0.6683310	0.0000000
S	-1.7780850	-0.5123050	0.0000000

HBT — K^* (S_1) — G= -1028.433139 au.

C	-0.5532160	-1.8939980	-0.0000000
C	-1.8453410	-1.3249690	-0.0000000
C	-2.9813800	-2.1252300	-0.0000000
C	-2.8148360	-3.5084360	-0.0000000
C	-1.5320080	-4.0751040	-0.0000000
C	-0.3910190	-3.2868530	-0.0000000
C	0.0000000	0.3556670	-0.0000000
H	-3.9710880	-1.6814440	-0.0000000
H	-3.6881060	-4.1513540	-0.0000000
H	-1.4268840	-5.1550910	-0.0000000
H	0.6022180	-3.7219910	0.0000000
C	0.8538100	1.4968390	0.0000000
C	2.3300890	1.3097830	0.0000000
C	0.3447280	2.7948970	0.0000000
C	3.1390180	2.4888090	0.0000000
C	1.1949420	3.9183310	0.0000000
H	-0.7306240	2.9546820	-0.0000000
C	2.5856430	3.7655010	0.0000000
H	4.2133440	2.3344030	0.0000000
H	0.7542680	4.9098560	0.0000000
H	3.2279600	4.6399180	0.0000000
N	0.4236490	-0.9426880	0.0000000
O	2.8306440	0.1532720	0.0000000
S	-1.7509150	0.4273860	-0.0000000
H	1.4402770	-1.0859290	0.0000000

HBT — TS^* (S_1) — G= -1028.424663 au, ν=1177.3 *i* cm^{-1}

C	-0.8318640	-1.6986190	0.0000000
C	-2.0548190	-0.9616610	0.0000000
C	-3.2874190	-1.6020380	0.0000000
C	-3.3112370	-2.9953550	0.0000000
C	-2.1134760	-3.7333030	0.0000000
C	-0.8793830	-3.1102640	0.0000000
C	0.0000000	0.4098350	-0.0000000
H	-4.2093340	-1.0298930	0.0000000
H	-4.2637430	-3.5140780	0.0000000
H	-2.1597210	-4.8178010	0.0000000
H	0.0458060	-3.6762510	0.0000000
C	1.0377430	1.3593780	-0.0000000
C	2.4323310	0.8489140	-0.0000000
C	0.8519520	2.7558240	-0.0000000
C	3.5093380	1.7630500	-0.0000000
C	1.9444480	3.6172410	-0.0000000

H	-0.1564520	3.1592210	-0.0000000
C	3.2719110	3.1287150	-0.0000000
H	4.5127350	1.3510660	-0.0000000
H	1.7725340	4.6887300	-0.0000000
H	4.1019620	3.8264550	-0.0000000
N	0.2724860	-0.9268430	-0.0000000
O	2.6434320	-0.4259750	-0.0000000
H	1.5867460	-0.9485050	-0.0000000
S	-1.7314090	0.7604030	0.0000000

HDMI 6 — E (S_0) — G= -1242.056643 au.

C	-1.8549230	-0.0746110	0.0053640
C	-2.8117690	1.1280670	0.0342890
C	-4.1309790	0.3890660	0.0091690
C	-5.4383570	0.8464630	0.0164090
C	-6.4704090	-0.0971140	-0.0132850
C	-6.1912060	-1.4657210	-0.0490200
C	-4.8756020	-1.9303730	-0.0560190
C	-3.8631490	-0.9804080	-0.0262870
H	-5.6639490	1.9094870	0.0443180
H	-7.5026310	0.2379520	-0.0085260
H	-7.0098720	-2.1778560	-0.0717100
H	-4.6447180	-2.9901340	-0.0837650
C	-0.3889710	-0.0324800	0.0087580
C	0.3091190	1.1815500	0.0248290
C	0.3548520	-1.2449220	-0.0057410
C	1.6986600	1.2381300	0.0239430
H	-0.2446460	2.1106700	0.0661890
C	1.7670660	-1.2027440	-0.0058790
C	2.4070810	0.0310200	0.0078250
C	-2.6919720	1.9438170	1.3344650
H	-1.7464220	2.4867660	1.3988650
H	-3.5045290	2.6757980	1.3711340
H	-2.7778030	1.2924510	2.2087140
C	-2.6851290	2.0167800	-1.2166110
H	-3.5021500	2.7447540	-1.2198140
H	-1.7431300	2.5695610	-1.2407710
H	-2.7577790	1.4158150	-2.1273660
O	-0.2345630	-2.4411390	-0.0379560
H	-1.2269330	-2.2926610	-0.0478140
N	-2.4742270	-1.2167760	-0.0269020
H	3.4938480	0.0507320	0.0019090
C	2.5760150	-2.4468270	-0.0458550
C	2.2816880	-3.5622850	0.7447090
C	3.7083920	-2.5264740	-0.8616930
C	3.1192910	-4.6703940	0.6862360
H	1.4175830	-3.5662620	1.3977570
C	4.4787020	-3.6846880	-0.8468240
H	3.9802610	-1.7038740	-1.5156650
N	4.2048810	-4.7507510	-0.0903740
H	2.9051460	-5.5417470	1.3010290
H	5.3595120	-3.7577150	-1.4807850
C	2.4059740	2.5386190	0.0432350
C	1.8973680	3.6556740	-0.6272300
C	3.6120670	2.7071250	0.7306280
C	2.5963560	4.8563780	-0.5754530
H	0.9812340	3.5892210	-1.2059780
C	4.2344200	3.9505720	0.7154650
H	4.0534720	1.8899480	1.2920590
N	3.7494780	5.0215100	0.0797630

H	2.2110420	5.7298230	-1.0965720
H	5.1705460	4.0931890	1.2504760

HDMI 6 — K^* (S_1) — G= -1241.952004 au.

C	-1.8334220	-0.0857130	-0.0367660
C	-2.8249890	1.0758750	0.0368790
C	-4.1460590	0.3283310	0.0339160
C	-5.4474270	0.7929810	0.0904180
C	-6.4951770	-0.1350640	0.0653330
C	-6.2318150	-1.5071440	-0.0162400
C	-4.9290940	-1.9932930	-0.0747140
C	-3.9003630	-1.0505170	-0.0472720
H	-5.6577470	1.8575930	0.1527750
H	-7.5220730	0.2119480	0.1090680
H	-7.0594310	-2.2090610	-0.0343780
H	-4.7197920	-3.0556790	-0.1379590
C	-0.4074460	-0.0361880	-0.0387480
C	0.2829170	1.1705150	-0.0290350
C	0.3884570	-1.3014650	-0.0509610
C	1.7026750	1.2399870	0.0096730
H	-0.2665730	2.1016520	-0.0068040
C	1.8397260	-1.1985220	-0.0087440
C	2.4517010	0.0617150	0.0215330
C	-2.6910160	1.8925830	1.3391840
H	-1.7473930	2.4407560	1.3849630
H	-3.5083110	2.6186550	1.3924100
H	-2.7543620	1.2371740	2.2118310
C	-2.7541410	1.9943670	-1.2028830
H	-3.5758900	2.7161070	-1.1602090
H	-1.8162260	2.5525690	-1.2497310
H	-2.8556130	1.4094760	-2.1208800
O	-0.1885680	-2.4053720	-0.1254120
H	-2.0385160	-2.1352330	-0.1437740
N	-2.5375960	-1.2467370	-0.0910960
H	3.5341420	0.1224870	0.0549030
C	2.6635010	-2.4105360	-0.0306650
C	2.2682690	-3.6271590	0.5549410
C	3.9390620	-2.3972910	-0.6248660
C	3.1340680	-4.7123570	0.5214130
H	1.3073780	-3.7185780	1.0422210
C	4.7204900	-3.5441020	-0.6076040
H	4.3084870	-1.5107790	-1.1294170
N	4.3463390	-4.6989490	-0.0457610
H	2.8341830	-5.6507540	0.9833490
H	5.7021230	-3.5343080	-1.0767350
C	2.3688050	2.5507400	0.0347740
C	1.7927290	3.6789470	-0.5670120
C	3.6108710	2.7355110	0.6593620
C	2.4669410	4.8935360	-0.5225870
H	0.8470140	3.6119710	-1.0945230
C	4.1966630	3.9948230	0.6498230
H	4.1036950	1.9186050	1.1751800
N	3.6500030	5.0708670	0.0729090
H	2.0311510	5.7705520	-0.9955000
H	5.1555210	4.1482020	1.1392330

HDMI 6.2H$^+$ — E (S_0) — G= -1242.897491 au.

C	1.8875640	-0.0317840	-0.0183920
C	2.8420490	1.1683690	0.0093150
C	4.1597260	0.4254810	0.0093720
C	5.4675020	0.8815470	0.0255130

C	6.4967520	-0.0650000	0.0206410
C	6.2169470	-1.4342290	-0.0002040
C	4.9016750	-1.8979900	-0.0168490
C	3.8929060	-0.9442410	-0.0118880
H	5.6948320	1.9441330	0.0416000
H	7.5293310	0.2682420	0.0331780
H	7.0352500	-2.1467660	-0.0035480
H	4.6693790	-2.9575280	-0.0331770
C	0.4191600	-0.0024780	-0.0163470
C	-0.2962020	1.1926520	-0.0127220
C	-0.3056010	-1.2303530	-0.0179010
C	-1.6935620	1.2249540	-0.0158510
H	0.2482450	2.1277700	-0.0470320
C	-1.7212770	-1.2078860	0.0007580
C	-2.3886210	0.0117730	-0.0017500
C	2.7327710	2.0471800	-1.2503190
H	1.7929150	2.6028790	-1.2935090
H	3.5508770	2.7735360	-1.2465520
H	2.8185030	1.4394750	-2.1551730
C	2.7007840	1.9916090	1.3030030
H	3.5111620	2.7248760	1.3477280
H	1.7535790	2.5351300	1.3486220
H	2.7724570	1.3463710	2.1828340
O	0.3008920	-2.4052720	-0.0105930
H	1.3036710	-2.2365980	-0.0137930
N	2.5021480	-1.1745130	-0.0265480
H	-3.4751230	0.0127530	0.0105940
C	-2.4949490	-2.4651680	0.0421100
C	-2.1294660	-3.5895390	-0.7170140
C	-3.6475600	-2.5511010	0.8390090
C	-2.9030370	-4.7278090	-0.6685920
H	-1.2509800	-3.5764970	-1.3468960
C	-4.3887350	-3.7123100	0.8599930
H	-3.9557280	-1.7247040	1.4679800
N	-3.9993790	-4.7587860	0.1114040
H	-2.6849680	-5.6235000	-1.2350090
H	-5.2789270	-3.8463730	1.4600800
C	-2.4134070	2.5075510	-0.0436430
C	-1.8773800	3.6544750	0.5677510
C	-3.6572310	2.6291940	-0.6872970
C	-2.5612510	4.8476450	0.5198720
H	-0.9385660	3.6191880	1.1063700
C	-4.3085240	3.8413260	-0.7075550
H	-4.1098260	1.7909430	-1.2022260
N	-3.7484990	4.9098210	-0.1110160
H	-2.2038820	5.7615610	0.9757970
H	-5.2615820	4.0010180	-1.1941440
H	-4.5525790	-5.6122080	0.1391430
H	-4.2412480	5.7995970	-0.1410880

HDMI 6.2H$^+$ — K* (S_1) — G= -1242.801102 au.

C	-1.8736210	-0.0944770	-0.0137570
C	-2.8659480	1.0688860	0.0526770
C	-4.1857550	0.3261650	0.0310670
C	-5.4882860	0.7906500	0.0684750
C	-6.5285700	-0.1431900	0.0282700
C	-6.2642230	-1.5172940	-0.0474940
C	-4.9613870	-2.0007880	-0.0850620
C	-3.9416150	-1.0506760	-0.0436210
H	-5.7039950	1.8537400	0.1260140
H	-7.5570550	0.2003940	0.0552730

H	-7.0915080	-2.2183150	-0.0774900
H	-4.7461260	-3.0619820	-0.1435180
C	-0.4529880	-0.0329000	-0.0056170
C	0.2335810	1.1872920	0.0145030
C	0.3460290	-1.2926700	-0.0241660
C	1.6436080	1.2421330	0.0384360
H	-0.3183430	2.1150650	0.0572700
C	1.8181440	-1.1966970	0.0146900
C	2.4130560	0.0673130	0.0477690
C	-2.7453670	1.8703390	1.3659020
H	-1.8065240	2.4241490	1.4275040
H	-3.5670630	2.5904810	1.4150730
H	-2.8160170	1.2063340	2.2311900
C	-2.7762520	1.9882550	-1.1846780
H	-3.6019780	2.7046980	-1.1502860
H	-1.8418250	2.5524740	-1.2153030
H	-2.8622280	1.4063390	-2.1058590
O	-0.2136610	-2.3905300	-0.1094980
H	-2.0947530	-2.1441740	-0.1226760
N	-2.5720770	-1.2456490	-0.0685110
H	3.4933940	0.1468780	0.0765040
C	2.6242310	-2.3975600	-0.0245580
C	2.1872970	-3.6557610	0.4738300
C	3.9469610	-2.3504550	-0.5470400
C	3.0202080	-4.7430070	0.4414930
H	1.2057310	-3.7716370	0.9068710
C	4.7360630	-3.4686480	-0.5685200
H	4.3435910	-1.4432990	-0.9845770
N	4.2679790	-4.6383580	-0.0756380
H	2.7388260	-5.7149100	0.8248930
H	5.7382960	-3.4818000	-0.9760360
C	2.3189200	2.5468020	0.0398680
C	1.7396170	3.6591100	-0.5977640
C	3.5610560	2.7263020	0.6750210
C	2.3896190	4.8725110	-0.5931870
H	0.7988010	3.5784630	-1.1278600
C	4.1734640	3.9588320	0.6563070
H	4.0413970	1.9185060	1.2123320
N	3.5776610	4.9896600	0.0274790
H	2.0019330	5.7608290	-1.0740390
H	5.1231750	4.1633210	1.1324180
H	4.8656760	-5.4581840	-0.0952050
H	4.0439010	5.8945070	0.0231020

HDMI 6 — D^* (S_1) — G= -1241.481006au.

C	1.8652840	-0.0717920	0.0108820
C	2.8163860	-1.2896470	0.0149080
C	4.1439260	-0.5647920	-0.0052320
C	5.4408060	-1.0410750	-0.0151700
C	6.5011490	-0.1229170	-0.0282880
C	6.2404410	1.2552940	-0.0303010
C	4.9407470	1.7466110	-0.0200780
C	3.8754610	0.8242700	-0.0074630
H	5.6429950	-2.1108050	-0.0127600
H	7.5269050	-0.4784070	-0.0364720
H	7.0739770	1.9526620	-0.0402580
H	4.7387120	2.8137450	-0.0220420
C	0.4354630	0.0006930	0.0014340
C	-0.1760360	1.2776460	-0.0088450
C	-0.4512340	-1.1893300	0.0076300
C	-1.5655680	1.4411700	-0.0321100

H	0.4760840	2.1405160	-0.0429850
C	-1.9050110	-0.9854880	-0.0140560
C	-2.4127350	0.3127750	-0.0373410
C	2.7270620	-2.1333730	1.3005660
H	1.7671940	-2.6460600	1.3606510
H	3.5335110	-2.8767110	1.3064070
H	2.8512910	-1.4955280	2.1818580
C	2.7004800	-2.1690650	-1.2434800
H	3.5084980	-2.9106650	-1.2469060
H	1.7416820	-2.6869460	-1.2671480
H	2.8022570	-1.5565890	-2.1453570
O	0.0273370	-2.3357920	0.0666200
N	2.5398930	1.1018460	0.0030530
H	-3.4871830	0.4621330	-0.0605550
C	-2.8142360	-2.1293720	0.0329730
C	-2.5184070	-3.4003410	-0.5053650
C	-4.1010550	-2.0048390	0.6016020
C	-3.4683870	-4.4091220	-0.4530210
H	-1.5613440	-3.5890060	-0.9708050
C	-4.9718920	-3.0831510	0.6034710
H	-4.4087970	-1.0784660	1.0752920
N	-4.6899310	-4.2868490	0.0873000
H	-3.2340370	-5.3829860	-0.8801490
H	-5.9572920	-2.9752310	1.0541210
C	-2.1530430	2.7935560	-0.0478510
C	-1.4959780	3.8861040	0.5369260
C	-3.3924920	3.0617680	-0.6468990
C	-2.0892670	5.1419280	0.5006110
H	-0.5433340	3.7544950	1.0383530
C	-3.8963060	4.3561660	-0.6297530
H	-3.9499230	2.2778770	-1.1483250
N	-3.2718340	5.3981140	-0.0690520
H	-1.5857240	5.9899580	0.9600580
H	-4.8544050	4.5685120	-1.0995120

HDMI 7 — E (S_0) — G= -1717.404489 au.

C	-1.9839830	1.4852300	0.0000000
C	-1.9874460	3.0212260	0.0000000
C	-3.4807170	3.2596130	0.0000000
C	-4.2227950	4.4292160	0.0000000
C	-5.6178480	4.3284290	0.0000000
C	-6.2479220	3.0813090	0.0000000
C	-5.5040290	1.9009260	0.0000000
C	-4.1203460	2.0187230	0.0000000
H	-3.7408510	5.4035790	0.0000000
H	-6.2199860	5.2313340	0.0000000
H	-7.3320050	3.0301450	0.0000000
H	-5.9802500	0.9260540	0.0000000
C	-0.8081630	0.6082500	0.0000000
C	0.4942130	1.1196620	0.0000000
C	-0.9826580	-0.8029510	0.0000000
C	1.6164770	0.2891970	0.0000000
H	0.6552080	2.1895030	0.0000000
C	0.1513260	-1.6494660	0.0000000
C	1.4296850	-1.0993590	0.0000000
C	-1.3597060	3.6102480	1.2763790
H	-0.2808810	3.4463220	1.3219220
H	-1.5379160	4.6897120	1.2956220
H	-1.8149990	3.1715910	2.1687180
C	-1.3597060	3.6102480	-1.2763790
H	-1.5379160	4.6897120	-1.2956220

H	-0.2808810	3.4463220	-1.3219220
H	-1.8149990	3.1715910	-2.1687180
O	-2.1776260	-1.3845160	0.0000000
H	-2.8690980	-0.6579620	0.0000000
N	-3.1773080	0.9714340	0.0000000
H	2.2900240	-1.7601380	0.0000000
C	-0.0319830	-3.0691730	0.0000000
C	-0.1713780	-4.2785870	0.0000000
C	2.9358220	0.8487870	0.0000000
C	4.0571770	1.3240250	0.0000000
Si	-0.4021390	-6.1138030	0.0000000
Si	5.7590230	2.0485170	0.0000000
C	-1.3597060	-6.5912410	-1.5426890
H	-1.5139410	-7.6753410	-1.5700290
H	-2.3413660	-6.1083960	-1.5630850
H	-0.8185260	-6.3027330	-2.4488660
C	1.2925190	-6.9218990	0.0000000
H	1.8671060	-6.6362140	0.8863320
H	1.1894930	-8.0123500	0.0000000
H	1.8671060	-6.6362140	-0.8863320
C	-1.3597060	-6.5912410	1.5426890
H	-0.8185260	-6.3027330	2.4488660
H	-2.3413660	-6.1083960	1.5630850
H	-1.5139410	-7.6753410	1.5700290
C	5.5997850	3.9193330	0.0000000
H	5.0630040	4.2706660	-0.8864440
H	5.0630040	4.2706660	0.8864440
H	6.5927830	4.3815310	0.0000000
C	6.6564870	1.4640890	1.5421180
H	6.1356270	1.7860190	2.4489450
H	6.7363740	0.3729890	1.5635300
H	7.6700950	1.8785380	1.5676390
C	6.6564870	1.4640890	-1.5421180
H	6.7363740	0.3729890	-1.5635300
H	6.1356270	1.7860190	-2.4489450
H	7.6700950	1.8785380	-1.5676390

HDMI 7 — K^* (S_1) — G= -1717.303952 au.

C	-1.9431730	1.4783670	0.0000000
C	-1.9740780	3.0059360	0.0000000
C	-3.4702290	3.2639510	0.0000000
C	-4.1826520	4.4492580	0.0000000
C	-5.5816580	4.3943730	0.0000000
C	-6.2470250	3.1636050	0.0000000
C	-5.5470030	1.9603190	0.0000000
C	-4.1538730	2.0388060	0.0000000
H	-3.6705480	5.4081510	0.0000000
H	-6.1562240	5.3145480	0.0000000
H	-7.3322280	3.1437800	0.0000000
H	-6.0583410	1.0036880	0.0000000
C	-0.8115900	0.6108420	0.0000000
C	0.4907180	1.0950060	0.0000000
C	-1.0063080	-0.8698370	0.0000000
C	1.6315580	0.2333380	0.0000000
H	0.6833160	2.1596440	0.0000000
C	0.1852880	-1.7083260	0.0000000
C	1.4742130	-1.1540020	0.0000000
C	-1.3423690	3.6104000	1.2719170
H	-0.2652270	3.4352340	1.3173850
H	-1.5113190	4.6918620	1.2772440
H	-1.8016010	3.1848420	2.1680890

C	-1.3423690	3.6104000	-1.2719170
H	-1.5113190	4.6918620	-1.2772440
H	-0.2652270	3.4352340	-1.3173850
H	-1.8016010	3.1848420	-2.1680890
O	-2.1436770	-1.3751350	0.0000000
H	-3.3990210	0.0165570	0.0000000
N	-3.2235550	1.0220040	0.0000000
H	2.3435040	-1.8014870	0.0000000
C	0.0007980	-3.1098800	0.0000000
C	-0.1392020	-4.3254280	0.0000000
C	2.9278880	0.8109630	0.0000000
C	4.0384530	1.3204740	0.0000000
Si	-0.3797900	-6.1552910	0.0000000
Si	5.7279750	2.0819590	0.0000000
C	-1.3423690	-6.6346460	-1.5405160
H	-1.5039570	-7.7180120	-1.5603870
H	-2.3206450	-6.1451030	-1.5627020
H	-0.8000680	-6.3555550	-2.4489010
C	1.3076270	-6.9796320	0.0000000
H	1.8850800	-6.6997420	0.8863100
H	1.1938670	-8.0690740	0.0000000
H	1.8850800	-6.6997420	-0.8863100
C	-1.3423690	-6.6346460	1.5405160
H	-0.8000680	-6.3555550	2.4489010
H	-2.3206450	-6.1451030	1.5627020
H	-1.5039570	-7.7180120	1.5603870
C	5.5281120	3.9476930	0.0000000
H	4.9841570	4.2871950	-0.8865870
H	4.9841570	4.2871950	0.8865870
H	6.5111170	4.4306750	0.0000000
C	6.6272910	1.5075020	1.5440290
H	6.0991910	1.8203940	2.4496690
H	6.7233900	0.4177990	1.5628940
H	7.6342300	1.9376900	1.5721080
C	6.6272910	1.5075020	-1.5440290
H	6.7233900	0.4177990	-1.5628940
H	6.0991910	1.8203940	-2.4496690
H	7.6342300	1.9376900	-1.5721080

HBI 8 — E (S_0) — G= -1654.945442 au.

C	-1.9311520	-1.9259970	0.0002030
C	-2.9981030	-3.8677930	-0.0000170
C	-3.4133820	-5.1999800	-0.0001450
C	-4.7823560	-5.4223730	-0.0003040
C	-5.7055520	-4.3574360	-0.0003330
C	-5.2864050	-3.0368220	-0.0002050
C	-3.9083760	-2.7933880	-0.0000450
H	-2.7024940	-6.0191030	-0.0001240
H	-5.1521410	-6.4425040	-0.0004090
H	-6.7673210	-4.5809740	-0.0004620
H	-5.9914740	-2.2124030	-0.0002290
C	-0.8514530	-0.9379980	0.0003390
C	0.4903320	-1.3190680	0.0005000
C	-1.1856400	0.4374910	0.0002690
C	1.5174950	-0.3727480	0.0005800
H	0.7630370	-2.3694420	0.0005560
C	-0.1491460	1.3992820	0.0003450
C	1.1813860	0.9874280	0.0005000
O	-2.4417890	0.8807930	0.0001240
H	-3.0551150	0.0919950	0.0000860
N	-3.2107010	-1.6013650	0.0000940

H	1.9660760	1.7362280	0.0005410
C	-0.4812870	2.7918080	0.0002320
C	-0.7473290	3.9797220	0.0001190
C	2.8892870	-0.7873100	0.0006630
C	4.0545390	-1.1412690	0.0006490
Si	-1.1597030	5.7831440	-0.0000880
Si	5.8253400	-1.6768190	-0.0000410
C	-2.1628240	6.1620510	1.5407740
H	-2.4247400	7.2252570	1.5683730
H	-3.0912410	5.5833520	1.5590420
H	-1.5971360	5.9284520	2.4477810
C	0.4476160	6.7537680	0.0037720
H	1.0492860	6.5258370	-0.8813140
H	0.2385200	7.8289220	0.0037330
H	1.0454550	6.5251460	0.8912720
C	-2.1561060	6.1632870	-1.5450140
H	-1.5864600	5.9304770	-2.4497440
H	-3.0844210	5.5845850	-1.5678180
H	-2.4179320	7.2265100	-1.5728540
C	6.9020600	-0.1446570	-0.1280470
H	6.6954150	0.4073750	-1.0499160
H	6.7340120	0.5284830	0.7180710
H	7.9603570	-0.4267610	-0.1318180
C	6.1696930	-2.5950330	1.6012630
H	5.9947020	-1.9535770	2.4702570
H	5.5314930	-3.4789280	1.6953550
H	7.2133040	-2.9264340	1.6288420
C	6.1034700	-2.8050770	-1.4749070
H	5.4639820	-3.6914080	-1.4211750
H	5.8903650	-2.2868550	-2.4147280
H	7.1457180	-3.1408130	-1.5014870
N	-1.7492860	-3.2793410	0.0001480
H	-0.8665530	-3.7706910	0.0001610

HBI 8 — E^* (S_1) — G= -1654.812245 au.

C	-1.7182110	-2.0802100	0.0004070
C	-2.7570870	-4.0551330	-0.0001030
C	-3.1431960	-5.3928740	-0.0004290
C	-4.5118380	-5.6519670	-0.0006920
C	-5.4598820	-4.6100220	-0.0006300
C	-5.0788180	-3.2759670	-0.0003070
C	-3.7037470	-2.9888050	-0.0000410
H	-2.4119250	-6.1937860	-0.0004780
H	-4.8555070	-6.6811470	-0.0009520
H	-6.5158330	-4.8609560	-0.0008450
H	-5.8068980	-2.4722840	-0.0002670
C	-0.7125930	-1.0944850	0.0006870
C	0.6763940	-1.3570750	0.0009290
C	-1.1445300	0.3045380	0.0006130
C	1.5981680	-0.2918170	0.0009290
H	1.0513310	-2.3735020	0.0010590
C	-0.1928850	1.3718320	0.0006820
C	1.1808510	1.0584690	0.0008430
O	-2.4060830	0.6012180	0.0004460
N	-3.0454960	-1.7993270	0.0002760
H	1.9170710	1.8522390	0.0008220
C	-0.6668530	2.7029060	0.0004610
C	-1.0597810	3.8621050	0.0002220
C	2.9905070	-0.5763490	0.0007940
C	4.1874330	-0.8199790	0.0004430
Si	-1.6685300	5.6040830	-0.0002810

Si	6.0070500	-1.1847600	-0.0003710
C	-2.7100620	5.8815160	1.5389540
H	-3.0929670	6.9078750	1.5535350
H	-3.5657100	5.1999970	1.5647910
H	-2.1216610	5.7256620	2.4481360
C	-0.1805800	6.7504390	0.0006650
H	0.4417970	6.5918980	-0.8852420
H	-0.5104970	7.7949410	0.0003590
H	0.4405850	6.5920300	0.8874440
C	-2.7079350	5.8813700	-1.5409810
H	-2.1182900	5.7253860	-2.4493350
H	-3.5635750	5.1998840	-1.5679170
H	-3.0907730	6.9077450	-1.5562070
C	6.9282020	0.4472620	-0.0764800
H	6.6743120	1.0021730	-0.9846160
H	6.6902360	1.0759880	0.7867250
H	8.0087650	0.2688700	-0.0787420
C	6.4091890	-2.1109050	1.5815420
H	6.1655170	-1.5117440	2.4638680
H	5.8537130	-3.0515550	1.6415480
H	7.4786160	-2.3451320	1.6148430
C	6.3822750	-2.2395020	-1.5065170
H	5.8277610	-3.1821780	-1.4772460
H	6.1209130	-1.7163700	-2.4311250
H	7.4513520	-2.4751830	-1.5403720
N	-1.5245540	-3.4485440	0.0002110
H	-0.6323610	-3.9216100	0.0000450
H	-2.9663580	-0.2964900	0.0003610

HBI 8 — K^* (S_1) — G= -1654.831304 au.

C	-2.6664210	-0.2927800	0.0064580
C	-4.7533390	-1.1661150	-0.0199960
C	-5.8803260	-1.9808030	-0.0457700
C	-7.1213030	-1.3434980	-0.0322500
C	-7.2281520	0.0531130	0.0054810
C	-6.1007540	0.8729610	0.0307270
C	-4.8594570	0.2412250	0.0169850
H	-5.7937770	-3.0610080	-0.0750480
H	-8.0235100	-1.9454890	-0.0513320
H	-8.2121190	0.5099100	0.0151230
H	-6.1797840	1.9536770	0.0591840
C	-1.2551250	-0.2032740	0.0146380
C	-0.4357160	-1.3348020	0.0202030
C	-0.6301060	1.1453350	0.0170260
C	0.9828790	-1.2114090	0.0097650
H	-0.8527990	-2.3357470	0.0355910
C	0.8241860	1.2178640	0.0087640
C	1.6023200	0.0462730	0.0029140
O	-1.3378990	2.1672870	0.0262300
N	-3.5762860	0.7313980	0.0324340
H	2.6838150	0.1145780	-0.0060680
C	1.4203070	2.4969200	0.0037990
C	1.9539720	3.5996230	-0.0009180
C	1.7767140	-2.3894750	0.0061270
C	2.4514940	-3.4078490	0.0022830
Si	2.7323350	5.2687420	-0.0096570
Si	3.4839870	-4.9457950	-0.0011520
C	2.1949670	6.2029760	1.5307780
H	2.6372610	7.2053500	1.5366970
H	1.1067630	6.3123020	1.5661240
H	2.5154230	5.6850680	2.4397900

C	4.5998900	5.0608530	-0.0232400
H	4.9308340	4.5130990	-0.9108590
H	5.0880720	6.0414680	-0.0289320
H	4.9442050	4.5167170	0.8615110
C	2.1720740	6.1969720	-1.5455790
H	2.4791250	5.6755760	-2.4572180
H	1.0834480	6.3060490	-1.5652430
H	2.6140890	7.1993530	-1.5619060
C	5.1506640	-4.5313260	-0.7573130
H	5.0409280	-4.1767550	-1.7865480
H	5.6634380	-3.7552990	-0.1811120
H	5.7888980	-5.4212980	-0.7711120
C	3.6843720	-5.5193590	1.7753830
H	4.1804660	-4.7570590	2.3834570
H	2.7151280	-5.7432570	2.2309040
H	4.2933130	-6.4292720	1.8079950
C	2.5936610	-6.2469450	-1.0199860
H	1.6108270	-6.4759750	-0.5970850
H	2.4529300	-5.9133510	-2.0524660
H	3.1783440	-7.1729110	-1.0394660
N	-3.4044010	-1.4537190	-0.0224640
H	-3.0109200	-2.3825610	-0.0698910
H	-3.2557040	1.6946530	0.0519350

HBI 8 — TS* (S_1) — G= -1654.813707 au, ν=556.5 i cm^{-1}

C	-1.7029020	-2.0898940	0.0001110
C	-2.8037920	-4.0325790	-0.0006320
C	-3.2253680	-5.3589870	-0.0011390
C	-4.6007670	-5.5829200	-0.0010690
C	-5.5196570	-4.5177430	-0.0005120
C	-5.1028340	-3.1929010	-0.0000110
C	-3.7226610	-2.9449880	-0.0000680
H	-2.5149790	-6.1784310	-0.0015600
H	-4.9707020	-6.6028960	-0.0014470
H	-6.5820740	-4.7395310	-0.0004680
H	-5.8096290	-2.3705370	0.0004330
C	-0.6895710	-1.1118970	0.0005170
C	0.6956500	-1.3717120	0.0001440
C	-1.1332600	0.2891000	0.0013340
C	1.6170750	-0.3019380	0.0007500
H	1.0738400	-2.3872260	-0.0006250
C	-0.1770790	1.3576940	0.0020850
C	1.1971540	1.0462860	0.0017900
O	-2.3898360	0.5673090	0.0013490
N	-3.0234940	-1.7759660	0.0003620
H	1.9322250	1.8411870	0.0022530
C	-0.6519540	2.6874720	0.0025670
C	-1.0469120	3.8463330	0.0029720
C	3.0091150	-0.5860480	0.0002790
C	4.2059680	-0.8302760	-0.0000840
Si	-1.6605960	5.5863670	-0.0000640
Si	6.0255650	-1.1952180	-0.0003140
C	-2.9778530	5.7624310	1.3276830
H	-3.3693570	6.7855900	1.3353270
H	-3.8144770	5.0808520	1.1465530
H	-2.5707480	5.5471670	2.3201590
C	-0.2120240	6.7274710	0.3562700
H	0.5713050	6.6210160	-0.4003360
H	-0.5457700	7.7707640	0.3533780
H	0.2278000	6.5154380	1.3354640
C	-2.3919950	5.9700990	-1.6881060

H	-1.6406070	5.8703840	-2.4771550
H	-3.2229390	5.2972560	-1.9205770
H	-2.7715290	6.9976740	-1.7079160
C	6.9467840	0.4373960	0.0571710
H	6.7063900	1.0572820	-0.8117430
H	6.6951590	1.0015010	0.9602490
H	8.0273890	0.2593090	0.0583390
C	6.4042410	-2.2352500	1.5149400
H	6.1448480	-1.7032310	2.4350250
H	5.8495720	-3.1781000	1.4959350
H	7.4733500	-2.4707590	1.5487910
C	6.4236370	-2.1368430	-1.5739830
H	5.8667640	-3.0772560	-1.6239300
H	6.1790150	-1.5459020	-2.4615700
H	7.4926490	-2.3729410	-1.6072280
N	-1.5518850	-3.4606720	-0.0005260
H	-0.6742360	-3.9601730	-0.0007030
H	-2.9624610	-0.3983620	0.0009370

HBO 9 — E (S_0) — G= -1674.805518 au.

C	2.7323390	0.0279910	0.0000000
C	4.7191930	0.8691280	0.0000000
C	5.8235920	1.7037870	0.0000000
C	7.0580720	1.0595740	0.0000000
C	7.1614360	-0.3422240	0.0000000
C	6.0365160	-1.1590380	0.0000000
C	4.7948840	-0.5244260	0.0000000
H	5.7288780	2.7831280	0.0000000
H	7.9636230	1.6567770	0.0000000
H	8.1467940	-0.7960050	0.0000000
H	6.1122840	-2.2405740	0.0000000
C	1.2780170	0.0376490	0.0000000
C	0.5750960	1.2437060	0.0000000
C	0.5854180	-1.1928280	0.0000000
C	-0.8199520	1.2572620	0.0000000
H	1.1250860	2.1785640	0.0000000
C	-0.8275040	-1.1812520	0.0000000
C	-1.5076720	0.0345590	0.0000000
O	1.1978220	-2.3781140	0.0000000
H	2.1773670	-2.2413040	0.0000000
N	3.4945500	-1.0246570	0.0000000
H	-2.5923840	0.0291750	0.0000000
C	-1.5439320	-2.4204530	0.0000000
C	-2.1670460	-3.4660370	0.0000000
C	-1.5399910	2.4966340	0.0000000
C	-2.1545940	3.5477420	0.0000000
Si	-3.0982450	-5.0656750	0.0000000
Si	-3.0919060	5.1433080	0.0000000
C	-2.6249030	-6.0235310	1.5434480
H	-3.1566260	-6.9807410	1.5709320
H	-1.5508880	-6.2313840	1.5649530
H	-2.8830670	-5.4661790	2.4489400
C	-4.9347120	-4.6766370	0.0000000
H	-5.2167500	-4.1003490	-0.8863590
H	-5.5164020	-5.6046780	0.0000000
H	-5.2167500	-4.1003490	0.8863590
C	-2.6249030	-6.0235310	-1.5434480
H	-2.8830670	-5.4661790	-2.4489400
H	-1.5508880	-6.2313840	-1.5649530
H	-3.1566260	-6.9807410	-1.5709320
C	-4.9261850	4.7444080	0.0000000

H	-5.2049140	4.1664800	-0.8863250
H	-5.2049140	4.1664800	0.8863250
H	-5.5130110	5.6692010	0.0000000
C	-2.6249030	6.1059730	1.5427410
H	-2.8784390	5.5473970	2.4488010
H	-1.5526450	6.3230940	1.5642720
H	-3.1641720	7.0589700	1.5697840
C	-2.6249030	6.1059730	-1.5427410
H	-1.5526450	6.3230940	-1.5642720
H	-2.8784390	5.5473970	-2.4488010
H	-3.1641720	7.0589700	-1.5697840
O	3.3925350	1.2118990	0.0000000

HBO 9 — E^* (S_1) — G= -1674.674508 au.

C	2.6916390	0.0522890	0.0000000
C	4.7515090	0.7356410	0.0000000
C	5.9130240	1.4794010	0.0000000
C	7.1059480	0.7478510	0.0000000
C	7.1046600	-0.6568330	0.0000000
C	5.9251870	-1.3933340	0.0000000
C	4.7201080	-0.6764420	0.0000000
H	5.8964820	2.5629800	0.0000000
H	8.0516700	1.2790160	0.0000000
H	8.0547980	-1.1813210	0.0000000
H	5.9262320	-2.4774180	0.0000000
C	1.2912200	0.1382000	0.0000000
C	0.5686140	1.3452000	0.0000000
C	0.5368750	-1.1164340	0.0000000
C	-0.8426700	1.3255610	0.0000000
H	1.0957600	2.2909890	0.0000000
C	-0.8887480	-1.1162740	0.0000000
C	-1.5729590	0.1151880	0.0000000
O	1.1577330	-2.2589490	0.0000000
H	2.1749330	-2.0985300	0.0000000
N	3.4144390	-1.0773140	0.0000000
H	-2.6551730	0.1329130	0.0000000
C	-1.5683120	-2.3568960	0.0000000
C	-2.1732590	-3.4196010	0.0000000
C	-1.5512540	2.5547650	0.0000000
C	-2.1608980	3.6137450	0.0000000
Si	-3.0706360	-5.0366320	0.0000000
Si	-3.0787320	5.2293870	0.0000000
C	-2.5786760	-5.9892550	1.5418680
H	-3.0877400	-6.9590500	1.5617360
H	-1.5001400	-6.1717310	1.5658200
H	-2.8534310	-5.4429230	2.4490810
C	-4.9146040	-4.6848680	0.0000000
H	-5.2087050	-4.1148970	-0.8864620
H	-5.4762900	-5.6251920	0.0000000
H	-5.2087050	-4.1148970	0.8864620
C	-2.5786760	-5.9892550	-1.5418680
H	-2.8534310	-5.4429230	-2.4490810
H	-1.5001400	-6.1717310	-1.5658200
H	-3.0877400	-6.9590500	-1.5617360
C	-4.9157810	4.8542320	0.0000000
H	-5.2017850	4.2805490	-0.8866050
H	-5.2017850	4.2805490	0.8866050
H	-5.4893390	5.7871980	0.0000000
C	-2.5786760	6.1657280	1.5468070
H	-2.8416400	5.6072220	2.4499740
H	-1.5014930	6.3561330	1.5623740

H	-3.0952450	7.1308520	1.5818400
C	-2.5786760	6.1657280	-1.5468070
H	-1.5014930	6.3561330	-1.5623740
H	-2.8416400	5.6072220	-2.4499740
H	-3.0952450	7.1308520	-1.5818400
O	3.4619910	1.1881550	0.0000000

HBO 9 — K^* (S_1) — G= -1674.689226 au.

C	2.6777580	0.0656150	0.0000000
C	4.7167810	0.8956240	0.0000000
C	5.8007820	1.7481090	0.0000000
C	7.0593490	1.1362650	0.0000000
C	7.1954200	-0.2567670	0.0000000
C	6.0902500	-1.1086940	0.0000000
C	4.8383450	-0.5002420	0.0000000
H	5.6756320	2.8241830	0.0000000
H	7.9476190	1.7581920	0.0000000
H	8.1900000	-0.6898740	0.0000000
H	6.1963380	-2.1869660	0.0000000
C	1.2688090	0.0692750	0.0000000
C	0.5414880	1.2529210	0.0000000
C	0.5666760	-1.2385010	0.0000000
C	-0.8876990	1.2272600	0.0000000
H	1.0507140	2.2099850	0.0000000
C	-0.8854680	-1.2091520	0.0000000
C	-1.5846940	0.0144200	0.0000000
O	1.2184240	-2.2979950	0.0000000
N	3.5474290	-0.9780680	0.0000000
H	-2.6684170	0.0145840	0.0000000
C	-1.5716570	-2.4427750	0.0000000
C	-2.1830940	-3.5035950	0.0000000
C	-1.5959010	2.4574560	0.0000000
C	-2.1947320	3.5223950	0.0000000
Si	-3.0855310	-5.1120010	0.0000000
Si	-3.1012510	5.1388720	0.0000000
C	-2.6047630	-6.0760080	1.5397220
H	-3.1205170	-7.0424690	1.5543770
H	-1.5275160	-6.2659280	1.5660450
H	-2.8778380	-5.5317100	2.4487360
C	-4.9308100	-4.7608960	0.0000000
H	-5.2251190	-4.1906230	-0.8862850
H	-5.4930480	-5.7009830	0.0000000
H	-5.2251190	-4.1906230	0.8862850
C	-2.6047630	-6.0760080	-1.5397220
H	-2.8778380	-5.5317100	-2.4487360
H	-1.5275160	-6.2659280	-1.5660450
H	-3.1205170	-7.0424690	-1.5543770
C	-4.9424470	4.7787720	0.0000000
H	-5.2331360	4.2070730	-0.8864320
H	-5.2331360	4.2070730	0.8864320
H	-5.5090260	5.7160700	0.0000000
C	-2.6047630	6.0833960	1.5442390
H	-2.8716050	5.5298770	2.4494370
H	-1.5270930	6.2714390	1.5630820
H	-3.1187340	7.0501860	1.5735370
C	-2.6047630	6.0833960	-1.5442390
H	-1.5270930	6.2714390	-1.5630820
H	-2.8716050	5.5298770	-2.4494370
H	-3.1187340	7.0501860	-1.5735370
O	3.3863020	1.2266320	0.0000000
H	3.1978100	-1.9333060	0.0000000

HBO 9 — TS* (S_1) — G= -1674.676057 au, ν=1127.0 *i* cm^{-1}

C	2.6839460	0.0848950	0.0000000
C	4.7907770	0.6144750	0.0000000
C	5.9965050	1.2830570	0.0000000
C	7.1422500	0.4789110	0.0000000
C	7.0529800	-0.9204400	0.0000000
C	5.8280540	-1.5831770	0.0000000
C	4.6757630	-0.7911720	0.0000000
H	6.0464220	2.3655680	0.0000000
H	8.1188010	0.9507410	0.0000000
H	7.9672400	-1.5050350	0.0000000
H	5.7620290	-2.6650050	0.0000000
C	1.2864130	0.1980730	0.0000000
C	0.5676640	1.3980680	0.0000000
C	0.5451740	-1.0771150	0.0000000
C	-0.8499780	1.3749070	0.0000000
H	1.0901050	2.3471390	0.0000000
C	-0.8878660	-1.0671650	0.0000000
C	-1.5726980	0.1643930	0.0000000
O	1.1870560	-2.1868600	0.0000000
H	2.3346540	-1.9486190	0.0000000
N	3.3398710	-1.0899150	0.0000000
H	-2.6552320	0.1800090	0.0000000
C	-1.5696480	-2.3048770	0.0000000
C	-2.1752190	-3.3678710	0.0000000
C	-1.5577890	2.6043600	0.0000000
C	-2.1638960	3.6652890	0.0000000
Si	-3.0708880	-4.9848770	0.0000000
Si	-3.0789090	5.2818200	0.0000000
C	-2.5787440	-5.9383910	1.5415060
H	-3.0868230	-6.9087470	1.5603240
H	-1.5000170	-6.1196900	1.5657710
H	-2.8544270	-5.3931150	2.4490760
C	-4.9157420	-4.6368630	0.0000000
H	-5.2110240	-4.0674450	-0.8864380
H	-5.4756320	-5.5782740	0.0000000
H	-5.2110240	-4.0674450	0.8864380
C	-2.5787440	-5.9383910	-1.5415060
H	-2.8544270	-5.3931150	-2.4490760
H	-1.5000170	-6.1196900	-1.5657710
H	-3.0868230	-6.9087470	-1.5603240
C	-4.9167590	4.9098410	0.0000000
H	-5.2037340	4.3365840	-0.8865770
H	-5.2037340	4.3365840	0.8865770
H	-5.4888210	5.8437350	0.0000000
C	-2.5787440	6.2188620	1.5464850
H	-2.8425550	5.6611060	2.4498860
H	-1.5013790	6.4083090	1.5625180
H	-3.0943630	7.1845260	1.5808770
C	-2.5787440	6.2188620	-1.5464850
H	-1.5013790	6.4083090	-1.5625180
H	-2.8425550	5.6611060	-2.4498860

H	-3.0943630	7.1845260	-1.5808770
O	3.5301220	1.1553220	0.0000000

HBT 10 — E (S_0) — G= -1997.774135 au.

C	2.5685600	0.0941120	0.0000000
C	4.9670640	0.6199860	0.0000000
C	6.2971900	1.0411970	0.0000000
C	7.2854110	0.0667710	0.0000000
C	6.9594470	-1.2997330	0.0000000
C	5.6390300	-1.7171800	0.0000000
C	4.6310920	-0.7460690	0.0000000
H	6.5510010	2.0956200	0.0000000
H	8.3276640	0.3680200	0.0000000
H	7.7548710	-2.0373940	0.0000000
H	5.3711400	-2.7683350	0.0000000
C	1.1043030	0.0991050	0.0000000
C	0.3882660	1.2986750	0.0000000
C	0.4015110	-1.1299520	0.0000000
C	-1.0063990	1.3165020	0.0000000
H	0.9199140	2.2460490	0.0000000
C	-1.0129150	-1.1170630	0.0000000
C	-1.6961340	0.0956020	0.0000000
O	1.0049630	-2.3177410	0.0000000
H	1.9873260	-2.1718660	0.0000000
N	3.2712030	-1.0005790	0.0000000
H	-2.7807860	0.0901980	0.0000000
C	-1.7272360	-2.3575860	0.0000000
C	-2.3493880	-3.4038210	0.0000000
C	-1.7224510	2.5579120	0.0000000
C	-2.3342390	3.6107190	0.0000000
Si	-3.2767090	-5.0052180	0.0000000
Si	-3.2693240	5.2074730	0.0000000
C	-2.8014130	-5.9626100	1.5432560
H	-3.3307390	-6.9211650	1.5703330
H	-1.7268760	-6.1677710	1.5649040
H	-3.0610750	-5.4062240	2.4489200
C	-5.1144070	-4.6216290	0.0000000
H	-5.3981520	-4.0461550	-0.8863490
H	-5.6933920	-5.5513700	0.0000000
H	-5.3981520	-4.0461550	0.8863490
C	-2.8014130	-5.9626100	-1.5432560
H	-3.0610750	-5.4062240	-2.4489200
H	-1.7268760	-6.1677710	-1.5649040
H	-3.3307390	-6.9211650	-1.5703330
C	-5.1040850	4.8106940	0.0000000
H	-5.3834530	4.2330670	-0.8863190
H	-5.3834530	4.2330670	0.8863190
H	-5.6898690	5.7361490	0.0000000
C	-2.8014130	6.1698430	1.5426790
H	-3.0555490	5.6115940	2.4487730
H	-1.7289490	6.3859540	1.5642900
H	-3.3397480	7.1233720	1.5696160
C	-2.8014130	6.1698430	-1.5426790
H	-1.7289490	6.3859540	-1.5642900
H	-3.0555490	5.6115940	-2.4487730
H	-3.3397480	7.1233720	-1.5696160
S	3.5121070	1.5803590	0.0000000

HBT 10 — E* (S_1) — G= -1997.650750 au.

C	2.5309010	0.1263000	0.0000000

C	4.9777030	0.4498710	0.0000000
C	6.3289320	0.7737230	0.0000000
C	7.2576180	-0.2642140	0.0000000
C	6.8343490	-1.6047740	0.0000000
C	5.4914860	-1.9374500	0.0000000
C	4.5336490	-0.9027650	0.0000000
H	6.6518610	1.8095580	0.0000000
H	8.3174790	-0.0334790	0.0000000
H	7.5776420	-2.3957790	0.0000000
H	5.1600770	-2.9703310	0.0000000
C	1.1240070	0.2090420	0.0000000
C	0.3922580	1.4063860	0.0000000
C	0.3648760	-1.0517680	0.0000000
C	-1.0188230	1.3910600	0.0000000
H	0.9068770	2.3612680	0.0000000
C	-1.0646570	-1.0456600	0.0000000
C	-1.7455700	0.1796110	0.0000000
O	0.9886210	-2.1828960	0.0000000
H	2.0436210	-1.9817290	0.0000000
N	3.1876220	-1.0548380	0.0000000
H	-2.8282170	0.1974950	0.0000000
C	-1.7476090	-2.2872560	0.0000000
C	-2.3506040	-3.3497420	0.0000000
C	-1.7280780	2.6204300	0.0000000
C	-2.3358530	3.6800310	0.0000000
Si	-3.2465420	-4.9689060	0.0000000
Si	-3.2519630	5.2965620	0.0000000
C	-2.7516720	-5.9181040	1.5425970
H	-3.2593440	-6.8885290	1.5648570
H	-1.6728550	-6.0989530	1.5655700
H	-3.0261380	-5.3705600	2.4491720
C	-5.0906410	-4.6187940	0.0000000
H	-5.3851740	-4.0490710	-0.8864770
H	-5.6515510	-5.5595640	0.0000000
H	-5.3851740	-4.0490710	0.8864770
C	-2.7516720	-5.9181040	-1.5425970
H	-3.0261380	-5.3705600	-2.4491720
H	-1.6728550	-6.0989530	-1.5655700
H	-3.2593440	-6.8885290	-1.5648570
C	-5.0893470	4.9227570	0.0000000
H	-5.3758340	4.3493220	-0.8866130
H	-5.3758340	4.3493220	0.8866130
H	-5.6621580	5.8561830	0.0000000
C	-2.7516720	6.2330430	1.5466510
H	-3.0153280	5.6750180	2.4499230
H	-1.6743360	6.4226280	1.5625740
H	-3.2673910	7.1986360	1.5813360
C	-2.7516720	6.2330430	-1.5466510
H	-1.6743360	6.4226280	-1.5625740
H	-3.0153280	5.6750180	-2.4499230
H	-3.2673910	7.1986360	-1.5813360
S	3.6029040	1.5337030	0.0000000

HBT 10 — K^* (S_1) — G= -1997.665902 au.

C	2.5199650	0.1365110	0.0000000
C	4.9596760	0.6690700	0.0000000
C	6.2692980	1.1343440	0.0000000
C	7.3003930	0.1983110	0.0000000
C	7.0208840	-1.1754380	0.0000000
C	5.7170480	-1.6494980	0.0000000
C	4.6775200	-0.7113830	0.0000000

H	6.4795700	2.1985690	0.0000000
H	8.3300110	0.5385900	0.0000000
H	7.8406160	-1.8862380	0.0000000
H	5.4977950	-2.7115500	0.0000000
C	1.0983630	0.1215410	0.0000000
C	0.3560080	1.2946190	0.0000000
C	0.3864090	-1.1853280	0.0000000
C	-1.0709550	1.2763350	0.0000000
H	0.8493020	2.2621810	0.0000000
C	-1.0687030	-1.1527840	0.0000000
C	-1.7677930	0.0628550	0.0000000
O	1.0189130	-2.2566660	0.0000000
N	3.3318230	-0.9595750	0.0000000
H	-2.8517180	0.0624290	0.0000000
C	-1.7547690	-2.3891990	0.0000000
C	-2.3644890	-3.4497690	0.0000000
C	-1.7770020	2.5072690	0.0000000
C	-2.3738820	3.5733240	0.0000000
Si	-3.2647160	-5.0609490	0.0000000
Si	-3.2778990	5.1913610	0.0000000
C	-2.7800050	-6.0208400	1.5405570
H	-3.2936800	-6.9883110	1.5578230
H	-1.7023250	-6.2083360	1.5657070
H	-3.0530380	-5.4753490	2.4488660
C	-5.1101550	-4.7120760	0.0000000
H	-5.4050610	-4.1421600	-0.8863090
H	-5.6712780	-5.6528050	0.0000000
H	-5.4050610	-4.1421600	0.8863090
C	-2.7800050	-6.0208400	-1.5405570
H	-3.0530380	-5.4753490	-2.4488660
H	-1.7023250	-6.2083360	-1.5657070
H	-3.2936800	-6.9883110	-1.5578230
C	-5.1194830	4.8334100	0.0000000
H	-5.4109030	4.2621240	-0.8864530
H	-5.4109030	4.2621240	0.8864530
H	-5.6848280	5.7714510	0.0000000
C	-2.7800050	6.1352250	1.5441820
H	-3.0480430	5.5823960	2.4494420
H	-1.7020200	6.3214390	1.5632410
H	-3.2922800	7.1029320	1.5731020
C	-2.7800050	6.1352250	-1.5441820
H	-1.7020200	6.3214390	-1.5632410
H	-3.0480430	5.5823960	-2.4494420
H	-3.2922800	7.1029320	-1.5731020
S	3.4748230	1.6039760	0.0000000
H	2.8807290	-1.8764240	0.0000000

HBT 10 — TS* (S_1) — G= -1997.651719 au, ν=290.5 *i* cm^{-1}

C	2.5302100	0.1342130	0.0000000
C	4.9827560	0.4152320	0.0000000
C	6.3385130	0.7192610	0.0000000
C	7.2520270	-0.3322240	0.0000000
C	6.8092200	-1.6657880	0.0000000
C	5.4611160	-1.9789380	0.0000000
C	4.5205200	-0.9300280	0.0000000
H	6.6764330	1.7502790	0.0000000
H	8.3151000	-0.1169250	0.0000000
H	7.5404870	-2.4679020	0.0000000
H	5.1148010	-3.0068950	0.0000000

C	1.1232420	0.2231870	0.0000000
C	0.3937980	1.4193060	0.0000000
C	0.3665860	-1.0416470	0.0000000
C	-1.0191190	1.4043650	0.0000000
H	0.9085680	2.3742450	0.0000000
C	-1.0650500	-1.0322190	0.0000000
C	-1.7451880	0.1935780	0.0000000
O	0.9944810	-2.1652780	0.0000000
H	2.0809260	-1.9445820	0.0000000
N	3.1708370	-1.0570340	0.0000000
H	-2.8278880	0.2118970	0.0000000
C	-1.7489040	-2.2727670	0.0000000
C	-2.3518950	-3.3354550	0.0000000
C	-1.7271710	2.6342320	0.0000000
C	-2.3338780	3.6944800	0.0000000
Si	-3.2460560	-4.9553580	0.0000000
Si	-3.2499650	5.3108620	0.0000000
C	-2.7501380	-5.9042960	1.5424880
H	-3.2565210	-6.8754060	1.5644550
H	-1.6710780	-6.0836920	1.5654960
H	-3.0253930	-5.3573410	2.4491800
C	-5.0907010	-4.6079750	0.0000000
H	-5.3860900	-4.0386860	-0.8864730
H	-5.6502310	-5.5495710	0.0000000
H	-5.3860900	-4.0386860	0.8864730
C	-2.7501380	-5.9042960	-1.5424880
H	-3.0253930	-5.3573410	-2.4491800
H	-1.6710780	-6.0836920	-1.5654960
H	-3.2565210	-6.8754060	-1.5644550
C	-5.0873430	4.9368330	0.0000000
H	-5.3737430	4.3633380	-0.8866040
H	-5.3737430	4.3633380	0.8866040
H	-5.6603150	5.8701630	0.0000000
C	-2.7501380	6.2477300	1.5465960
H	-3.0136910	5.6897030	2.4499010
H	-1.6728690	6.4377050	1.5626400
H	-3.2661940	7.2131500	1.5811510
C	-2.7501380	6.2477300	-1.5465960
H	-1.6728690	6.4377050	-1.5626400
H	-3.0136910	5.6897030	-2.4499010
H	-3.2661940	7.2131500	-1.5811510
S	3.6235470	1.5211920	0.0000000

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