Supporting Information

Mutual Interference between Intramolecular Proton Transfer Sites through the Adjoining π-Conjugated System in Schiff Bases of Double-headed, Fused Salicylaldehydes

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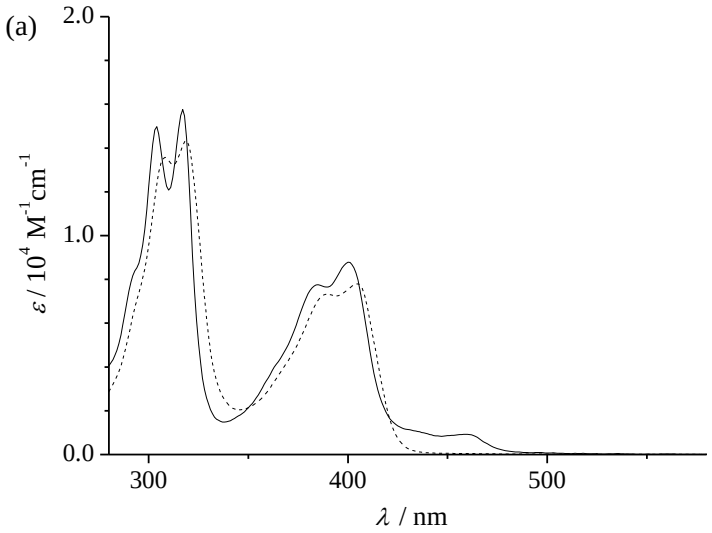
1. General Procedures of Experiments

All the chemicals were used as purchased, without further purification. FT-IR spectra were recorded with a conventional transmission-type spectrometer. NMR spectra were obtained with a spectrometer with field gradient amplifier (400 MHz for ^{1}H). Solution UV–vis spectra were measured for $1x10^{5}$ M solution of spectrograde solvents, with a conventional spectrophotometer. Solid-state UV–vis spectra were measured for samples smeared on slide glass, with a fiber optic, portable spectrophotometer equipped with a conventional optical microscope.

2. Supplementary Figures, Schemes, and Tables



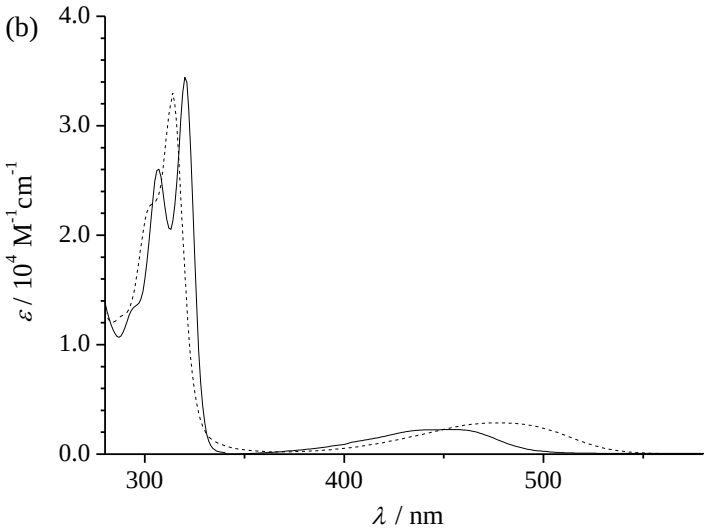


Figure S1 Comparison of the UV spectra of dihydroxynaphthalene-dialdimines with their corresponding dialdehydes; (a) α,α-diimine (**1b**), and (b) β,β-diimine (**2b**).

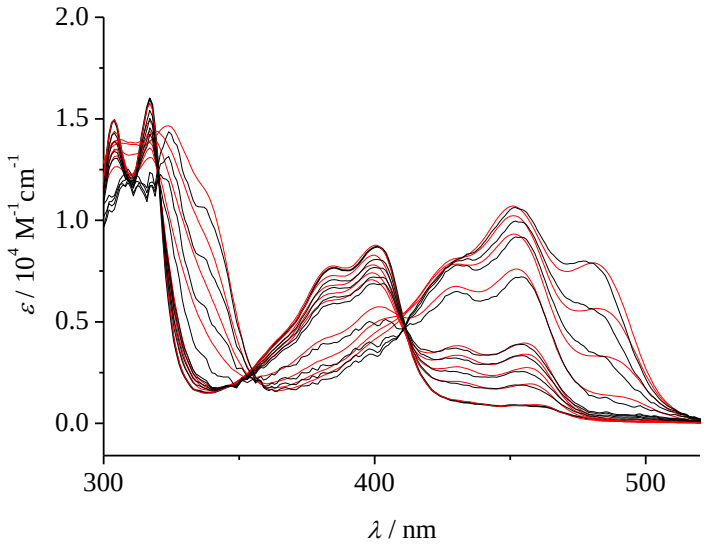


Figure S2 Original (black line) and reconstituted (red line) UV–vis spectra of **1b**.

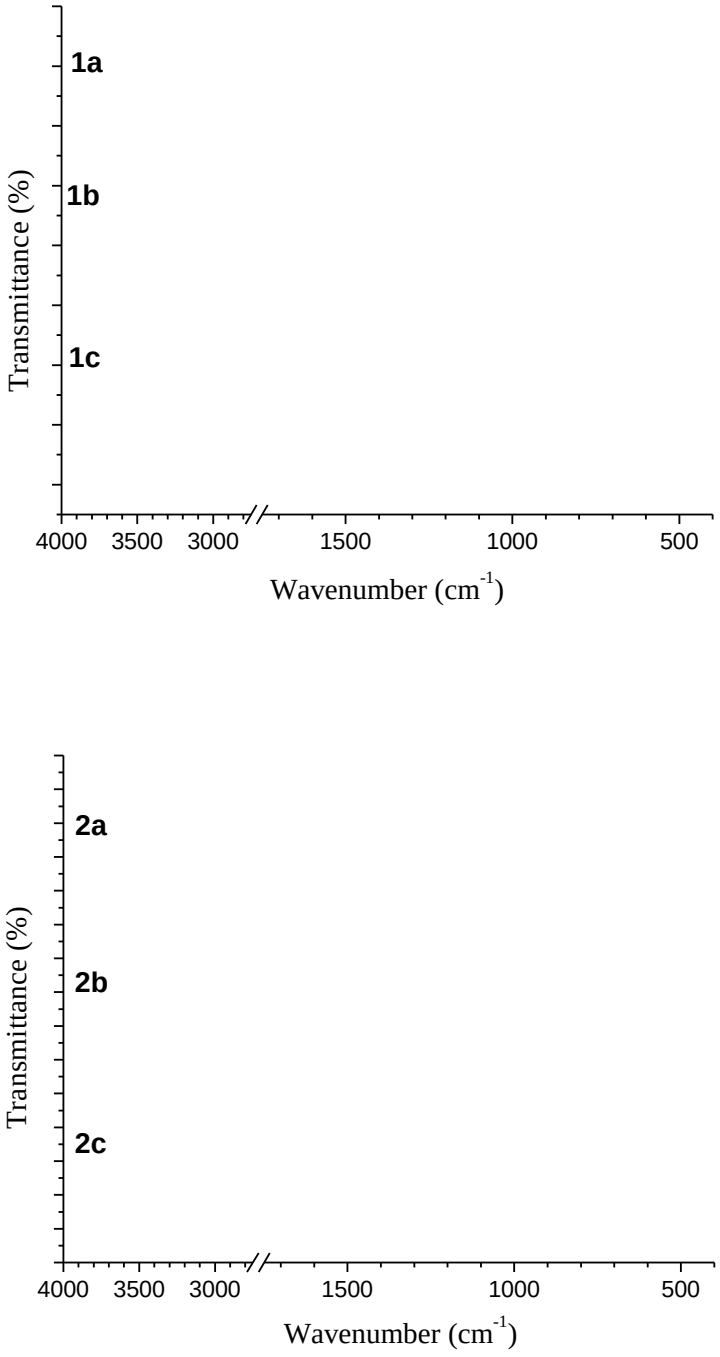


Figure S3 FT-IR spectra of **1a-c** and **2a-c**.

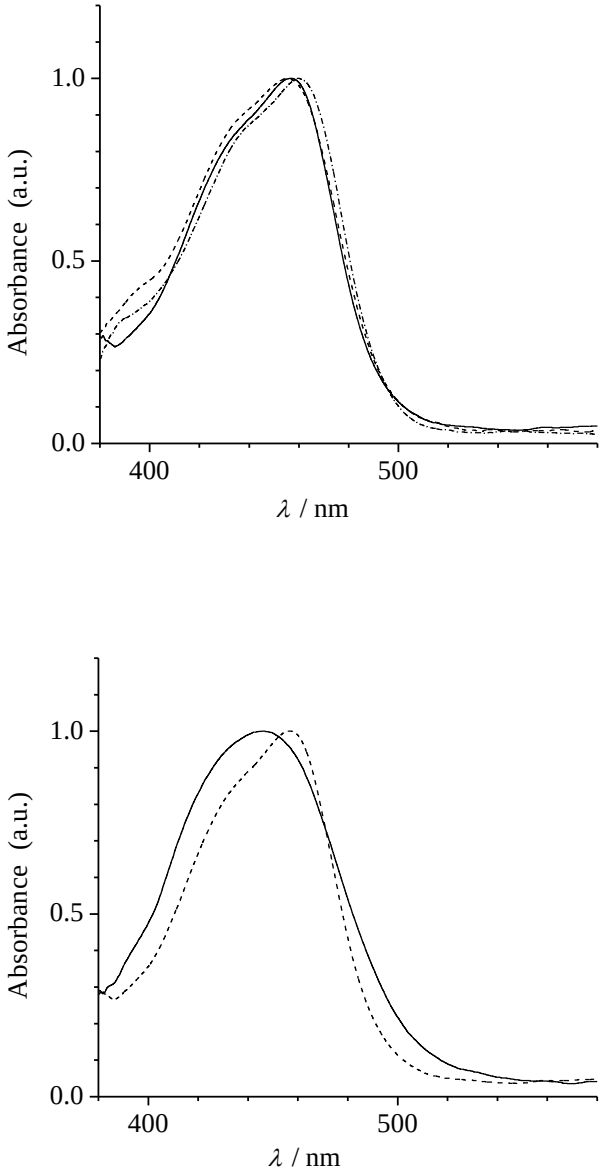


Figure S4 Absorption spectra of **2a** (dashed line), **2b** (solid line), and **2c** (dotted line); (a) smeared solid films at 273 K, and (b) molten liquid films (only **2a** and **2b**).

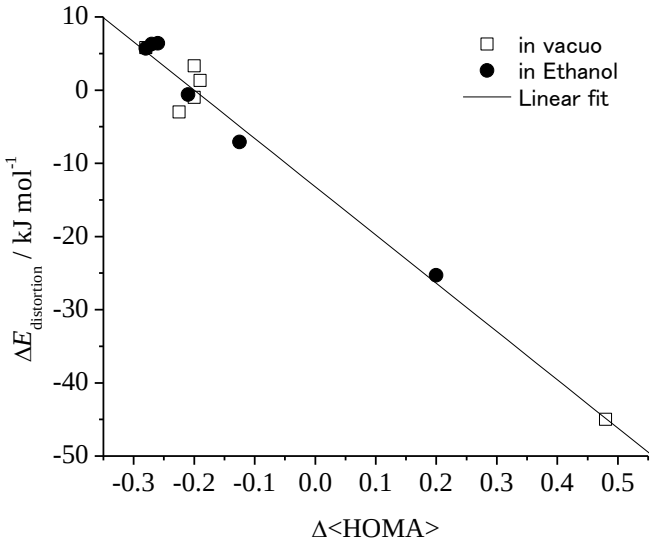
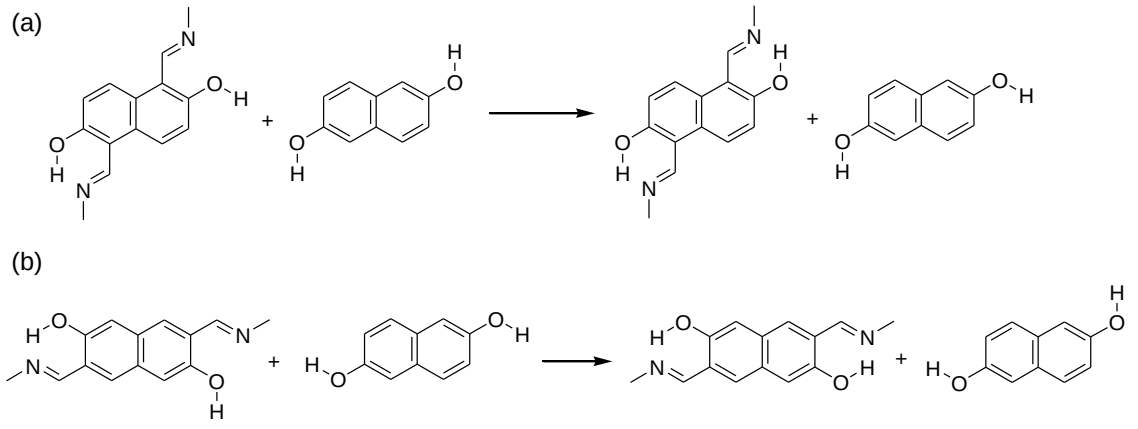


Figure S5 Correlation between $\Delta E_{\text{distortion}}$ and $\Delta\langle\text{HOMA}\rangle$ calculated by B3LYP method with or without solvent effects.



Scheme S1 Isodesmic reaction for estimating the intramolecular hydrogen bonding energy

Table S1 Energy (in kJ/mol) of the selected conformers of **1** and **2** in each tautomer, and energies related to the intramolecular hydrogen bond (B3LYP/6-311G(d,p)//HF/6-311G(d,p))

	$\Delta E_{I \rightarrow II}$	$\Delta E_{O/C}$	ΔE_{HB}	ΔE_{RA}
$\mathbf{1}_{OH/OH}$ (I-I → I-II)	66.5	63.8	57.4	6.4
$\mathbf{1}_{OH/OH}$ (I-II → II-II)	66.4	64.0	57.3	6.7
$\mathbf{1}_{OH/OH}$ (I-I → II-II)	132.9	127.8	114.7	13.1
$\mathbf{1}_{NH/OH}$ (I → II)	65.5	62.8	56.0	6.8
$\mathbf{2}_{OH/OH}$ (I-I → I-II)	53.3	55.7	48.1	7.6
$\mathbf{2}_{OH/OH}$ (I-II → II-II)	53.1	55.8	48.1	7.7
$\mathbf{2}_{OH/OH}$ (I-I → II-II)	106.4	111.4	96.4	15.1
$\mathbf{2}_{NH/OH}$ (I → II)	51.0	53.6	46.0	7.6
$\mathbf{3}_{OH}$ (I → II)	57.2	57.2	48.9	8.3

Table S2 Calculated energies (in kJ/mol) based on a hypothetic homodesmotic reaction shown in Scheme 3.

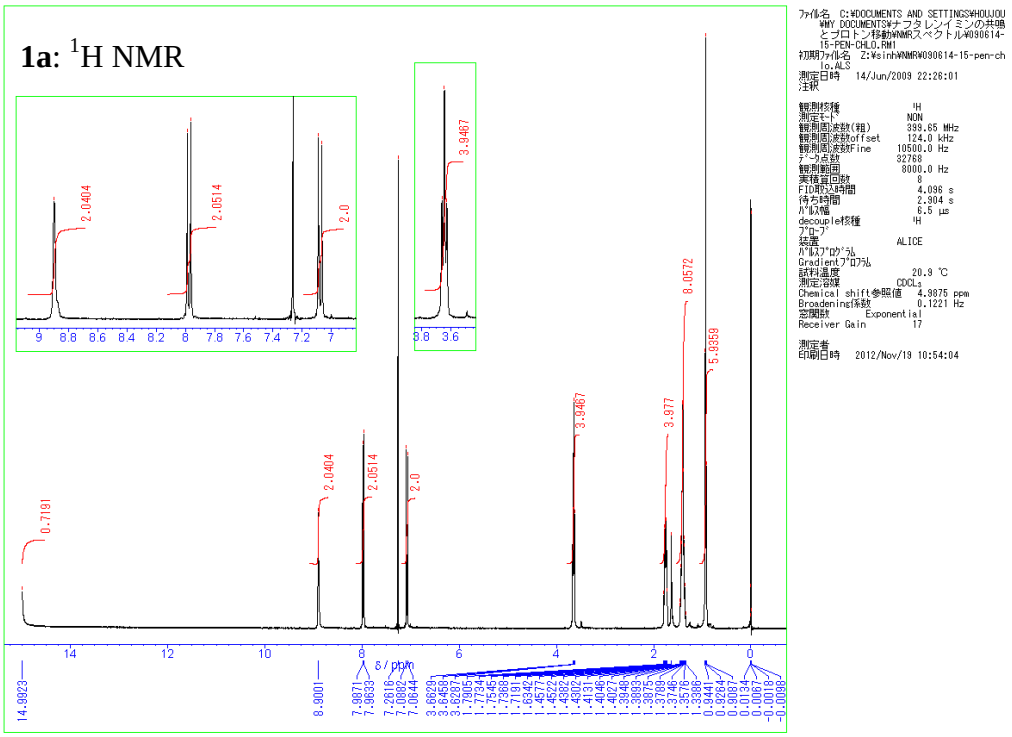
	ΔE_{fusion}		$\Delta E_{distortion}$		ΔE_{RAHB}	
	ε = 1	ε = 25	ε = 1	ε = 25	ε = 1	ε = 25
$\mathbf{1}_{OH/OH}$	+23.4	+28.6	+5.8	+5.7	+17.6	+22.9
$\mathbf{1}_{NH/OH}$	+7.5	+16.7	+3.3	+6.4	+4.2	+10.3
$\mathbf{1}_{NH/NH}$	-1.9	+10.4	+1.3	+6.3	-3.2	+4.1

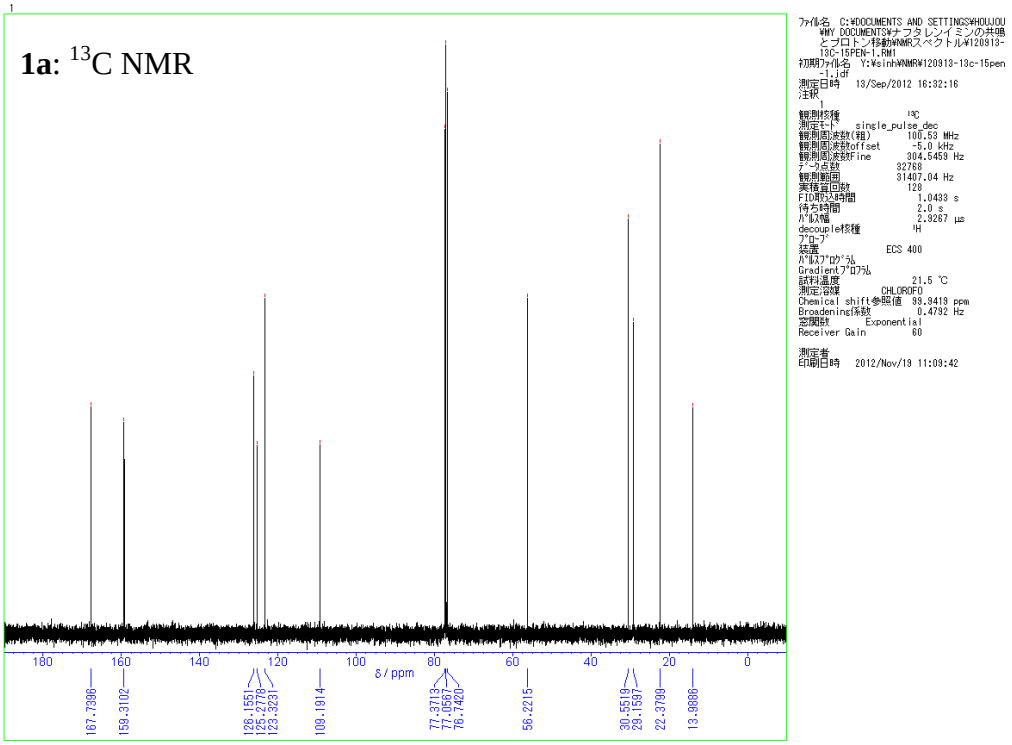
$\mathbf{2}_{OH/OH}$	+11.1	+13.2	-1.0	-0.6	+12.1	+13.8
$\mathbf{2}_{NH/OH}$	+33.4	+30.2	-3.0	-7.1	+36.4	+37.3
$\mathbf{2}_{NH/NH}$	+55.2	+56.7	-45.0	-25.3	+100.2	+82.0

Table S3 Calculated energies (in kJ/mol) related to the intramolecular proton transfer.

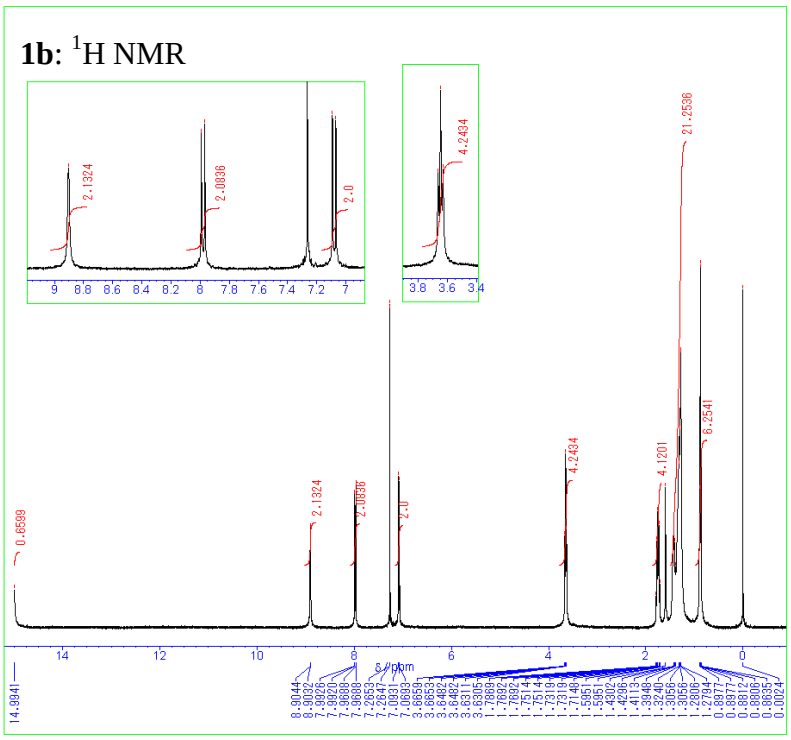
	ΔE_{PT}		ΔE_{AB}		ΔE_{RE}	
	ε = 1	ε=25	ε = 1	ε=25	ε = 1	ε=25
$\mathbf{1}_{OH/OH} \rightarrow \mathbf{1}_{NH/OH}$	+6.9	-7.7	+52.0	+29.4	-45.1	-37.1
$\mathbf{1}_{NH/OH} \rightarrow \mathbf{1}_{NH/NH}$	+13.5	-2.2	+58.3	+22.0	-44.8	-24.2
$\mathbf{2}_{OH/OH} \rightarrow \mathbf{2}_{NH/OH}$	+45.1	+21.2	+93.0	+43.1	-47.9	-21.9
$\mathbf{2}_{NH/OH} \rightarrow \mathbf{2}_{NH/NH}$	+44.7	+30.7	+113.3	+52.4	-68.6	-21.8
$\mathbf{3}_{OH} \rightarrow \mathbf{3}_{NH}$	+22.8	+4.2	+70.5	+30.9	-47.7	-26.7

3. ^{1}H and ^{13}C NMR spectra of Novel Compounds





1b: ^{1}H NMR



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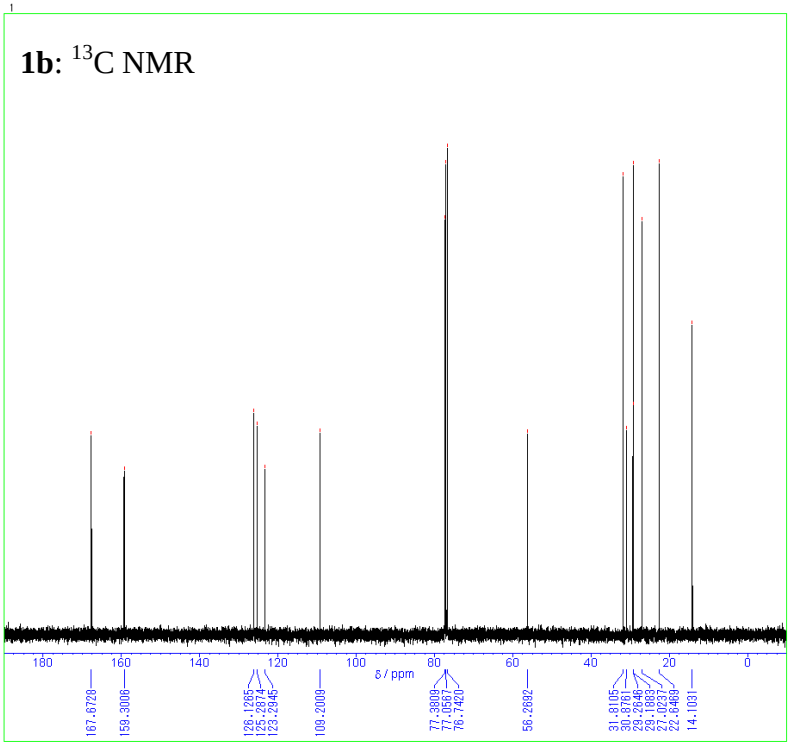
1b: ^{13}C NMR



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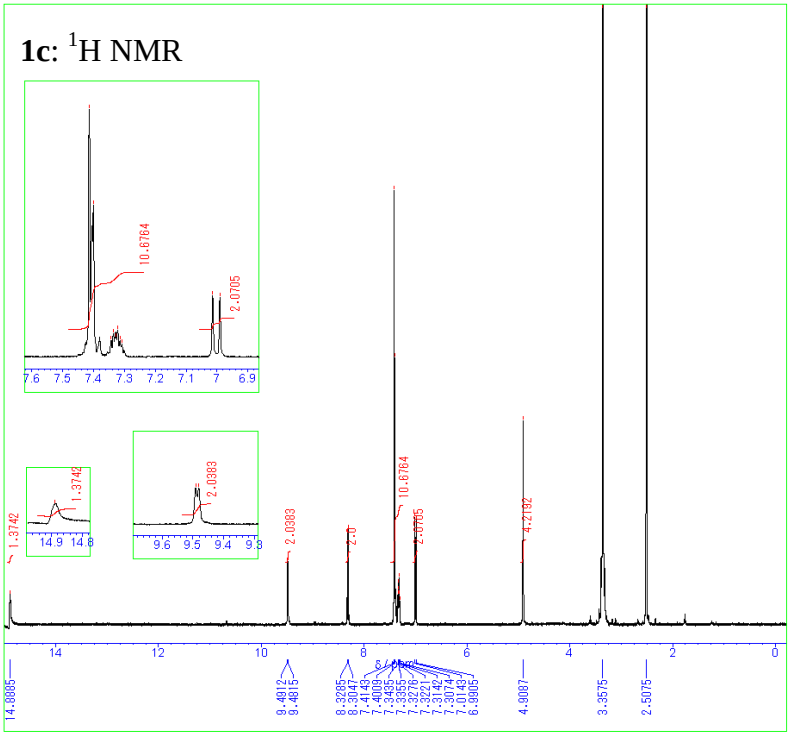

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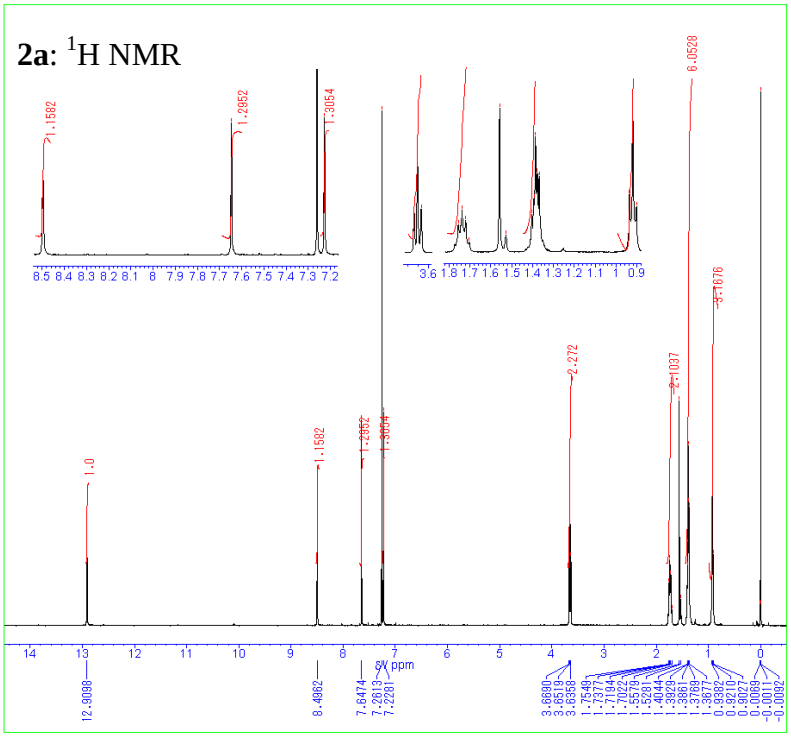
2a: ^{1}H NMR



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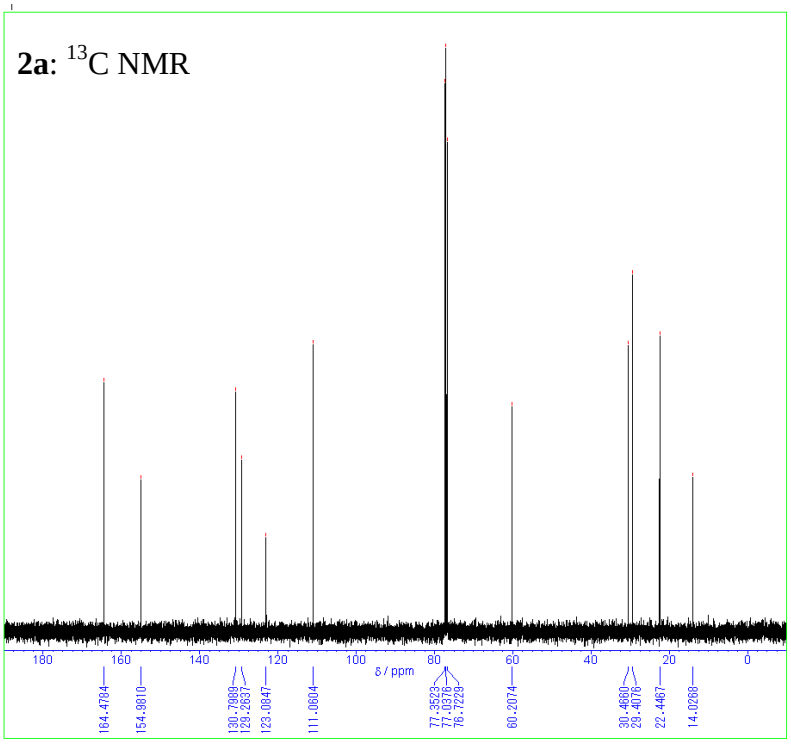

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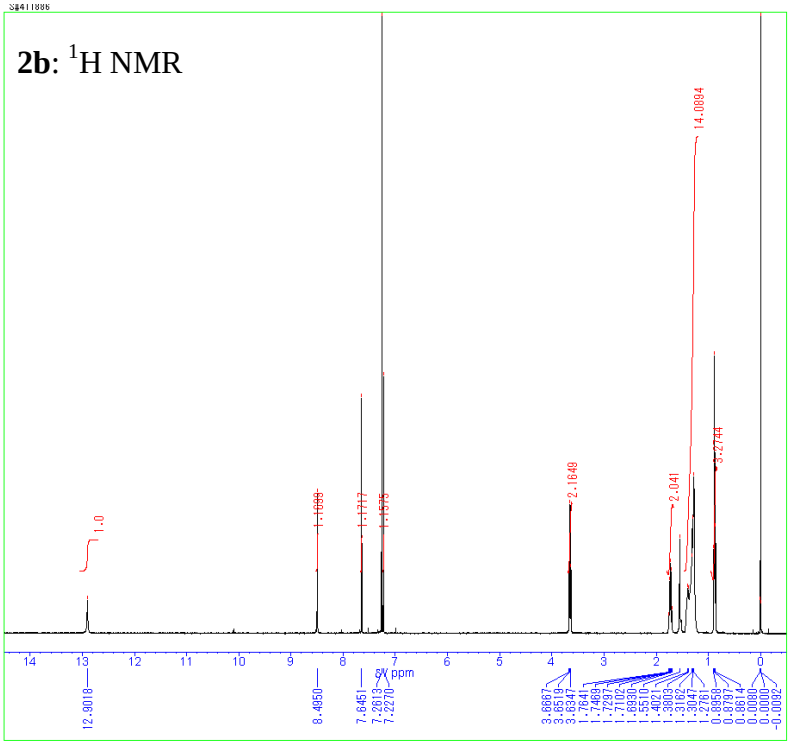

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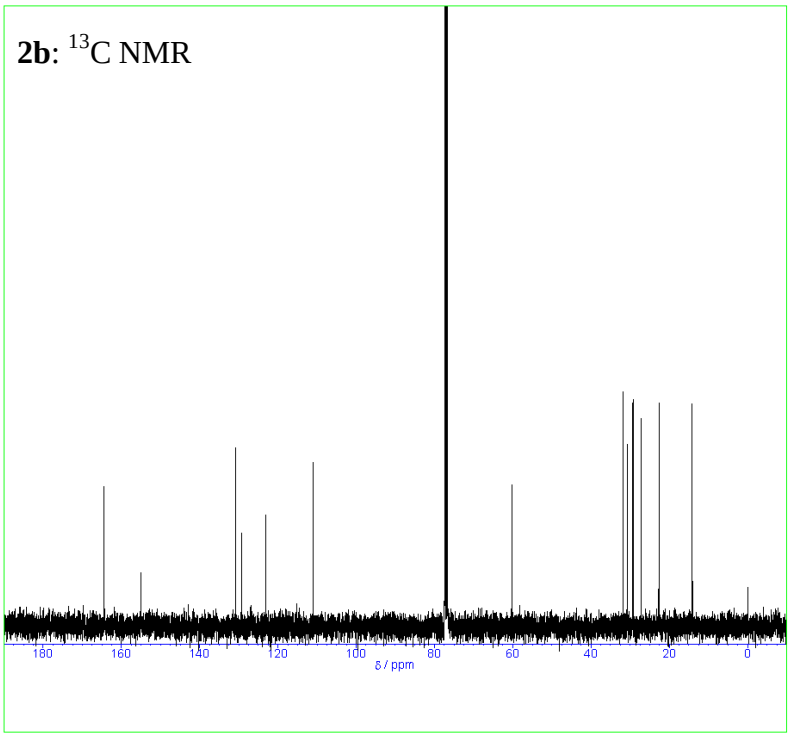

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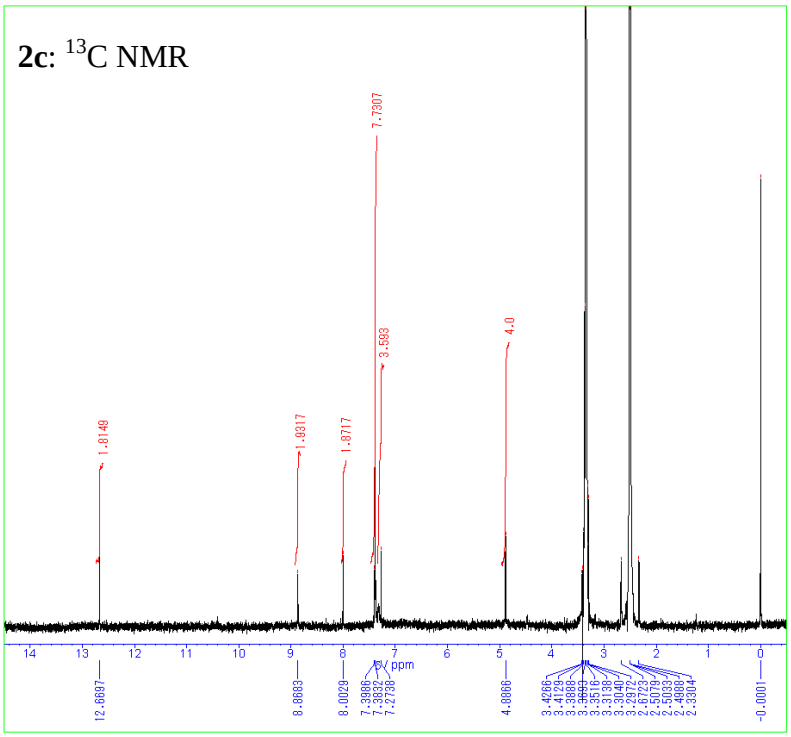

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測定者
印刷日時 2012/Nov/26 21:34:20

4. Numerical data for ab initio calculation

Compound **1** OH/OH-form (closed/closed) in vacuo

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.703680	0.000000
2	6	0	1.239151	1.443234	0.000000
3	6	0	2.431839	0.755465	0.000000
4	6	0	2.427795	-0.656997	0.000000
5	6	0	1.269675	-1.350806	0.000000
6	6	0	0.000038	-0.703700	0.000000
7	6	0	-1.239146	-1.443237	0.000000
8	6	0	-2.431828	-0.755457	0.000000
9	6	0	-2.427747	0.657009	0.000000
10	6	0	-1.269622	1.350805	0.000000
11	6	0	1.247121	2.917821	0.000000
12	7	0	2.297947	3.605672	0.000000
13	8	0	3.630442	1.326106	0.000000
14	6	0	-1.247167	-2.917825	0.000000
15	7	0	-2.297989	-3.605696	0.000000
16	8	0	-3.630452	-1.326055	0.000000
17	1	0	0.288752	3.418290	0.000000
18	1	0	3.528442	2.275801	0.000000
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E(RB+HF-LYP) = -802.070047505 A.U.

Compound **1** NH/OH-form (closed) in vacuo

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6	6	0	0.058083	-0.704139	0.000000
7	6	0	-1.180894	-1.505670	0.000000
8	6	0	-2.477149	-0.852554	0.000000
9	6	0	-2.458906	0.608926	0.000000
10	6	0	-1.324326	1.305102	0.000000
11	6	0	1.131632	2.957995	0.000000
12	7	0	2.149309	3.693042	0.000000
13	8	0	3.595389	1.482916	0.000000
14	6	0	-1.147389	-2.882594	0.000000
15	7	0	-2.180321	-3.702381	0.000000
16	8	0	-3.540031	-1.449295	0.000000
17	1	0	0.152936	3.415891	0.000000
18	1	0	3.444683	2.424791	0.000000
19	1	0	3.445746	-1.015929	0.000000
20	1	0	1.450698	-2.358170	0.000000
21	1	0	-0.197803	-3.385301	0.000000
22	1	0	-3.080452	-3.265363	0.000000
23	1	0	-3.416849	1.095444	0.000000
24	1	0	-1.409471	2.372767	0.000000
25	6	0	1.984090	5.127186	0.000000
26	1	0	0.938405	5.432589	0.000000
27	1	0	2.470544	5.545424	0.875008
28	1	0	2.470544	5.545424	-0.875008
29	6	0	-2.076439	-5.142644	0.000000
30	1	0	-1.034226	-5.436890	0.000000
31	1	0	-2.550742	-5.561734	0.881058
32	1	0	-2.550742	-5.561734	-0.881058

E(RHF) = -797.093447910 A.U.

E(RB+HF-LYP) = -802.067447666 A.U.

Compound **1** NH/NH-form in vacuo

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.682971	0.000000
2	6	0	1.257463	1.443138	0.000000
3	6	0	2.532496	0.745410	0.000000
4	6	0	2.457103	-0.709776	0.000000
5	6	0	1.288575	-1.354296	0.000000
6	6	0	0.000457	-0.683208	0.000000
7	6	0	-1.257096	-1.443193	0.000000
8	6	0	-2.532130	-0.745560	0.000000
9	6	0	-2.456634	0.709578	0.000000
10	6	0	-1.288032	1.354025	0.000000
11	6	0	1.275178	2.823232	0.000000
12	7	0	2.340356	3.598899	0.000000
13	8	0	3.616601	1.308028	0.000000
14	6	0	-1.275362	-2.823268	0.000000
15	7	0	-2.340902	-3.598374	0.000000
16	8	0	-3.616154	-1.308389	0.000000
17	1	0	0.347513	3.364497	0.000000
18	1	0	3.220982	3.121930	0.000000
19	1	0	3.392806	-1.237804	0.000000
20	1	0	1.325455	-2.426859	0.000000
21	1	0	-0.347835	-3.364760	0.000000
22	1	0	-3.221307	-3.120949	0.000000
23	1	0	-3.392300	1.237659	0.000000
24	1	0	-1.324820	2.426605	0.000000
25	6	0	2.296838	5.042092	0.000000
26	1	0	1.268022	5.380348	0.000000
27	1	0	2.788711	5.440553	0.880996
28	1	0	2.788711	5.440553	-0.880996
29	6	0	-2.298139	-5.041589	0.000000
30	1	0	-1.269504	-5.380390	0.000000
31	1	0	-2.790242	-5.439756	0.880996
32	1	0	-2.790242	-5.439756	-0.880996

E(RHF) = -797.083722340 A.U.

E(RB+HF-LYP) = -802.062288429 A.U.

Compound **1** OH/OH-form (closed/closed) in ethanol (ε = 25)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000769	-0.704745	0.000000
2	6	0	-1.238471	-1.443728	0.000000
3	6	0	-2.428246	-0.752355	0.000000
4	6	0	-2.426542	0.659731	0.000000
5	6	0	-1.267871	1.355139	0.000000
6	6	0	0.000000	0.704302	0.000000
7	6	0	1.239049	1.443516	0.000000
8	6	0	2.428945	0.752213	0.000000
9	6	0	2.427319	-0.659883	0.000000
10	6	0	1.268736	-1.355441	0.000000
11	6	0	-1.248125	-2.921465	0.000000
12	7	0	-2.306067	-3.598792	0.000000
13	8	0	-3.628777	-1.331202	0.000000
14	6	0	1.247797	2.921301	0.000000
15	7	0	2.305110	3.599626	0.000000
16	8	0	3.629545	1.330874	0.000000
17	1	0	-0.293881	-3.426383	0.000000
18	1	0	-3.513662	-2.282457	0.000000
19	1	0	-3.374302	1.165415	0.000000
20	1	0	-1.334958	2.423233	0.000000
21	1	0	0.293144	3.425480	0.000000
22	1	0	3.514537	2.282164	0.000000
23	1	0	3.375128	-1.165479	0.000000
24	1	0	1.336015	-2.423504	0.000000
25	6	0	-2.219003	-5.043012	0.000000
26	1	0	-1.191998	-5.401058	0.000000
27	1	0	-2.727732	-5.432996	0.875071
28	1	0	-2.727732	-5.432996	-0.875071
29	6	0	2.216716	5.043770	0.000000
30	1	0	1.189382	5.400865	0.000000
31	1	0	2.725082	5.434227	0.875071
32	1	0	2.725082	5.434227	-0.875071

E(RHF) = -797.109206297 A.U.

E(RB3LYP) = -802.078918596 A.U.

Compound **1** NH/OH-form (closed) in ethanol (ε = 25)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.555523	-0.432330	0.000000
2	6	0	1.907631	0.147654	0.000000
3	6	0	2.090494	1.574967	0.000000
4	6	0	0.874156	2.377835	0.000000
5	6	0	-0.343514	1.831844	0.000000
6	6	0	-0.572591	0.395305	0.000000
7	6	0	-1.895182	-0.150562	0.000000
8	6	0	-2.054527	-1.526828	0.000000
9	6	0	-0.925986	-2.353095	0.000000
10	6	0	0.329132	-1.825094	0.000000
11	6	0	3.036625	-0.669982	0.000000
12	7	0	4.283811	-0.283346	0.000000
13	8	0	3.189053	2.130672	0.000000
14	6	0	-3.089418	0.724259	0.000000
15	7	0	-4.263718	0.279686	0.000000
16	8	0	-3.242531	-2.141723	0.000000
17	1	0	2.912719	-1.736001	0.000000
18	1	0	4.437526	0.704751	0.000000
19	1	0	1.002040	3.445086	0.000000
20	1	0	-1.178280	2.502345	0.000000
21	1	0	-2.927146	1.791007	0.000000
22	1	0	-3.933268	-1.479481	0.000000
23	1	0	-1.073881	-3.417346	0.000000
24	1	0	1.148156	-2.516296	0.000000
25	6	0	5.421833	-1.182564	0.000000
26	1	0	5.077799	-2.207620	0.000000
27	1	0	6.028977	-1.015580	-0.881366
28	1	0	6.028977	-1.015580	0.881366
29	6	0	-5.370454	1.211621	0.000000
30	1	0	-5.045259	2.249468	0.000000
31	1	0	-5.986762	1.035547	-0.875056
32	1	0	-5.986762	1.035547	0.875056

E(RHF) = -797.110202899 A.U.

E(RB3LYP) = -802.081848339 A.U.

Compound **1** NH/NH-form in ethanol (ε = 25)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000137	-0.687082	0.000000
2	6	0	-1.253674	-1.447206	0.000000
3	6	0	-2.519841	-0.762289	0.000000
4	6	0	-2.452245	0.688007	0.000000
5	6	0	-1.287369	1.348074	0.000000
6	6	0	0.000000	0.687008	0.000000
7	6	0	1.253667	1.447123	0.000000
8	6	0	2.519870	0.762338	0.000000
9	6	0	2.452407	-0.687873	0.000000
10	6	0	1.287488	-1.347986	0.000000
11	6	0	-1.253285	-2.844162	0.000000
12	7	0	-2.300374	-3.622228	0.000000
13	8	0	-3.615805	-1.331707	0.000000
14	6	0	1.253135	2.844104	0.000000
15	7	0	2.300203	3.622073	0.000000
16	8	0	3.615780	1.331988	0.000000
17	1	0	-0.319396	-3.372351	0.000000
18	1	0	-3.188188	-3.160180	0.000000
19	1	0	-3.387733	1.217603	0.000000
20	1	0	-1.337397	2.419329	0.000000
21	1	0	0.319186	3.372209	0.000000
22	1	0	3.187987	3.159908	0.000000
23	1	0	3.387888	-1.217466	0.000000
24	1	0	1.337628	-2.419229	0.000000
25	6	0	-2.246777	-5.071473	0.000000
26	1	0	-1.216438	-5.399243	0.000000
27	1	0	-2.740336	-5.462398	0.881365
28	1	0	-2.740336	-5.462398	-0.881365
29	6	0	2.246729	5.071334	0.000000
30	1	0	1.216416	5.399181	0.000000
31	1	0	2.740333	5.462183	0.881367
32	1	0	2.740333	5.462183	-0.881367

E(RHF) = -797.106969219 A.U.

E(RB3LYP) = -802.082679525 A.U.

Compound **2** OH/OH-form (closed/closed) in vacuo

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.702347	-0.017619	0.000000
2	6	0	-1.382363	-1.259608	0.000000
3	6	0	-0.701579	-2.435088	0.000000
4	6	0	0.731423	-2.414986	0.000000
5	6	0	1.388052	-1.218378	0.000000
6	6	0	0.702310	0.017618	0.000000
7	6	0	1.382330	1.259602	0.000000
8	6	0	0.701535	2.435072	0.000000
9	6	0	-0.731460	2.414971	0.000000
10	6	0	-1.388123	1.218379	0.000000
11	6	0	1.537218	-3.650625	0.000000
12	7	0	1.046489	-4.801694	0.000000
13	8	0	-1.388123	-3.583120	0.000000
14	6	0	-1.537209	3.650633	0.000000
15	7	0	-1.046406	4.801668	0.000000
16	8	0	1.388052	3.583123	0.000000
17	1	0	2.613758	-3.495525	0.000000
18	1	0	-0.786069	-4.318776	0.000000
19	1	0	-2.456724	-1.287616	0.000000
20	1	0	2.464497	-1.209893	0.000000
21	1	0	-2.613756	3.495578	0.000000
22	1	0	0.785983	4.318765	0.000000
23	1	0	2.456691	1.287615	0.000000
24	1	0	-2.464567	1.209912	0.000000
25	6	0	1.925289	-5.947880	0.000000
26	1	0	2.979235	-5.673660	0.000000
27	1	0	1.719842	-6.555409	0.874826
28	1	0	1.719842	-6.555409	-0.874826
29	6	0	-1.925135	5.947907	0.000000
30	1	0	-2.979098	5.673753	0.000000
31	1	0	-1.719648	6.555423	0.874826
32	1	0	-1.719648	6.555423	-0.874826

E(RHF) = -797.106614494 A.U.

E(RB+HF-LYP) = -802.074738854 A.U.

Compound **2** NH/OH-form (closed) in vacuo

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.026661	-0.752331	0.000000
2	6	0	1.218155	-1.484177	0.000000
3	6	0	2.404204	-0.864927	0.000000
4	6	0	2.447819	0.597120	0.000000
5	6	0	1.304825	1.308384	0.000000
6	6	0	0.000000	0.687271	0.000000
7	6	0	-1.143452	1.438220	0.000000
8	6	0	-2.444785	0.842130	0.000000
9	6	0	-2.451038	-0.614340	0.000000
10	6	0	-1.248610	-1.358677	0.000000
11	6	0	3.719005	1.350519	0.000000
12	7	0	4.848393	0.814052	0.000000
13	8	0	3.539541	-1.584982	0.000000
14	6	0	-3.669541	-1.300350	0.000000
15	7	0	-4.842374	-0.739741	0.000000
16	8	0	-3.488836	1.501167	0.000000
17	1	0	3.606444	2.432088	0.000000
18	1	0	4.290719	-1.005355	0.000000
19	1	0	1.197041	-2.559062	0.000000
20	1	0	1.347250	2.383530	0.000000
21	1	0	-3.654419	-2.379491	0.000000
22	1	0	-4.812521	0.270767	0.000000
23	1	0	-1.098546	2.512215	0.000000
24	1	0	-1.304537	-2.435185	0.000000
25	6	0	6.028320	1.646608	0.000000
26	1	0	5.795789	2.710495	0.000000
27	1	0	6.626866	1.416701	0.874897
28	1	0	6.626866	1.416701	-0.874897
29	6	0	-6.102754	-1.448270	0.000000
30	1	0	-5.924833	-2.516189	0.000000
31	1	0	-6.678401	-1.189974	0.881193
32	1	0	-6.678401	-1.189974	-0.881193

E(RHF) = -797.079240663 A.U.

E(RB+HF-LYP) = -802.057546570 A.U.

Compound **2** NH/NH-form in vacuo

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.079760	0.708916	-0.000052
2	6	0	1.022869	1.590132	-0.000057
3	6	0	2.330788	1.136970	-0.000136
4	6	0	2.474941	-0.316097	-0.000029
5	6	0	1.405117	-1.180188	-0.000022
6	6	0	0.080016	-0.708649	-0.000060
7	6	0	-1.023526	-1.589843	-0.000049
8	6	0	-2.330519	-1.136450	-0.000082
9	6	0	-2.474618	0.316924	-0.000021
10	6	0	-1.405506	1.180783	-0.000019
11	6	0	3.802021	-0.861803	0.000028
12	7	0	4.829513	-0.104871	0.000019
13	8	0	3.366055	1.874823	0.000095
14	6	0	-3.802424	0.862444	0.000029
15	7	0	-4.828604	0.104240	0.000010
16	8	0	-3.366972	-1.873670	0.000074
17	1	0	3.939481	-1.933625	0.000077
18	1	0	4.516737	0.917871	-0.000016
19	1	0	0.856293	2.652452	0.000008
20	1	0	1.578306	-2.243881	0.000020
21	1	0	-3.940509	1.934185	0.000086
22	1	0	-4.512483	-0.919253	-0.000056
23	1	0	-0.857097	-2.652185	-0.000007
24	1	0	-1.578570	2.244496	0.000006
25	6	0	6.203315	-0.554789	0.000058
26	1	0	6.245572	-1.637365	0.000087
27	1	0	6.710066	-0.178515	-0.880128
28	1	0	6.710015	-0.178483	0.880260
29	6	0	-6.202995	0.552357	0.000061
30	1	0	-6.246930	1.634866	0.000118
31	1	0	-6.709123	0.175246	-0.880125
32	1	0	-6.709091	0.175146	0.880223

E(RHF) = -797.037939259 A.U.

E(RB+HF-LYP) = -802.040551356 A.U.

Compound **2** OH/OH-form (closed/closed) in ethanol (ε = 25)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.702165	0.000000
2	6	0	-1.227584	1.411457	0.000000
3	6	0	-2.415784	0.753382	0.000000
4	6	0	-2.432005	-0.679719	0.000000
5	6	0	-1.251230	-1.363679	0.000000
6	6	0	-0.000010	-0.702503	0.000000
7	6	0	1.227694	-1.411563	0.000000
8	6	0	2.415881	-0.753450	0.000000
9	6	0	2.432028	0.679626	0.000000
10	6	0	1.251174	1.363460	0.000000
11	6	0	-3.690398	-1.453679	0.000000
12	7	0	-4.823410	-0.920953	0.000000
13	8	0	-3.555300	1.462438	0.000000
14	6	0	3.690323	1.453747	0.000000
15	7	0	4.823420	0.921197	0.000000
16	8	0	3.555373	-1.462533	0.000000
17	1	0	-3.568666	-2.532376	0.000000
18	1	0	-4.297925	0.863656	0.000000
19	1	0	-1.226162	2.486454	0.000000
20	1	0	-1.267840	-2.439346	0.000000
21	1	0	3.568455	2.532428	0.000000
22	1	0	4.298000	-0.863750	0.000000
23	1	0	1.226380	-2.486564	0.000000
24	1	0	1.267700	2.439137	0.000000
25	6	0	-6.000940	-1.762261	0.000000
26	1	0	-5.758914	-2.822392	0.000000
27	1	0	-6.600250	-1.535996	0.875051
28	1	0	-6.600250	-1.535996	-0.875051
29	6	0	6.000824	1.762684	0.000000
30	1	0	5.758638	2.822778	0.000000
31	1	0	6.600170	1.536512	0.875051
32	1	0	6.600170	1.536512	-0.875051

E(RHF) = -797.118798203 A.U.

E(RB3LYP) = -802.084802142 A.U.

Compound **2** NH/OH-form (closed) in ethanol (ε = 25)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012892	-0.724194	0.000000
2	6	0	1.223998	-1.452627	0.000000
3	6	0	2.410976	-0.820809	0.000000
4	6	0	2.444371	0.629237	0.000000
5	6	0	1.288456	1.332926	0.000000
6	6	0	0.000000	0.698341	0.000000
7	6	0	-1.174825	1.437910	0.000000
8	6	0	-2.448869	0.830851	0.000000
9	6	0	-2.436390	-0.622406	0.000000
10	6	0	-1.249359	-1.348833	0.000000
11	6	0	3.713757	1.389195	0.000000
12	7	0	4.840409	0.844734	0.000000
13	8	0	3.554115	-1.538547	0.000000
14	6	0	-3.660333	-1.356595	0.000000
15	7	0	-4.826434	-0.823765	0.000000
16	8	0	-3.524718	1.475997	0.000000
17	1	0	3.602783	2.468931	0.000000
18	1	0	4.298271	-0.944204	0.000000
19	1	0	1.202746	-2.528026	0.000000
20	1	0	1.325698	2.407892	0.000000
21	1	0	-3.613100	-2.432975	0.000000
22	1	0	-4.821340	0.187011	0.000000
23	1	0	-1.132471	2.512937	0.000000
24	1	0	-1.295246	-2.424718	0.000000
25	6	0	6.026593	1.673826	0.000000
26	1	0	5.795718	2.736355	0.000000
27	1	0	6.623237	1.440729	0.875038
28	1	0	6.623237	1.440729	-0.875038
29	6	0	-6.083708	-1.552720	0.000000
30	1	0	-5.888264	-2.615331	0.000000
31	1	0	-6.652456	-1.290157	0.882054
32	1	0	-6.652456	-1.290157	-0.882054

E(RHF) = -797.102982894 A.U.

E(RB3LYP) = -802.076717822 A.U.

Compound **2** NH/NH-form in ethanol (ε = 25)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.099315	-0.701568	0.000002
2	6	0	0.984971	-1.610716	0.000003
3	6	0	2.308245	-1.195460	0.000000
4	6	0	2.491260	0.254738	-0.000003
5	6	0	1.441015	1.140661	-0.000004
6	6	0	0.099915	0.703025	-0.000002
7	6	0	-0.985785	1.611263	0.000001
8	6	0	-2.308613	1.195589	0.000000
9	6	0	-2.491171	-0.254767	-0.000005
10	6	0	-1.440583	-1.139819	-0.000008
11	6	0	3.820556	0.814384	-0.000002
12	7	0	4.879815	0.105278	0.000003
13	8	0	3.315349	-1.971310	0.000005
14	6	0	-3.820239	-0.814951	-0.000003
15	7	0	-4.879476	-0.105992	0.000003
16	8	0	-3.316322	1.970983	0.000006
17	1	0	3.932337	1.885969	-0.000008
18	1	0	4.691297	-0.896742	0.000005
19	1	0	0.783191	-2.668034	0.000009
20	1	0	1.641658	2.198603	-0.000004
21	1	0	-3.931671	-1.886573	-0.000010
22	1	0	-4.690765	0.896093	0.000007
23	1	0	-0.784829	2.668840	0.000001
24	1	0	-1.640489	-2.197900	-0.000009
25	6	0	6.239960	0.618073	0.000000
26	1	0	6.222327	1.698329	-0.000006
27	1	0	6.755260	0.262624	0.882032
28	1	0	6.755261	0.262613	-0.882027
29	6	0	-6.239598	-0.618848	0.000002
30	1	0	-6.222012	-1.699105	-0.000006
31	1	0	-6.754925	-0.263360	0.882002
32	1	0	-6.754928	-0.263348	-0.881992

E(RHF) = -797.079588182 A.U.

E(RB3LYP) = -802.065029507 A.U.