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Supporting information available for

ESIPT Emission Behavior of Methoxy-Substituted 2-Hydroxyphenylbenzimidazole Isomers

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S1. NMR spectra

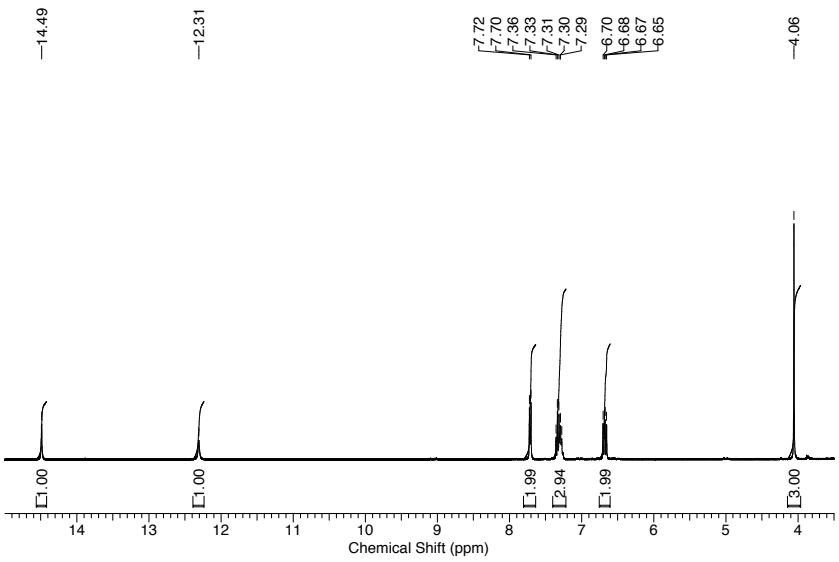

Figure S1. NMR spectra of **1** in DMSO-d_6.

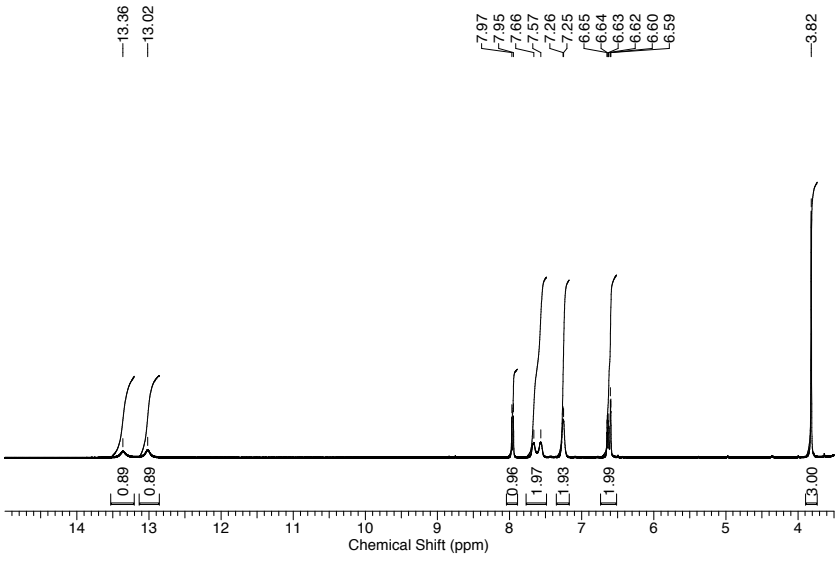

Figure S2. NMR spectra of **2** in DMSO-d_6.

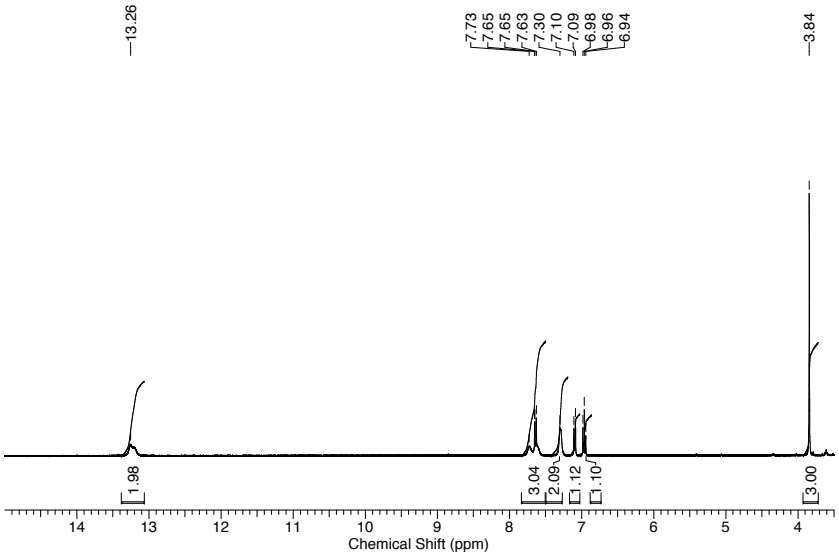

Figure S3. NMR spectra of **3** in DMSO-d_6.

S2. Optical properties

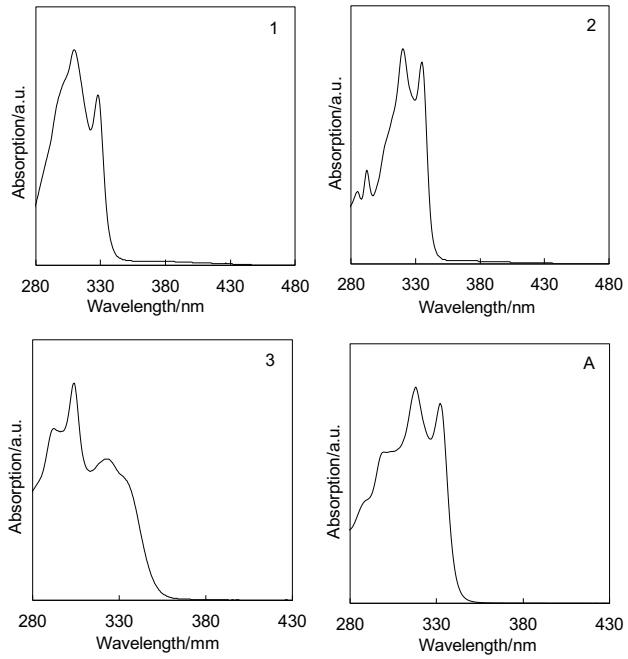

Figure S4. UV-vis absorption spectrum of **1**, **2**, **3**, and **A** in THF (10 μM).

Table S1. Absorption characteristics in THF (10 μM).

	λ_{ab}/nm	$\varepsilon/M^{-1}\cdot cm^{-1}$
1	307	27700
2	320	19300
3	304	32000
A	318	30100

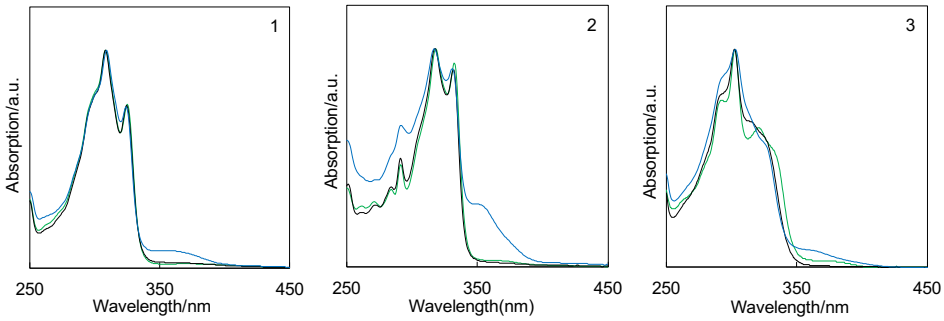

Figure S5. UV-vis absorption spectrum of **1**, **2**, and **3** in MeCN (black line), MeOH (green line), and THF/water mixed solvent in the volume ratio of 1/9 (blue line) (10 μM).

Table S2. Emission characteristics of **1** in various solvents (10 μM).

	λ_{em}/nm	Φ[a]	LE/ESIPT[b]	Stokes shift[c]/cm^{-1}
THF	458	0.31	0/1	10400
MeCN	456	0.27	0/1	10400
MeOH	446	0.30	0/1	10000
T1W9[d]	446	0.28	0/1	9900

[a] Calculated based on quinine sulfate as a standard (0.55).
[b] Relative peak intensity of LE and ESIPT emission.
[c] Calculated for ESIPT emission.
[d] THF/water mixed solvent in the volume ratio of 1/9.

Table S3. Emission characteristics of **2** in various solvents (10 μM).

	λ_{em}/nm	Φ[a]	LE/ESIPT[b]	Stokes shift[c]/cm^{-1}
THF	450	0.17	0/1	9300
MeCN	444	0.21	0/1	8900
MeOH	351, 433	0.21	0.29/1	8200
T1W9[d]	353, 419	0.37	1.89/1	7700

[a] Calculated based on quinine sulfate as a standard (0.55).
[b] Relative peak intensity of LE and ESIPT emission.
[c] Calculated for ESIPT emission.
[d] THF/water mixed solvent in the volume ratio of 1/9.

Table S4. Emission characteristics of **3** in various solvents (10 μM).

	λ_{em}/nm	Φ[a]	LE/ESIPT[b]	Stokes shift[c]/cm^{-1}
THF	345, 486	0.04	0.91/1	12300
MeCN	345, 433	0.06	0.34/1	9900
MeOH	359, 462	0.10	3.23/1	11500
T1W9[d]	354, 431	0.08	0.08/1	9800

[a] Calculated based on quinine sulfate as a standard (0.55).
[b] Relative peak intensity of LE and ESIPT emission.
[c] Calculated for ESIPT emission.
[d] THF/water mixed solvent in the volume ratio of 1/9.

S3. Computational results

Table S5. TDDFT calculations for the excitation energies (EE in eV), absorption wavelengths (Abs in nm), and oscillator strengths (*f*) of **1**, **2**, and **3** in several solvents.

	THF			MeCN			MeOH			H_2O		
State	EE/eV	Abs/nm	*f*	EE/eV	Abs/nm	*f*	EE/eV	Abs/nm	*f*	EE/eV	Abs/nm	*f*
1												
$1^1A'$	4.068	305	0.688	4.088	303	0.677	4.091	303	0.665	4.092	303	0.672
$2^1A'$	4.236	293	0.265	4.227	293	0.252	4.229	293	0.256	4.226	293	0.251
$3^1A'$	4.698	264	0.028	4.700	264	0.027	4.701	264	0.027	4.701	264	0.027
$4^1A'$	5.270	235	0.032	5.277	235	0.032	5.277	235	0.032	5.278	235	0.032
$5^1A'$	5.488	226	0.021	5.492	226	0.019	5.492	226	0.019	5.492	226	0.019
$1^1A''$	5.506	225	0.001	5.543	224	0.001	5.542	224	0.001	5.547	224	0.001
2												
$1^1A'$	3.973	312	0.949	3.992	311	0.932	3.994	310	0.926	3.995	310	0.929
$2^1A'$	4.607	269	0.077	4.613	269	0.074	4.613	269	0.074	4.613	269	0.074
$3^1A'$	4.784	259	0.065	4.785	259	0.061	4.786	259	0.061	4.786	259	0.060
$4^1A'$	5.077	244	0.052	5.091	244	0.053	5.092	243	0.052	5.094	243	0.053
$5^1A'$	5.275	235	0.105	5.278	235	0.100	5.279	235	0.099	5.279	235	0.099
$1^1A''$	5.275	235	0.001	5.329	233	0.002	5.328	233	0.002	5.335	232	0.002
3												
$1^1A'$	3.890	319	0.346	3.912	317	0.327	3.913	317	0.323	3.916	317	0.324
$2^1A'$	4.289	289	0.601	4.296	289	0.597	4.298	288	0.594	4.297	289	0.595
$3^1A'$	4.703	264	0.052	4.700	264	0.050	4.701	264	0.050	4.700	264	0.050
$4^1A'$	5.196	239	0.023	5.218	238	0.021	5.218	238	0.020	5.221	237	0.020
$5^1A'$	5.365	231	0.070	5.381	230	0.052	5.381	230	0.052	5.384	230	0.050
$1^1A''$	5.365	231	0.001	5.407	229	0.001	5.407	229	0.001	5.411	229	0.001

Table S6. DFT/TDDFT calculations for emission energy (EmE in eV) and fluorescence wavelength (Flu in nm) of **1**, **2**, and **3** in several solvents.

Solvent	**1** (keto)		**2** (enol)		**2** (keto)		**3** (keto)	
	EmE/eV	Flu/nm	EmE/eV	Flu/nm	EmE/eV	Flu/nm	EmE/eV	Flu/nm
THF	2.851	435	3.413	363	2.995	414	2.572	482
MeCN	2.821	439	3.360	369	2.978	426	2.530	490
MeOH	2.820	440	3.362	369	2.978	416	2.529	490
H_2O	2.817	440	3.353	370	2.977	416	2.525	491

Table S7. Activation energy (ΔE_a) and heat of reaction (ΔH) for ESIPT reaction of **2** in kcal·mol^{-1}.

Solvent	ΔE_a	ΔH
THF	2.27	4.25
MeCN	2.36	4.14
MeOH	2.36	4.14
H_2O	2.37	4.13

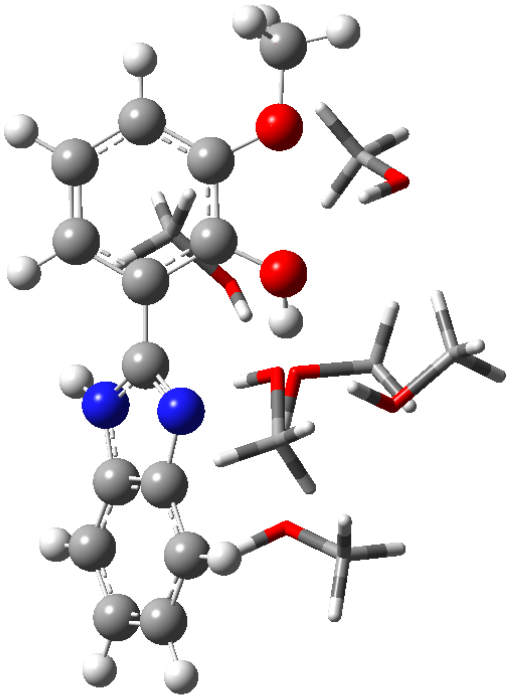

Figure S6. A typical solvation structure of **3** with six MeOH molecules in ground state optimized by ωB97XD/6-31G(d,p) in PCM (methanol).

Cartesian Coordinates

Optimized geometries of **1** in the ground state in THF (angstrom)

C	2.17660	0.70654	-0.00003
C	2.26057	-0.70360	0.00001
C	3.51018	-1.33361	0.00004
C	4.64142	-0.52514	0.00002
C	4.54221	0.88017	-0.00002
C	3.30768	1.52284	-0.00005
N	0.82961	0.98493	-0.00005
C	0.15369	-0.20058	-0.00003
N	0.99069	-1.23635	0.00002
H	3.58819	-2.42127	0.00007
H	5.63001	-0.98667	0.00005
H	5.45426	1.47881	-0.00003
H	3.23338	2.61051	-0.00008
H	0.36947	1.88505	-0.00008
C	-1.29165	-0.35938	-0.00002
C	-1.82910	-1.67371	-0.00003
C	-2.19469	0.73364	0.00002
C	-3.21569	-1.87301	0.00002
C	-3.57146	0.52921	0.00006
C	-4.06463	-0.77913	0.00006
H	-3.59615	-2.89396	0.00001
H	-4.26390	1.36688	0.00009
H	-5.14445	-0.93631	0.00010
O	-1.04359	-2.75766	-0.00011
H	-0.08924	-2.44119	-0.00020
O	-1.63345	1.97254	0.00002
C	-2.49495	3.10330	0.00007
H	-3.12564	3.11791	-0.90013
H	-3.12559	3.11787	0.90031
H	-1.83726	3.97818	0.00007

Optimized geometries of **1** in the ground state in MeCN (angstrom)

C	2.17583	0.70565	-0.00001
C	2.26014	-0.70449	-0.00003
C	3.50998	-1.33451	-0.00005
C	4.64103	-0.52525	-0.00005
C	4.54125	0.88041	-0.00003
C	3.30643	1.52282	-0.00001
N	0.82921	0.98459	0.00001
C	0.15316	-0.20009	0.00000
N	0.98994	-1.23711	-0.00002
H	3.58946	-2.42209	-0.00006
H	5.62978	-0.98637	-0.00007
H	5.45308	1.47929	-0.00003
H	3.23009	2.61020	0.00001
H	0.37158	1.88624	0.00003
C	-1.29208	-0.35958	0.00001
C	-1.83019	-1.67334	0.00000
C	-2.19458	0.73431	0.00002
C	-3.21624	-1.87306	0.00000
C	-3.57185	0.52990	0.00002
C	-4.06512	-0.77816	0.00001
H	-3.59852	-2.89341	0.00000
H	-4.26391	1.36783	0.00003
H	-5.14491	-0.93515	0.00001
O	-1.04267	-2.75807	0.00000
H	-0.08808	-2.43990	0.00001
O	-1.63235	1.97090	0.00003
C	-2.49114	3.10530	0.00004
H	-3.12120	3.12099	-0.90018
H	-3.12119	3.12097	0.90027
H	-1.82985	3.97705	0.00005

Optimized geometries of **1** in the ground state in MeOH (angstrom)

C	2.17585	0.70577	-0.00002
C	2.26027	-0.70445	-0.00001
C	3.51027	-1.33424	-0.00001
C	4.64125	-0.52501	-0.00001
C	4.54138	0.88057	-0.00002
C	3.30655	1.52285	-0.00003
N	0.82918	0.98444	-0.00002
C	0.15325	-0.20025	-0.00001
N	0.99004	-1.23707	-0.00001
H	3.58945	-2.42191	0.00000
H	5.63006	-0.98612	-0.00001
H	5.45319	1.47958	-0.00003
H	3.22996	2.61028	-0.00003
H	0.37080	1.88586	-0.00002
C	-1.29218	-0.35944	-0.00001
C	-1.82981	-1.67334	-0.00001
C	-2.19480	0.73440	0.00002
C	-3.21601	-1.87310	0.00001
C	-3.57202	0.52947	0.00004
C	-4.06521	-0.77857	0.00004
H	-3.59763	-2.89375	0.00001
H	-4.26402	1.36756	0.00006
H	-5.14501	-0.93573	0.00006
O	-1.04230	-2.75774	-0.00006
H	-0.08806	-2.43953	-0.00010
O	-1.63289	1.97090	0.00003
C	-2.49165	3.10505	0.00006
H	-3.12199	3.12075	-0.90015
H	-3.12197	3.12072	0.90028
H	-1.83056	3.97707	0.00006

Optimized geometries of **1** in the ground state in H2O (angstrom)

C	2.17574	0.70551	-0.00002
C	2.26033	-0.70470	-0.00002
C	3.51046	-1.33439	-0.00002
C	4.64135	-0.52489	-0.00002
C	4.54123	0.88076	-0.00002
C	3.30627	1.52287	-0.00002
N	0.82917	0.98422	-0.00001
C	0.15319	-0.20024	-0.00001
N	0.99000	-1.23729	-0.00001
H	3.59001	-2.42205	-0.00002
H	5.63024	-0.98583	-0.00003
H	5.45294	1.47992	-0.00003
H	3.22893	2.61023	-0.00002
H	0.37129	1.88601	-0.00001
C	-1.29229	-0.35949	0.00000
C	-1.83010	-1.67328	-0.00001
C	-2.19482	0.73455	0.00002
C	-3.21623	-1.87303	0.00001
C	-3.57215	0.52968	0.00004
C	-4.06541	-0.77827	0.00003
H	-3.59825	-2.89357	0.00000
H	-4.26400	1.36791	0.00005
H	-5.14522	-0.93534	0.00005
O	-1.04224	-2.75787	-0.00004
H	-0.08799	-2.43924	-0.00006
O	-1.63276	1.97053	0.00003
C	-2.49097	3.10537	0.00005
H	-3.12124	3.12128	-0.90015
H	-3.12122	3.12126	0.90027
H	-1.82914	3.97677	0.00006

Optimized geometries of **1** in the S1 state in THF (angstrom)

C	2.19328	0.68679	-0.00041
C	2.31388	-0.72454	0.00024
C	3.56464	-1.34589	0.00051
C	4.69089	-0.50760	0.00010
C	4.57096	0.88501	-0.00054
C	3.31460	1.51497	-0.00082
N	0.84733	0.95987	-0.00054
C	0.11690	-0.20789	0.00001
N	1.04053	-1.22326	0.00056
H	3.65949	-2.43117	0.00100
H	5.68506	-0.95712	0.00030
H	5.47232	1.49953	-0.00085
H	3.22191	2.60059	-0.00136
H	0.40541	1.86756	-0.00064
C	-1.30113	-0.36254	-0.00003
C	-1.87662	-1.71365	-0.00001
C	-2.19201	0.71741	-0.00005
C	-3.29957	-1.85903	-0.00010
C	-3.60663	0.52642	-0.00028
C	-4.15401	-0.75155	-0.00029
H	-3.68622	-2.87877	-0.00013
H	-4.26485	1.39231	-0.00050
H	-5.23600	-0.87885	-0.00044
O	-1.12227	-2.73475	0.00006
H	0.70013	-2.18391	0.00058
O	-1.64426	1.96273	-0.00006
C	-2.49583	3.10269	0.00122
H	-3.12462	3.12928	-0.89984
H	-3.12421	3.12754	0.90262
H	-1.82732	3.96925	0.00188

Optimized geometries of **1** in the S1 state in MeCN (angstrom)

C	2.19073	0.68416	-0.00035
C	2.31319	-0.72776	0.00018
C	3.56446	-1.34720	0.00041
C	4.68969	-0.50805	0.00008
C	4.56787	0.88545	-0.00044
C	3.31140	1.51342	-0.00068
N	0.84607	0.95673	-0.00049
C	0.11487	-0.21211	-0.00003
N	1.04075	-1.22808	0.00045
H	3.66042	-2.43243	0.00081
H	5.68437	-0.95649	0.00024
H	5.46851	1.50108	-0.00068
H	3.21558	2.59874	-0.00110
H	0.40448	1.86512	-0.00054
C	-1.29979	-0.36374	-0.00004
C	-1.88222	-1.71489	0.00000
C	-2.19011	0.72128	-0.00006
C	-3.30581	-1.85607	-0.00004
C	-3.60081	0.53244	-0.00022
C	-4.15500	-0.74644	-0.00018
H	-3.69664	-2.87442	-0.00003
H	-4.25738	1.39978	-0.00041
H	-5.23758	-0.86805	-0.00028
O	-1.12954	-2.73745	0.00003
H	0.70653	-2.18997	0.00044
O	-1.63620	1.96383	-0.00012
C	-2.48394	3.10716	0.00109
H	-3.11285	3.13492	-0.89980
H	-3.11242	3.13331	0.90232
H	-1.81216	3.97100	0.00168

Optimized geometries of **1** in the S1 state in MeOH (angstrom)

C	2.19089	0.68413	-0.00029
C	2.31329	-0.72774	0.00011
C	3.56449	-1.34729	0.00027
C	4.68979	-0.50822	0.00001
C	4.56805	0.88528	-0.00038
C	3.31163	1.51331	-0.00054
N	0.84617	0.95668	-0.00037
C	0.11485	-0.21215	-0.00002
N	1.04077	-1.22801	0.00031
H	3.66021	-2.43253	0.00056
H	5.68451	-0.95659	0.00013
H	5.46880	1.50076	-0.00056
H	3.21585	2.59863	-0.00086
H	0.40431	1.86497	-0.00041
C	-1.29996	-0.36364	-0.00002
C	-1.88237	-1.71489	-0.00001
C	-2.19029	0.72131	-0.00001
C	-3.30601	-1.85625	-0.00003
C	-3.60102	0.53230	-0.00013
C	-4.15513	-0.74667	-0.00012
H	-3.69687	-2.87457	-0.00004
H	-4.25792	1.39934	-0.00025
H	-5.23773	-0.86827	-0.00018
O	-1.12961	-2.73738	0.00000
H	0.70641	-2.18987	0.00032
O	-1.63628	1.96406	-0.00005
C	-2.48367	3.10765	0.00091
H	-3.11251	3.13560	-0.90001
H	-3.11214	3.13434	0.90213
H	-1.81153	3.97121	0.00136

Optimized geometries of **1** in the S1 state in H2O (angstrom)

C	2.19038	0.68362	-0.00024
C	2.31319	-0.72836	0.00005
C	3.56453	-1.34748	0.00016
C	4.68956	-0.50812	-0.00004
C	4.56737	0.88556	-0.00032
C	3.31089	1.51313	-0.00043
N	0.84594	0.95607	-0.00029
C	0.11450	-0.21298	-0.00002
N	1.04085	-1.22898	0.00023
H	3.66053	-2.43270	0.00038
H	5.68441	-0.95621	0.00003
H	5.46794	1.50131	-0.00047
H	3.21421	2.59837	-0.00066
H	0.40425	1.86454	-0.00031
C	-1.29963	-0.36389	-0.00001
C	-1.88332	-1.71517	0.00000
C	-2.18990	0.72203	0.00000
C	-3.30709	-1.85573	0.00000
C	-3.59984	0.53348	-0.00008
C	-4.15520	-0.74572	-0.00007
H	-3.69881	-2.87376	-0.00001
H	-4.25636	1.40085	-0.00018
H	-5.23791	-0.86628	-0.00011
O	-1.13080	-2.73787	0.00000
H	0.70771	-2.19109	0.00022
O	-1.63484	1.96425	-0.00004
C	-2.48179	3.10824	0.00079
H	-3.11066	3.13612	-0.90011
H	-3.11033	3.13505	0.90195
H	-1.80928	3.97147	0.00117

Optimized geometries of **2** in the ground state in THF (angstrom)

C	2.81295	-0.77820	0.00005
C	2.66267	0.62602	-0.00003
C	3.79112	1.45199	-0.00008
C	5.04110	0.84080	-0.00004
C	5.17436	-0.56052	0.00004
C	4.06126	-1.39768	0.00008
N	1.52675	-1.27545	0.00006
C	0.66627	-0.21329	0.00002
N	1.32036	0.94333	-0.00005
H	3.68870	2.53762	-0.00014
H	5.93992	1.45919	-0.00008
H	6.17209	-1.00164	0.00006
H	4.16615	-2.48298	0.00014
H	1.26870	-2.25096	0.00017
C	-0.77964	-0.30648	0.00002
C	-1.54925	0.88178	0.00001
C	-1.46348	-1.53585	0.00001
C	-2.94884	0.82186	-0.00001
C	-2.84179	-1.60581	-0.00001
H	-0.90062	-2.47075	0.00000
C	-3.59080	-0.41401	-0.00002
H	-3.49545	1.76250	-0.00001
H	-3.36193	-2.56288	-0.00003
O	-0.98156	2.09586	0.00004
H	0.01076	1.96117	0.00010
O	-4.93387	-0.56797	-0.00004
C	-5.73768	0.60259	-0.00004
H	-6.77499	0.25343	-0.00006
H	-5.55460	1.20887	0.89946
H	-5.55458	1.20888	-0.89954

Optimized geometries of **2** in the ground state in MeCN (angstrom)

C	2.81257	-0.77806	0.00005
C	2.66275	0.62639	-0.00002
C	3.79119	1.45281	-0.00003
C	5.04143	0.84134	0.00002
C	5.17431	-0.56041	0.00008
C	4.06117	-1.39780	0.00009
N	1.52709	-1.27548	0.00002
C	0.66661	-0.21444	-0.00002
N	1.32007	0.94337	-0.00006
H	3.68932	2.53862	-0.00008
H	5.94030	1.45969	0.00001
H	6.17196	-1.00179	0.00012
H	4.16520	-2.48301	0.00014
H	1.27022	-2.25189	0.00020
C	-0.77990	-0.30749	-0.00003
C	-1.54940	0.88083	-0.00004
C	-1.46378	-1.53704	-0.00003
C	-2.94904	0.82233	-0.00002
C	-2.84231	-1.60583	-0.00002
H	-0.90131	-2.47187	-0.00004
C	-3.59114	-0.41380	-0.00001
H	-3.49618	1.76279	-0.00002
H	-3.36199	-2.56325	-0.00002
O	-0.97966	2.09532	-0.00006
H	0.01288	1.95849	-0.00009
O	-4.93417	-0.56718	0.00001
C	-5.73837	0.60395	0.00002
H	-6.77560	0.25490	0.00004
H	-5.55535	1.21018	0.89940
H	-5.55538	1.21018	-0.89936

Optimized geometries of **2** in the ground state in MeOH (angstrom)

C	2.81262	-0.77801	0.00005
C	2.66274	0.62640	-0.00003
C	3.79121	1.45276	-0.00008
C	5.04130	0.84130	-0.00003
C	5.17423	-0.56038	0.00005
C	4.06114	-1.39774	0.00009
N	1.52697	-1.27554	0.00006
C	0.66656	-0.21454	0.00001
N	1.32011	0.94328	-0.00006
H	3.68948	2.53855	-0.00015
H	5.94019	1.45961	-0.00007
H	6.17193	-1.00161	0.00008
H	4.16511	-2.48298	0.00016
H	1.27018	-2.25183	0.00022
C	-0.77976	-0.30739	0.00000
C	-1.54925	0.88078	0.00000
C	-1.46370	-1.53684	-0.00002
C	-2.94875	0.82237	-0.00001
C	-2.84226	-1.60564	-0.00003
H	-0.90123	-2.47175	-0.00003
C	-3.59118	-0.41369	-0.00002
H	-3.49576	1.76284	-0.00001
H	-3.36186	-2.56307	-0.00004
O	-0.97951	2.09519	0.00003
H	0.01298	1.95746	0.00006
O	-4.93416	-0.56711	-0.00003
C	-5.73885	0.60389	-0.00002
H	-6.77597	0.25443	-0.00003
H	-5.55574	1.20989	0.89946
H	-5.55573	1.20990	-0.89950

Optimized geometries of **2** in the ground state in H2O (angstrom)

C	2.81263	-0.77791	0.00005
C	2.66249	0.62649	-0.00003
C	3.79093	1.45304	-0.00008
C	5.04109	0.84165	-0.00004
C	5.17419	-0.56010	0.00004
C	4.06121	-1.39761	0.00009
N	1.52705	-1.27575	0.00007
C	0.66657	-0.21518	0.00002
N	1.31980	0.94307	-0.00005
H	3.68932	2.53886	-0.00015
H	5.93994	1.46004	-0.00008
H	6.17199	-1.00112	0.00007
H	4.16501	-2.48284	0.00015
H	1.27077	-2.25225	0.00018
C	-0.77975	-0.30780	0.00001
C	-1.54917	0.88041	0.00001
C	-1.46382	-1.53722	0.00000
C	-2.94861	0.82230	-0.00001
C	-2.84243	-1.60575	-0.00002
H	-0.90152	-2.47221	-0.00001
C	-3.59133	-0.41376	-0.00002
H	-3.49575	1.76273	-0.00001
H	-3.36184	-2.56330	-0.00003
O	-0.97899	2.09497	0.00004
H	0.01374	1.95710	0.00008
O	-4.93418	-0.56681	-0.00004
C	-5.73868	0.60478	-0.00004
H	-6.77580	0.25545	-0.00004
H	-5.55520	1.21047	0.89951
H	-5.55519	1.21048	-0.89957

Optimized geometries of **2** in the S1 state keto form in THF (angstrom)

C	2.82127	-0.76990	0.00006
C	2.72063	0.64509	-0.00004
C	3.86235	1.45372	-0.00009
C	5.10043	0.79819	-0.00004
C	5.19799	-0.59900	0.00006
C	4.05639	-1.41594	0.00012
N	1.53229	-1.24772	0.00008
C	0.63385	-0.20400	0.00003
N	1.38827	0.93903	-0.00006
H	3.78887	2.54038	-0.00016
H	6.01429	1.39425	-0.00008
H	6.18413	-1.06514	0.00010
H	4.13184	-2.50290	0.00020
H	1.27539	-2.22340	0.00021
C	-0.78728	-0.29328	-0.00001
C	-1.58947	0.94577	0.00000
C	-1.46632	-1.51534	-0.00005
C	-3.00952	0.84012	-0.00002
C	-2.87616	-1.57673	-0.00004
H	-0.91912	-2.45887	-0.00008
C	-3.64643	-0.40818	-0.00003
H	-3.56144	1.77835	-0.00001
H	-3.38042	-2.54351	-0.00005
O	-1.01012	2.07476	0.00002
H	0.89982	1.83463	-0.00008
O	-4.99549	-0.58368	-0.00002
C	-5.80639	0.57881	0.00001
H	-6.84213	0.22387	0.00001
H	-5.62912	1.18921	0.89874
H	-5.62913	1.18925	-0.89870

Optimized geometries of **2** in the S1 state keto form in MeCN (angstrom)

C	2.81810	-0.77028	0.00006
C	2.72094	0.64648	-0.00004
C	3.86449	1.45217	-0.00009
C	5.10084	0.79424	-0.00004
C	5.19506	-0.60448	0.00007
C	4.05256	-1.41864	0.00012
N	1.53037	-1.24552	0.00008
C	0.63203	-0.19937	0.00003
N	1.39056	0.94399	-0.00007
H	3.79277	2.53896	-0.00017
H	6.01612	1.38814	-0.00008
H	6.18029	-1.07264	0.00011
H	4.12488	-2.50572	0.00021
H	1.27314	-2.22154	0.00023
C	-0.78495	-0.28888	-0.00001
C	-1.59179	0.95107	0.00000
C	-1.46328	-1.51588	-0.00006
C	-3.01159	0.84221	-0.00001
C	-2.86951	-1.57661	-0.00005
H	-0.91434	-2.45804	-0.00010
C	-3.64363	-0.40664	-0.00003
H	-3.56709	1.77844	0.00000
H	-3.37318	-2.54390	-0.00007
O	-1.01314	2.08007	0.00002
H	0.90911	1.84241	-0.00009
O	-4.99213	-0.58853	-0.00002
C	-5.80866	0.57081	0.00001
H	-6.84283	0.21155	0.00002
H	-5.63348	1.18175	0.89865
H	-5.63350	1.18179	-0.89860

Optimized geometries of **2** in the S1 state keto form in MeOH (angstrom)

C	2.81810	-0.77028	0.00006
C	2.72094	0.64648	-0.00004
C	3.86449	1.45217	-0.00009
C	5.10084	0.79424	-0.00004
C	5.19506	-0.60448	0.00007
C	4.05256	-1.41864	0.00012
N	1.53037	-1.24552	0.00008
C	0.63203	-0.19937	0.00003
N	1.39056	0.94399	-0.00007
H	3.79277	2.53896	-0.00017
H	6.01612	1.38814	-0.00008
H	6.18029	-1.07264	0.00011
H	4.12488	-2.50572	0.00021
H	1.27314	-2.22154	0.00023
C	-0.78495	-0.28888	-0.00001
C	-1.59179	0.95107	0.00000
C	-1.46328	-1.51588	-0.00006
C	-3.01159	0.84221	-0.00001
C	-2.86951	-1.57661	-0.00005
H	-0.91434	-2.45804	-0.00010
C	-3.64363	-0.40664	-0.00003
H	-3.56709	1.77844	0.00000
H	-3.37318	-2.54390	-0.00007
O	-1.01314	2.08007	0.00002
H	0.90911	1.84241	-0.00009
O	-4.99213	-0.58853	-0.00002
C	-5.80866	0.57081	0.00001
H	-6.84283	0.21155	0.00002
H	-5.63348	1.18175	0.89865
H	-5.63350	1.18179	-0.89860

Optimized geometries of **2** in the S1 state keto form in H2O (angstrom)

C	2.81742	-0.77050	0.00006
C	2.72048	0.64660	-0.00004
C	3.86416	1.45224	-0.00008
C	5.10030	0.79420	-0.00003
C	5.19436	-0.60485	0.00006
C	4.05204	-1.41895	0.00011
N	1.53015	-1.24567	0.00008
C	0.63160	-0.19924	0.00002
N	1.39045	0.94436	-0.00006
H	3.79218	2.53901	-0.00015
H	6.01579	1.38779	-0.00007
H	6.17966	-1.07286	0.00010
H	4.12403	-2.50602	0.00019
H	1.27296	-2.22179	0.00020
C	-0.78466	-0.28869	-0.00001
C	-1.59163	0.95182	0.00000
C	-1.46315	-1.51654	-0.00004
C	-3.01146	0.84281	-0.00002
C	-2.86854	-1.57676	-0.00004
H	-0.91370	-2.45832	-0.00007
C	-3.64283	-0.40598	-0.00002
H	-3.56748	1.77876	-0.00001
H	-3.37324	-2.54356	-0.00005
O	-1.01243	2.08048	0.00000
H	0.90931	1.84293	-0.00008
O	-4.99127	-0.58878	-0.00002
C	-5.80871	0.57006	0.00001
H	-6.84262	0.21011	0.00001
H	-5.63386	1.18109	0.89863
H	-5.63388	1.18112	-0.89860

Optimized geometries of **2** in the S1 state enol form in THF (angstrom)

C	2.80553	-0.79289	0.00003
C	2.64136	0.64062	-0.00002
C	3.78928	1.47329	-0.00004
C	5.03263	0.85400	0.00001
C	5.17180	-0.55329	0.00006
C	4.05751	-1.40405	0.00007
N	1.53954	-1.29868	0.00001
C	0.63917	-0.23187	-0.00001
N	1.33780	0.95481	-0.00005
H	3.68688	2.55818	-0.00007
H	5.93538	1.46752	0.00000
H	6.17319	-0.98641	0.00009
H	4.16719	-2.48834	0.00011
H	1.29740	-2.27796	0.00018
C	-0.75326	-0.32749	-0.00001
C	-1.55706	0.89490	-0.00003
C	-1.46529	-1.57386	0.00000
C	-2.94292	0.84406	-0.00002
C	-2.84381	-1.60308	0.00001
H	-0.91555	-2.51477	-0.00001
C	-3.59383	-0.40138	0.00000
H	-3.48572	1.78699	-0.00004
H	-3.38407	-2.55037	0.00002
O	-0.96039	2.08291	-0.00005
H	0.04061	1.93031	-0.00007
O	-4.93585	-0.55603	0.00001
C	-5.74480	0.61027	0.00001
H	-6.78061	0.25702	0.00002
H	-5.56194	1.21730	0.89952
H	-5.56196	1.21727	-0.89953

Optimized geometries of **2** in the S1 state enol form in MeCN (angstrom)

C	2.80485	-0.79339	0.00004
C	2.64109	0.64119	-0.00002
C	3.78974	1.47383	-0.00005
C	5.03306	0.85397	-0.00001
C	5.17154	-0.55385	0.00005
C	4.05717	-1.40470	0.00008
N	1.54005	-1.29898	0.00002
C	0.63855	-0.23262	0.00001
N	1.33858	0.95568	-0.00004
H	3.68824	2.55891	-0.00010
H	5.93614	1.46707	-0.00003
H	6.17289	-0.98715	0.00008
H	4.16597	-2.48892	0.00013
H	1.29936	-2.27904	0.00020
C	-0.75262	-0.32709	0.00000
C	-1.55746	0.89509	-0.00002
C	-1.46573	-1.57409	0.00000
C	-2.94247	0.84408	-0.00002
C	-2.84328	-1.60375	0.00000
H	-0.91563	-2.51468	-0.00001
C	-3.59408	-0.40173	-0.00001
H	-3.48657	1.78639	-0.00003
H	-3.38234	-2.55177	0.00000
O	-0.96015	2.08467	-0.00003
H	0.04003	1.93109	-0.00003
O	-4.93528	-0.55605	0.00000
C	-5.74635	0.61025	0.00000
H	-6.78148	0.25547	0.00001
H	-5.56375	1.21681	0.89960
H	-5.56376	1.21680	-0.89961

Optimized geometries of **2** in the S1 state enol form in MeOH (angstrom)

C	2.80496	-0.79334	0.00003
C	2.64128	0.64109	-0.00002
C	3.79001	1.47360	-0.00005
C	5.03324	0.85357	-0.00001
C	5.17162	-0.55421	0.00005
C	4.05711	-1.40490	0.00007
N	1.53993	-1.29857	0.00003
C	0.63856	-0.23213	0.00001
N	1.33873	0.95586	-0.00004
H	3.68855	2.55866	-0.00009
H	5.93640	1.46654	-0.00003
H	6.17292	-0.98764	0.00007
H	4.16581	-2.48913	0.00012
H	1.29905	-2.27854	0.00017
C	-0.75267	-0.32670	0.00000
C	-1.55768	0.89531	-0.00002
C	-1.46558	-1.57380	0.00000
C	-2.94275	0.84414	-0.00002
C	-2.84313	-1.60365	0.00000
H	-0.91558	-2.51444	0.00000
C	-3.59407	-0.40180	-0.00001
H	-3.48682	1.78642	-0.00003
H	-3.38206	-2.55173	0.00001
O	-0.96057	2.08506	-0.00003
H	0.03955	1.93237	-0.00002
O	-4.93528	-0.55649	0.00000
C	-5.74632	0.60964	-0.00001
H	-6.78133	0.25452	-0.00001
H	-5.56388	1.21626	0.89960
H	-5.56389	1.21624	-0.89964

Optimized geometries of **2** in the S1 state enol form in H2O (angstrom)

C	2.80484	-0.79343	0.00004
C	2.64108	0.64119	-0.00002
C	3.78979	1.47385	-0.00004
C	5.03315	0.85387	0.00000
C	5.17158	-0.55398	0.00006
C	4.05718	-1.40484	0.00008
N	1.54015	-1.29883	0.00002
C	0.63836	-0.23262	0.00000
N	1.33862	0.95574	-0.00004
H	3.68840	2.55894	-0.00009
H	5.93627	1.46691	-0.00002
H	6.17293	-0.98731	0.00009
H	4.16586	-2.48904	0.00013
H	1.29974	-2.27900	0.00019
C	-0.75264	-0.32704	-0.00001
C	-1.55759	0.89522	-0.00003
C	-1.46589	-1.57412	-0.00001
C	-2.94255	0.84420	-0.00002
C	-2.84330	-1.60378	0.00000
H	-0.91598	-2.51478	-0.00002
C	-3.59414	-0.40171	-0.00001
H	-3.48676	1.78644	-0.00003
H	-3.38219	-2.55190	0.00000
O	-0.95994	2.08487	-0.00004
H	0.04023	1.93127	-0.00005
O	-4.93524	-0.55613	0.00000
C	-5.74640	0.61016	0.00000
H	-6.78136	0.25499	0.00002
H	-5.56390	1.21668	0.89963
H	-5.56392	1.21667	-0.89963

Optimized geometries of **2** in the S1 state TS in THF (angstrom)

C	2.82251	0.79016	0.00003
C	2.61398	-0.62997	-0.00005
C	3.71902	-1.50635	0.00003
C	4.98930	-0.93156	0.00021
C	5.18061	0.46396	0.00030
C	4.09723	1.35484	0.00020
N	1.57491	1.35191	-0.00008
C	0.63014	0.33769	-0.00022
N	1.28572	-0.86602	-0.00026
H	3.57710	-2.58644	-0.00006
H	5.86629	-1.58128	0.00028
H	6.19676	0.86088	0.00043
H	4.24433	2.43473	0.00026
H	1.37579	2.34091	-0.00009
C	-0.77000	0.41800	-0.00028
C	-1.51359	-0.86014	-0.00013
C	-1.51806	1.62380	-0.00025
C	-2.91569	-0.85404	0.00005
C	-2.90644	1.59110	-0.00013
H	-1.00845	2.58729	-0.00030
C	-3.60917	0.36119	0.00003
H	-3.42098	-1.81758	0.00018
H	-3.48435	2.51600	-0.00011
O	-0.84946	-1.97811	-0.00014
H	0.32929	-1.69164	-0.00057
O	-4.95935	0.47358	0.00018
C	-5.72331	-0.72126	0.00037
H	-6.77206	-0.40788	0.00047
H	-5.51857	-1.32221	-0.89876
H	-5.51835	-1.32207	0.89954

Optimized geometries of **2** in the S1 state TS in MeCN (angstrom)

C	2.82085	0.79119	-0.00004
C	2.61212	-0.63051	0.00005
C	3.71731	-1.50738	0.00004
C	4.98760	-0.93290	-0.00008
C	5.17899	0.46358	-0.00017
C	4.09641	1.35489	-0.00016
N	1.57532	1.35349	0.00001
C	0.62835	0.33982	0.00010
N	1.28525	-0.86598	0.00016
H	3.57512	-2.58748	0.00012
H	5.86472	-1.58245	-0.00009
H	6.19535	0.86004	-0.00026
H	4.24337	2.43456	-0.00023
H	1.37818	2.34336	-0.00008
C	-0.76928	0.41830	0.00010
C	-1.51273	-0.86088	0.00006
C	-1.51925	1.62608	0.00006
C	-2.91381	-0.85431	0.00001
C	-2.90545	1.59283	0.00002
H	-1.00875	2.58895	0.00006
C	-3.60775	0.36127	-0.00001
H	-3.42083	-1.81710	-0.00003
H	-3.48389	2.51748	-0.00001
O	-0.84779	-1.97999	0.00007
H	0.33265	-1.69108	0.00029
O	-4.95725	0.47259	-0.00006
C	-5.72235	-0.72275	-0.00009
H	-6.77076	-0.40867	-0.00013
H	-5.51731	-1.32314	-0.89928
H	-5.51738	-1.32315	0.89910

Optimized geometries of **2** in the S1 state TS in MeOH (angstrom)

C	2.82093	0.79113	0.00004
C	2.61233	-0.63055	-0.00006
C	3.71748	-1.50737	0.00002
C	4.98780	-0.93277	0.00021
C	5.17909	0.46364	0.00032
C	4.09643	1.35493	0.00022
N	1.57532	1.35338	-0.00008
C	0.62844	0.33969	-0.00023
N	1.28535	-0.86597	-0.00027
H	3.57552	-2.58749	-0.00008
H	5.86487	-1.58237	0.00028
H	6.19540	0.86025	0.00046
H	4.24335	2.43460	0.00029
H	1.37828	2.34327	-0.00008
C	-0.76926	0.41834	-0.00030
C	-1.51282	-0.86099	-0.00014
C	-1.51921	1.62603	-0.00027
C	-2.91398	-0.85437	0.00005
C	-2.90553	1.59269	-0.00015
H	-1.00898	2.58905	-0.00032
C	-3.60786	0.36119	0.00003
H	-3.42091	-1.81719	0.00019
H	-3.48378	2.51745	-0.00013
O	-0.84781	-1.97985	-0.00015
H	0.33322	-1.69087	-0.00058
O	-4.95745	0.47263	0.00019
C	-5.72269	-0.72261	0.00039
H	-6.77108	-0.40847	0.00050
H	-5.51785	-1.32314	-0.89876
H	-5.51762	-1.32298	0.89958

Optimized geometries of **2** in the S1 state TS in H2O (angstrom)

C	2.82065	0.79137	-0.00004
C	2.61184	-0.63057	0.00005
C	3.71700	-1.50758	0.00003
C	4.98734	-0.93320	-0.00008
C	5.17878	0.46341	-0.00016
C	4.09637	1.35483	-0.00014
N	1.57545	1.35381	0.00001
C	0.62811	0.34025	0.00010
N	1.28517	-0.86589	0.00016
H	3.57474	-2.58766	0.00010
H	5.86444	-1.58278	-0.00010
H	6.19519	0.85978	-0.00024
H	4.24340	2.43443	-0.00020
H	1.37868	2.34385	-0.00007
C	-0.76915	0.41844	0.00009
C	-1.51259	-0.86092	0.00006
C	-1.51949	1.62647	0.00004
C	-2.91351	-0.85433	0.00001
C	-2.90538	1.59308	0.00001
H	-1.00892	2.58928	0.00004
C	-3.60759	0.36127	-0.00001
H	-3.42073	-1.81704	-0.00002
H	-3.48388	2.51771	-0.00002
O	-0.84752	-1.98022	0.00006
H	0.33315	-1.69092	0.00029
O	-4.95701	0.47236	-0.00006
C	-5.72224	-0.72310	-0.00008
H	-6.77061	-0.40896	-0.00011
H	-5.51716	-1.32341	-0.89927
H	-5.51722	-1.32341	0.89912

Optimized geometries of **3** in the ground state in THF (angstrom)

C	-2.78551	0.68959	-0.00002
C	-2.46935	-0.68658	-0.00003
C	-3.49010	-1.64301	-0.00005
C	-4.80326	-1.18610	-0.00006
C	-5.10303	0.19020	-0.00005
C	-4.09976	1.15498	-0.00004
N	-1.56853	1.33622	-0.00001
C	-0.58832	0.38418	0.00001
N	-1.09930	-0.84102	-0.00001
H	-3.25763	-2.70831	-0.00006
H	-5.62202	-1.90700	-0.00008
H	-6.14654	0.50833	-0.00006
H	-4.33497	2.21936	-0.00003
H	-1.42925	2.33574	0.00000
C	0.84090	0.65314	0.00001
C	1.72883	-0.44228	0.00006
C	1.35326	1.96535	-0.00004
C	3.12493	-0.20421	0.00002
C	2.71761	2.18371	-0.00007
H	0.67723	2.82070	-0.00007
C	3.60763	1.09951	-0.00004
H	3.11010	3.20061	-0.00012
H	4.67971	1.28876	-0.00006
O	1.31518	-1.71615	0.00015
H	0.31465	-1.69870	0.00022
O	3.89478	-1.31980	0.00007
C	5.30028	-1.14035	0.00005
H	5.73094	-2.14681	0.00010
H	5.63411	-0.60021	-0.89922
H	5.63412	-0.60013	0.89926

Optimized geometries of **3** in the ground state in MeCN (angstrom)

C	-2.78531	0.68930	-0.00003
C	-2.46882	-0.68685	-0.00002
C	-3.48932	-1.64395	-0.00004
C	-4.80267	-1.18703	-0.00005
C	-5.10273	0.18961	-0.00005
C	-4.09976	1.15479	-0.00004
N	-1.56930	1.33691	-0.00001
C	-0.58878	0.38680	0.00001
N	-1.09844	-0.83991	-0.00001
H	-3.25747	-2.70947	-0.00004
H	-5.62133	-1.90810	-0.00006
H	-6.14636	0.50735	-0.00007
H	-4.33367	2.21941	-0.00004
H	-1.43295	2.33714	-0.00002
C	0.84101	0.65525	0.00001
C	1.72838	-0.44066	0.00005
C	1.35463	1.96693	-0.00004
C	3.12432	-0.20498	0.00002
C	2.71971	2.18311	-0.00006
H	0.68001	2.82319	-0.00007
C	3.60885	1.09833	-0.00003
H	3.11335	3.19954	-0.00010
H	4.68107	1.28658	-0.00005
O	1.31156	-1.71531	0.00014
H	0.30997	-1.69394	0.00020
O	3.89366	-1.32178	0.00006
C	5.30066	-1.14242	0.00005
H	5.73108	-2.14890	0.00009
H	5.63387	-0.60225	-0.89906
H	5.63388	-0.60217	0.89912

Optimized geometries of **3** in the ground state in MeOH (angstrom)

6	-2.78531	0.68930	-0.00003
6	-2.46882	-0.68685	-0.00002
6	-3.48932	-1.64395	-0.00004
6	-4.80267	-1.18703	-0.00005
6	-5.10273	0.18961	-0.00005
6	-4.09976	1.15479	-0.00004
7	-1.56930	1.33691	-0.00001
6	-0.58878	0.38680	0.00001
7	-1.09844	-0.83991	-0.00001
1	-3.25747	-2.70947	-0.00004
1	-5.62133	-1.90810	-0.00006
1	-6.14636	0.50735	-0.00007
1	-4.33367	2.21941	-0.00004
1	-1.43295	2.33714	-0.00002
6	0.84101	0.65525	0.00001
6	1.72838	-0.44066	0.00005
6	1.35463	1.96693	-0.00004
6	3.12432	-0.20498	0.00002
6	2.71971	2.18311	-0.00006
1	0.68001	2.82319	-0.00007
6	3.60885	1.09833	-0.00003
1	3.11335	3.19954	-0.00010
1	4.68107	1.28658	-0.00005
8	1.31156	-1.71531	0.00014
1	0.30997	-1.69394	0.00020
8	3.89366	-1.32178	0.00006
6	5.30066	-1.14242	0.00005
1	5.73108	-2.14890	0.00009
1	5.63387	-0.60225	-0.89906
1	5.63388	-0.60217	0.89912

Optimized geometries of **3** in the ground state in H2O (angstrom)

6	0	-2.78529	0.68920	-0.00002
6	0	-2.46886	-0.68700	-0.00005
6	0	-3.48942	-1.64414	-0.00009
6	0	-4.80280	-1.18709	-0.00009
6	0	-5.10275	0.18969	-0.00007
6	0	-4.09972	1.15487	-0.00003
7	0	-1.56947	1.33688	0.00001
6	0	-0.58893	0.38709	0.00002
7	0	-1.09842	-0.83988	-0.00003
1	0	-3.25776	-2.70974	-0.00011
1	0	-5.62149	-1.90813	-0.00012
1	0	-6.14637	0.50749	-0.00007
1	0	-4.33323	2.21958	-0.00001
1	0	-1.43353	2.33725	0.00002
6	0	0.84102	0.65556	0.00003
6	0	1.72839	-0.44044	0.00008
6	0	1.35478	1.96721	-0.00004
6	0	3.12432	-0.20501	0.00002
6	0	2.71997	2.18308	-0.00009
1	0	0.68035	2.82357	-0.00008
6	0	3.60905	1.09823	-0.00006
1	0	3.11378	3.19943	-0.00015
1	0	4.68128	1.28634	-0.00010
8	0	1.31121	-1.71531	0.00022
1	0	0.30942	-1.69379	0.00034
8	0	3.89366	-1.32198	0.00007
6	0	5.30095	-1.14267	0.00004
1	0	5.73140	-2.14913	0.00009
1	0	5.63415	-0.60250	-0.89901
1	0	5.63418	-0.60239	0.89900

Optimized geometries of **3** in the S1 state in THF (angstrom)

C	-2.80185	0.68579	0.00019
C	-2.52951	-0.70363	-0.00069
C	-3.56248	-1.64489	-0.00125
C	-4.87457	-1.14726	-0.00090
C	-5.14155	0.22448	-0.00004
C	-4.10533	1.17523	0.00055
N	-1.57844	1.31975	0.00053
C	-0.56012	0.39375	0.00010
N	-1.16821	-0.83229	-0.00096
H	-3.35567	-2.71440	-0.00188
H	-5.70741	-1.85211	-0.00131
H	-6.17666	0.56863	0.00021
H	-4.31356	2.24456	0.00127
H	-1.44741	2.31957	0.00157
C	0.85028	0.63872	0.00001
C	1.76574	-0.50349	0.00041
C	1.37788	1.92305	-0.00043
C	3.18216	-0.21351	0.00027
C	2.77940	2.15662	-0.00036
H	0.71989	2.79365	-0.00093
C	3.68066	1.10942	-0.00005
H	3.14139	3.18495	-0.00058
H	4.75022	1.30828	-0.00006
O	1.33811	-1.69590	0.00092
H	-0.56967	-1.65942	-0.00057
O	3.96079	-1.30470	0.00062
C	5.37166	-1.13660	0.00067
H	5.78999	-2.14769	0.00100
H	5.70506	-0.60006	-0.89952
H	5.70494	-0.59950	0.90057

Optimized geometries of **3** in the S1 state in MeCN (angstrom)

C	-2.80097	0.68464	0.00017
C	-2.53269	-0.70619	-0.00067
C	-3.56820	-1.64368	-0.00123
C	-4.87890	-1.14307	-0.00092
C	-5.14187	0.23033	-0.00010
C	-4.10322	1.17724	0.00048
N	-1.57749	1.31582	0.00052
C	-0.55959	0.38760	0.00015
N	-1.17196	-0.83918	-0.00091
H	-3.36448	-2.71387	-0.00183
H	-5.71352	-1.84583	-0.00133
H	-6.17594	0.57768	0.00012
H	-4.30717	2.24748	0.00116
H	-1.44619	2.31581	0.00159
C	0.84682	0.63468	0.00004
C	1.76972	-0.50509	0.00042
C	1.37301	1.92202	-0.00039
C	3.18533	-0.21216	0.00026
C	2.77292	2.15549	-0.00032
H	0.71474	2.79201	-0.00085
C	3.67997	1.11124	-0.00004
H	3.13279	3.18470	-0.00054
H	4.74854	1.31456	-0.00005
O	1.34460	-1.69905	0.00095
H	-0.58226	-1.67086	-0.00049
O	3.96723	-1.30245	0.00059
C	5.37860	-1.12807	0.00061
H	5.80161	-2.13715	0.00092
H	5.70893	-0.58970	-0.89935
H	5.70885	-0.58918	0.90028

Optimized geometries of **3** in the S1 state in MeOH (angstrom)

C	-2.80101	0.68481	0.00009
C	-2.53272	-0.70590	-0.00054
C	-3.56801	-1.64371	-0.00101
C	-4.87874	-1.14333	-0.00084
C	-5.14190	0.23006	-0.00022
C	-4.10350	1.17714	0.00027
N	-1.57750	1.31597	0.00041
C	-0.55952	0.38775	0.00015
N	-1.17185	-0.83859	-0.00063
H	-3.36393	-2.71381	-0.00146
H	-5.71342	-1.84604	-0.00118
H	-6.17611	0.57708	-0.00011
H	-4.30768	2.24730	0.00077
H	-1.44578	2.31587	0.00124
C	0.84707	0.63506	0.00009
C	1.76958	-0.50500	0.00034
C	1.37338	1.92223	-0.00018
C	3.18514	-0.21237	0.00025
C	2.77343	2.15538	-0.00013
H	0.71535	2.79234	-0.00048
C	3.68017	1.11076	0.00005
H	3.13390	3.18436	-0.00028
H	4.74874	1.31405	0.00004
O	1.34400	-1.69877	0.00068
H	-0.58252	-1.67040	-0.00040
O	3.96706	-1.30299	0.00048
C	5.37827	-1.12820	0.00048
H	5.80142	-2.13723	0.00068
H	5.70860	-0.58975	-0.89945
H	5.70857	-0.58941	0.90021

Optimized geometries of **3** in the S1 state in H2O (angstrom)

C	-2.80089	0.68456	0.00013
C	-2.53326	-0.70644	-0.00061
C	-3.56908	-1.64353	-0.00113
C	-4.87957	-1.14245	-0.00090
C	-5.14197	0.23118	-0.00017
C	-4.10303	1.17763	0.00038
N	-1.57733	1.31530	0.00047
C	-0.55958	0.38669	0.00016
N	-1.17252	-0.83993	-0.00076
H	-3.36568	-2.71377	-0.00166
H	-5.71455	-1.84482	-0.00129
H	-6.17595	0.57889	-0.00001
H	-4.30640	2.24799	0.00098
H	-1.44569	2.31524	0.00143
C	0.84646	0.63412	0.00007
C	1.77016	-0.50548	0.00041
C	1.37243	1.92179	-0.00029
C	3.18570	-0.21220	0.00026
C	2.77224	2.15517	-0.00024
H	0.71420	2.79171	-0.00068
C	3.67995	1.11113	0.00000
H	3.13205	3.18438	-0.00044
H	4.74841	1.31494	-0.00002
O	1.34526	-1.69960	0.00081
H	-0.58406	-1.67224	-0.00044
O	3.96836	-1.30229	0.00055
C	5.37965	-1.12636	0.00054
H	5.80376	-2.13497	0.00079
H	5.70940	-0.58759	-0.89936
H	5.70937	-0.58714	0.90017

Optimized geometries of **3**+$(MeOH)_6$ in the ground state in MeOH (angstrom)

C	-2.66592	-1.85799	-0.10177
C	-2.64154	-0.68222	-0.87508
C	-3.82251	0.02717	-1.11277
C	-4.99121	-0.45643	-0.54384
C	-4.99700	-1.62611	0.24241
C	-3.83574	-2.35235	0.47453
N	-1.35593	-2.28183	-0.06292
C	-0.61041	-1.38451	-0.77074
N	-1.34505	-0.41612	-1.27646
H	-3.81579	0.93314	-1.70827
H	-5.92257	0.07678	-0.69991
H	-5.93002	-1.96804	0.67665
H	-3.83842	-3.25172	1.07938
H	-0.99541	-3.07535	0.44427
C	0.83828	-1.53840	-0.95144
C	1.69245	-0.43976	-0.81732
C	1.36198	-2.80030	-1.27791
C	3.06927	-0.60678	-1.08272
C	2.71671	-2.95837	-1.49489
H	0.68791	-3.64404	-1.38277
C	3.57463	-1.85783	-1.40899
H	3.12027	-3.93153	-1.74992
H	4.63354	-1.98950	-1.59493
O	1.29721	0.79554	-0.44194
H	0.50107	0.74817	0.13819
O	3.80476	0.52542	-0.96716
C	5.21307	0.42250	-1.07983
H	5.60238	1.41783	-0.87126
H	5.61829	-0.28697	-0.34928
H	5.50931	0.11677	-2.08902
O	3.23319	2.02955	1.45892
H	2.85027	1.68782	0.63727
O	-0.74423	3.10284	-0.29699
H	-0.54758	2.65581	-1.14308
O	-0.53843	1.80777	-2.71912
H	-0.75132	0.96538	-2.25349
O	-0.30446	0.48363	1.67626
H	-1.27594	0.35996	1.75529
O	-2.97913	0.54384	2.15223
H	-3.50026	-0.10319	1.66226
O	1.13847	-1.47244	3.05594
H	0.61938	-0.89629	2.46656
C	0.02878	1.61409	2.48550
H	1.06936	1.86934	2.27816
H	-0.59887	2.46783	2.21954
H	-0.09018	1.37889	3.54820
C	-3.34655	1.84675	1.69753
H	-4.42255	1.91039	1.51299
H	-3.08334	2.55098	2.48955
H	-2.79828	2.12056	0.78956
C	3.62193	0.90306	2.22080
H	4.32082	0.25807	1.67139
H	4.12906	1.26776	3.11781
H	2.76508	0.29243	2.53720
C	1.85799	-2.39538	2.27082
H	2.53143	-1.90871	1.55129
H	2.46619	-3.00568	2.94401
H	1.20193	-3.07297	1.70621
C	-1.72602	2.24591	-3.35075
H	-1.46492	3.02923	-4.06644
H	-2.22047	1.43235	-3.89591
H	-2.44127	2.66900	-2.63113
C	0.31517	3.98938	-0.02050

H	0.06814	4.53659	0.89413
H	1.26476	3.46552	0.15099
H	0.46576	4.72510	-0.82345