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Supplementary information

Harnessing Remote Synergistic Effect for Regulating Photoinduced Electron Transfer: A Novel Strategy for Absorption/Fluorescence Dual-Mode Hydrochromism

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1. Experimental section

Materials.

Methyl iodide (98%), sodium hydride (98%), and acryloyl chloride (98%) were purchased from Energy Chemical (Shanghai, China). Rhodamine B (**RhB**) (95 %) was purchased from Aladdin (Shanghai, China). Unless otherwise noted, all the other materials were purchased from Sinopharm Chemical Reagent Company Limited (Beijing, China), without further purification. Water (H_2O) was purified by the Milli-Q system for labpartner technology development company limited (Changchun, China). Polyethylene glycol (PEG) 20000 (molecular weight: 17000-22000) was purchased from Guangfu Fine Chemical Research Institute (Tianjin, China). Cellulose filter paper (Whatman-Xinhua, grade 91, Hangzhou, China) was selected as the solid substrate.

Instrument.

Absorption spectra and reflective UV-vis spectra (by reflective mode of integrating sphere, using barium sulfate as background) were measured using a Analitik Jena Specord®210 plus UV-vis spectrophotometer. Steady State fluorescence spectra were measured using a Shimadzu RF-5301 PC spectrophotometer. The fluorescence quantum yields were recorded on FLS 920 lifetime and steady state spectrometer. Proton nuclear magnetic resonance spectra (^{1}H NMR) (500 MHz) and ^{13}C NMR (126 MHz) spectra were recorded on a Bruker AVANCE500 at room temperature. ^{1}H NMR (400 MHz) spectra and ^{13}C NMR (101 MHz) spectra were recorded on a Zhongke Oxford Instrument Company AS 400 at room temperature. LC-HRMS analysis was performed on an Agilent 1290-micro TOF-Q II mass spectrometer.

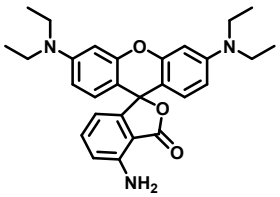
Calculation Method.

The ground and excited state geometries and electronic structures of **RhB** derivatives were optimized using density functional theory (DFT) and time-dependent DFT (TD-DFT) with the consideration of the Solvation Model Based on Density (SMD) to simulate the aqueous environment[1]. Frequency analysis was conducted on the optimized structures, revealing no imaginary frequencies, indicating that all optimized

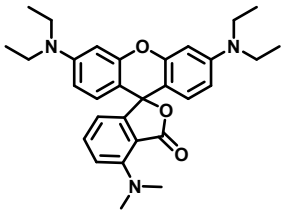
geometries are stable. The hole electron orbitals and frontier molecular orbitals of RhB derivatives were analyzed using Multiwfn 3.8 and VMD 1.9.4 programs[2-4]. The root mean square displacement (RMSD) calculations between molecules were performed using the PyMol program[5]. All calculations were conducted at the M06-2X/TZVP level using Gaussian 16 software[6-8].

2. Preparation/Synthesis

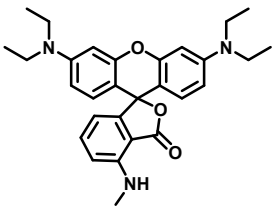
Synthesis of RhB derivatives.



NH_2-RhB was synthesized according to reported literature[9]. ^{1}H NMR (500 MHz, dimethyl sulfoxide-d_6 (DMSO-d_6)) δ 7.34 (t, *J* = 7.7 Hz, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 6.55 (d, *J* = 8.8 Hz, 2H), 6.47 – 6.38 (m, 6H), 6.18 (d, *J* = 7.2 Hz, 1H), 3.36 (q, *J* = 13.8, 6.8 Hz, 8H), 1.09 (t, *J* = 6.9 Hz, 12H). LC-HRMS (ESI) calculated for $C_{28}H_{31}N_3O_3$ $[M + H]^+$: 458.2438, found: 458.2435.

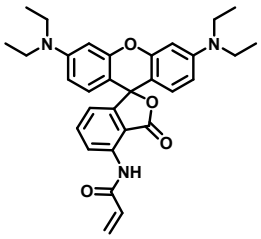


NMe_2-RhB was obtained as a dark red solid powder (166 mg, 70%). **NH_2-RhB** (0.5 mmol, 228.8 mg) and sodium hydroxide (2.0 mmol, 80 mg) were added to a 50 ml round bottom flask. Under the protection of argon, dry tetrahydrofuran (20 mL) was added to the flask and stirred to change color, then methyl iodide (0.7 mmol, 50 μl) was added into the bottom flask. The reaction was stirred for 18 hours at room temperature. H_2O (10 mL) was added into the flask to quench the reaction. The reaction mixture was extracted with ethyl acetate (30 mL), and then the combined organic layers were washed with saturated sodium chloride solution (30 mL), dried over anhydrous sodium sulfate. Finally, the column chromatography was performed using petroleum ether, ethyl acetate, and methanol as eluent to afford the products **NMe_2-RhB**. Melt point: 183.7-184.8 °C. ^{1}H NMR (400 MHz, deuterium chloroform ($CDCl_3$)) δ 7.41 (t, *J* = 8.0 Hz, 1H), 6.85 (d, *J* =8.0 Hz 1H), 6.68 (d, *J* = 12 Hz, 2H), 6.54 (d, *J* = 8.0 Hz, 1H), 6.42 (s, 2H), 6.34 (d, *J* = 12.0 Hz, 2H), 3.34 (m, 8H), 3.14 (s, 6H), 1.16 (t, *J* = 8.0 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.55, 157.03, 153.11, 151.48, 149.25, 135.31, 128.95, 115.18, 114.54, 114.25, 108.02, 106.88, 97.59, 82.15, 44.48, 43.78, 12.56. LC-HRMS calculated for $C_{30}H_{35}N_3O_3$ $[M + H]^+$: 486.2751, found: 486.2755.



NHMe-RhB: NHMe-RhB was obtained as a magenta solid powder (8 mg, 10%). Melt point: 179.2-180.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (t, *J* = 8.0 Hz, 1H), 6.70 (d, *J* = 8.0

Hz, 2H), 6.59 (d, *J* = 4.0 Hz, 1H), 6.54 (s, 1H), 6.42 (s, 2H), 6.34 (m, 3H), 3.34 (m, 8H), 3.00 (s, 3H), 1.17 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.63, 154.46, 153.24, 149.36, 148.17, 136.54, 128.97, 110.17, 109.67, 108.34, 107.96, 106.60, 97.66, 85.32, 44.49, 29.34, 12.58. LC-HRMS calculated for $C_{29}H_{33}N_3O_3$ $[M + H]^+$: 472.2595, found: 472.2592.



$NHCOC_2H_3$-RhB was synthesized according to reported literature[10]. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.23 (s, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.63 - 6.55 (m, 3H), 6.48 – 6.44 (m, 4H), 6.36 (d, *J* = 16 Hz, 1H), 5.91(d, J = 4.0 Hz, 1H), 3.36 (m, 8H), 1.10 (m, 12H). LC-HRMS calculated for $C_{31}H_{33}N_3O_4$ $[M + H]^+$: 512.2544, found: 512.2540.

Preparation for solutions of RhB derivatives in binary* acetonitrile (MeCN) *and H_2O solvents.

Firstly, prepare a stock solution of RhB derivatives (**NMe_2-RhB**, **NH_2-RhB**, **NHMe-RhB**, **$NHCOC_2H_3$-RhB**, and **RhB**) (C = 1 × 10^{-4} M) in MeCN. Taking **NMe_2-RhB** as an example, transfer its 1 mL stock solution to ten 10 mL volumetric flasks. Then add 0, 1, 2, 3, 4, 5, 6, 7, 8, and 9 mL H_2O to the ten flasks. Finally, fill the flasks to the mark with MeCN, obtaining **RhB** derivatives (C = 1 × 10^{-5} M) solutions with different H_2O content (from 0% to 90%, by volume), respectively.

Preparation of dual-mode hydrochromic material.

The hydrochromic **NMe_2-RhB** material was prepared in a layer-by-layer way, referring to previous work[11]. The filter paper substrate was coated with 10 wt % PEG aqueous solution and dried at 70 °C. Then the solution including **NMe_2-RhB** (1 × 10^{-4} M) and 6 wt % PEG in MeCN-H_2O (v/v = 2/3, by volume) was coated over the PEG-modified paper and dried at 70 °C.

3. Nuclear magnetic resonance spectra of NHMe-RhB and NMe_2-RhB.

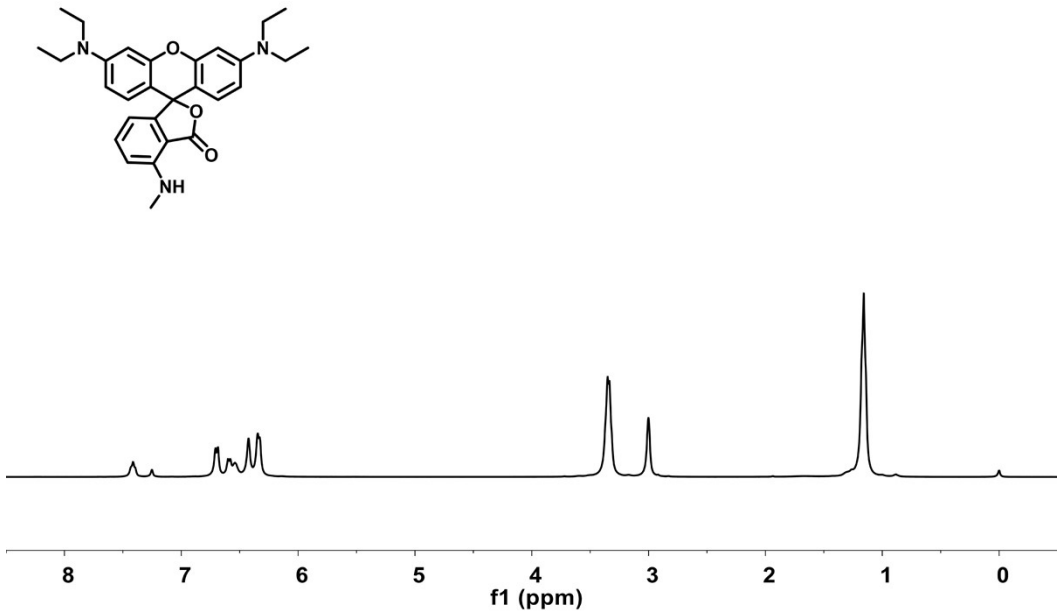


Figure S1. ^{1}H NMR spectrum of **NHMe-RhB** in $CDCl_3$.

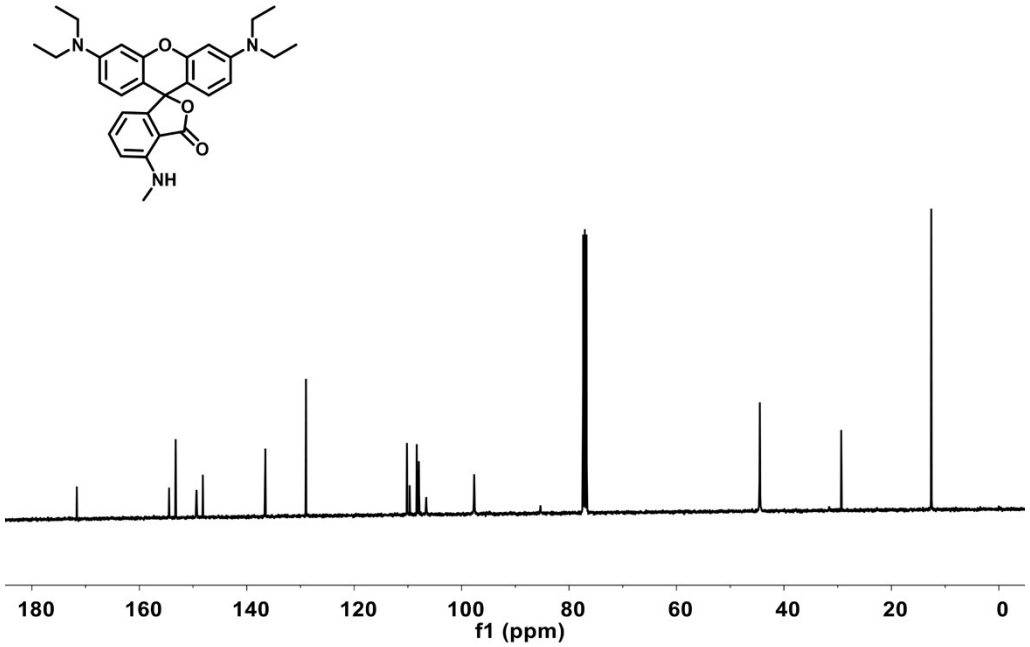


Figure S2. ^{13}C NMR spectrum of **NHMe-RhB** in $CDCl_3$.

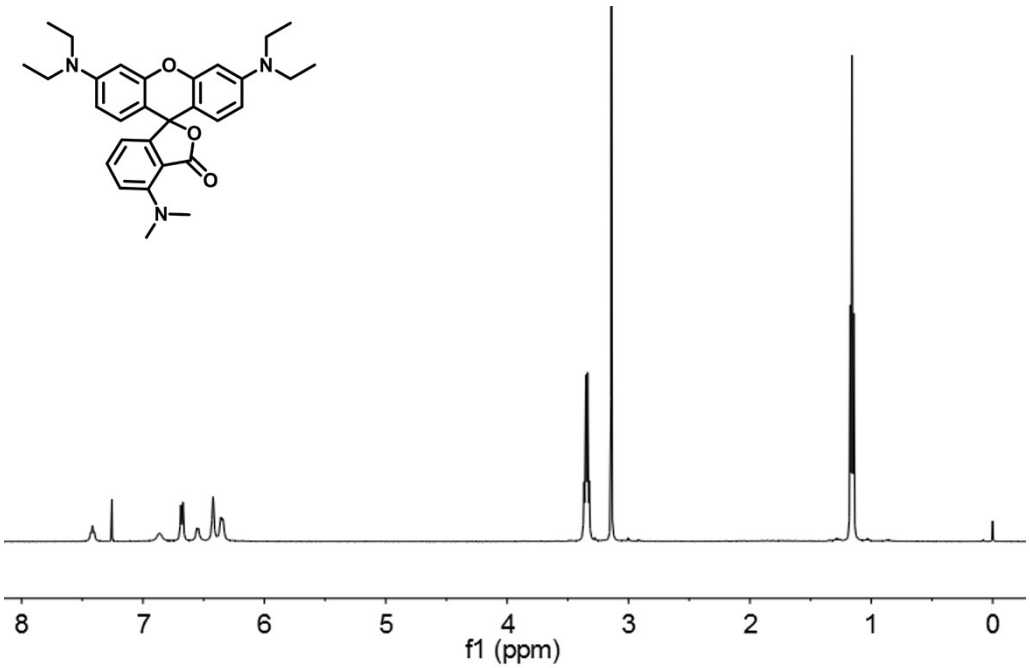


Figure S3 ^{1}H NMR spectrum of **NMe_2-RhB** in $CDCl_3$.

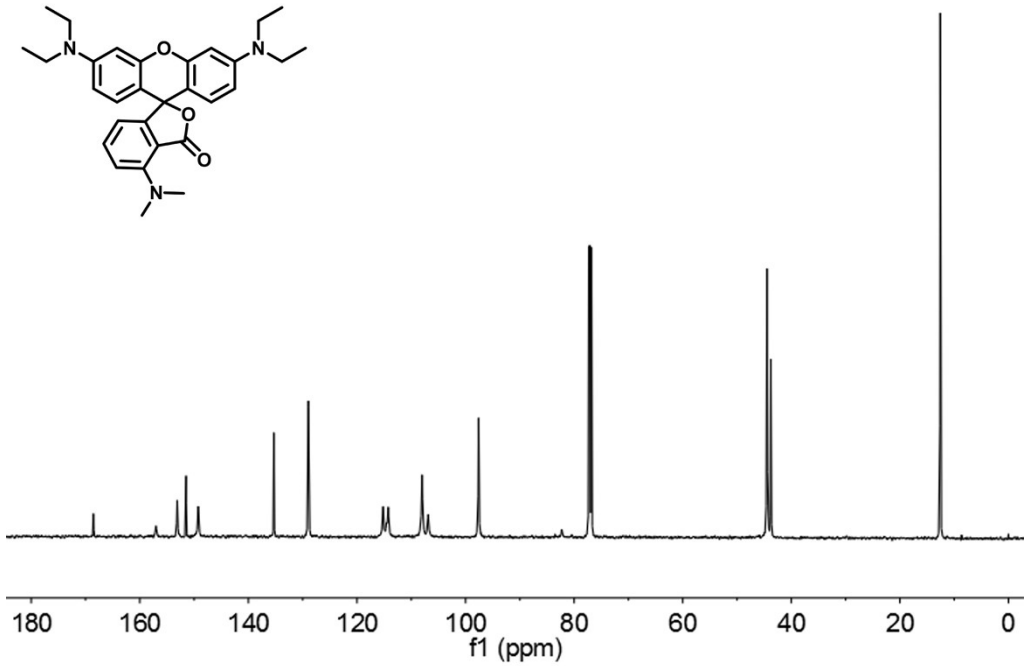


Figure S4 ^{13}C NMR spectrum of **NMe_2-RhB** in $CDCl_3$.

4. Test for dual-mode hydrochromic properties of RhB derivatives

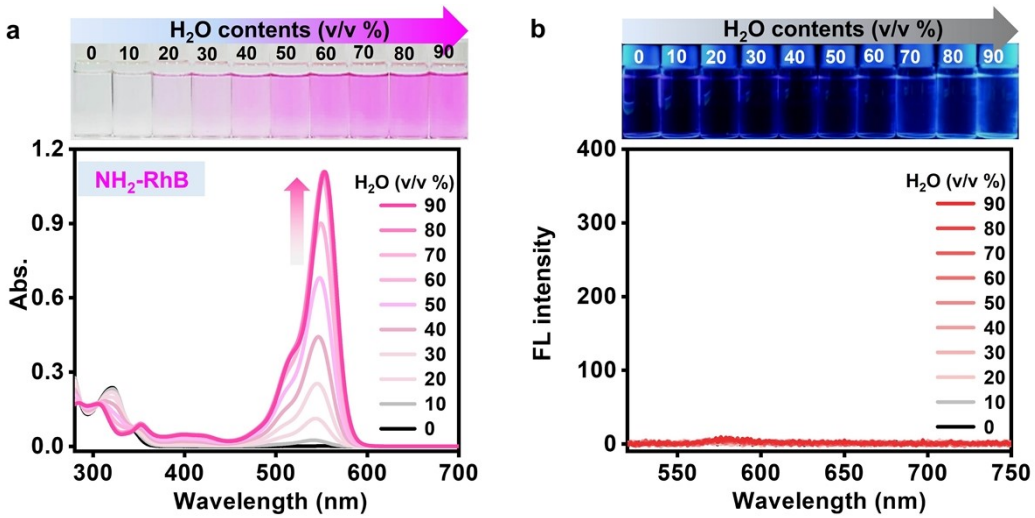


Figure S5. (a) Photographs and corresponding UV-vis absorption spectra of **NH_2-RhB** (1×10^{-5} M) in binary MeCN-H_2O solutions with H_2O percentage from 0% to 90% by volume. (b) Photographs (under 365 nm UV (ultraviolet) irradiation) and fluorescence emission spectra (λ_{ex} = 568 nm, slit width = 1.5, 1.5) of **NH_2-RhB** (1×10^{-5} M) in variable MeCN-H_2O mixtures with H_2O percentage (0% - 90%, by volume).

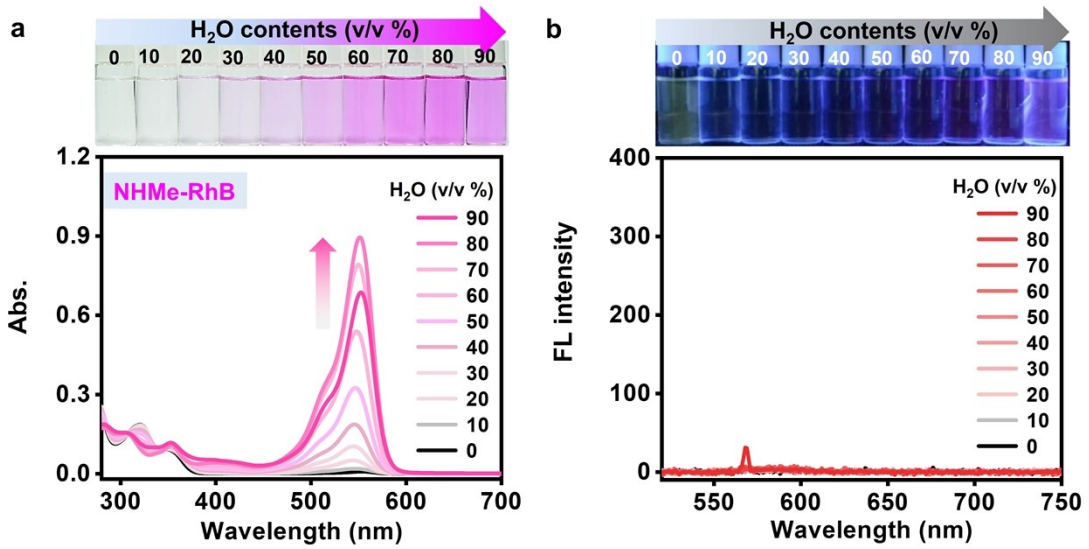


Figure S6. (a) Photographs and corresponding UV-vis absorption spectra of **NHMe-RhB** (1×10^{-5} M) in binary MeCN-H_2O solutions with H_2O percentage from 0% to 90% by volume. (b) Photographs (under 365 nm UV irradiation) and fluorescence emission spectra (λ_{ex} = 568 nm, slit width = 1.5, 1.5) of **NHMe-RhB** (1×10^{-5} M) in variable MeCN-H_2O mixtures with H_2O contents (0% - 90%, by volume).

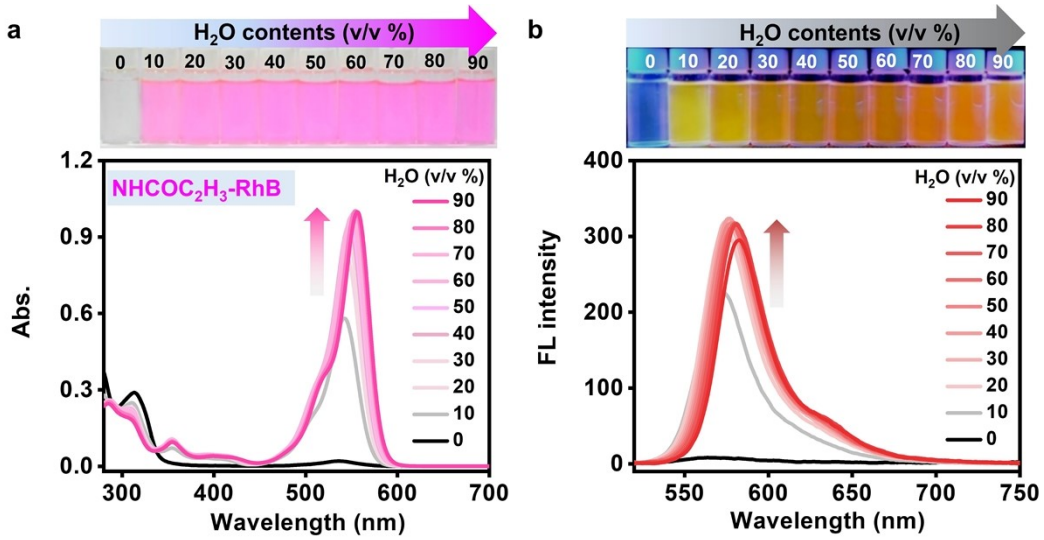


Figure S7. (a) Photographs and corresponding UV-vis absorption spectra of **$NHCOC_2H_3$-RhB** (1×10^{-5} M) in binary MeCN-H_2O solutions as increasing percentage of H_2O by volume from 0% to 90%. (b) Photographs (under 365 nm UV irradiation) and fluorescence emission spectra (λ_{ex} = 568 nm, slit width = 1.5, 1.5) of **$NHCOC_2H_3$-RhB** (1×10^{-5} M) in variable MeCN-H_2O mixtures as increasing percentage of H_2O by volume from 0% to 90%.

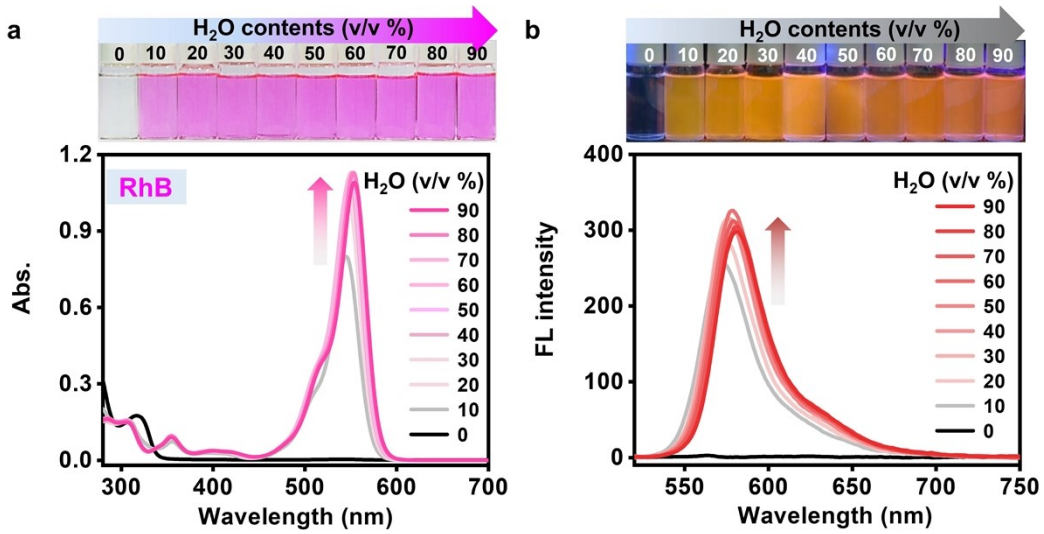


Figure S8. (a) Photographs and corresponding UV-vis absorption spectra of **RhB** (1×10^{-5} M) in binary MeCN-H_2O solutions as increasing percentage of H_2O by volume from 0% to 90%. (b) Photographs (under 365 nm UV irradiation) and fluorescence emission spectra (λ_{ex} = 568 nm, slit width = 1.5, 1.5) of **RhB** (1×10^{-5} M) in variable MeCN-H_2O mixtures as increasing percentage of H_2O by volume from 0% to 90%.

5. Base state geometry and dihedral angles of RhB derivatives

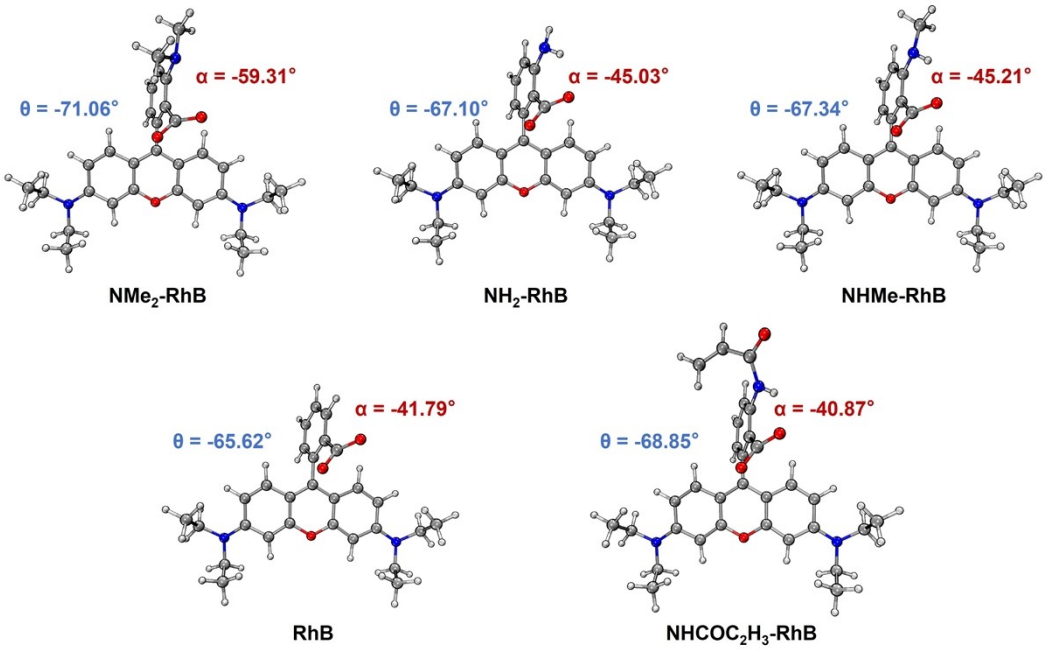


Figure S9. Base state geometry and dihedral angles α and θ of the studied molecules.

6. Absorption characteristics of RhB derivatives

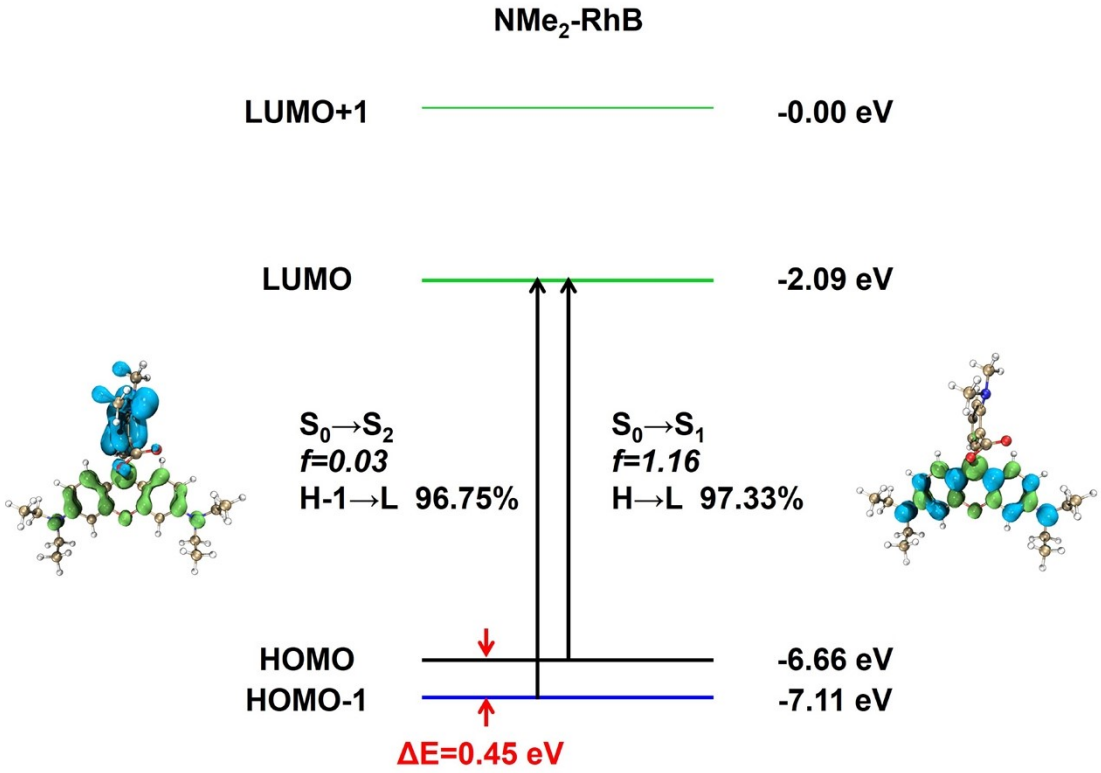


Figure S10. The absorption spectra oscillator strengths and orbital transition forms, as well as hole-electron distribution diagrams of **NMe_2-RhB**. Green represents electron distribution, and blue represents hole distribution.

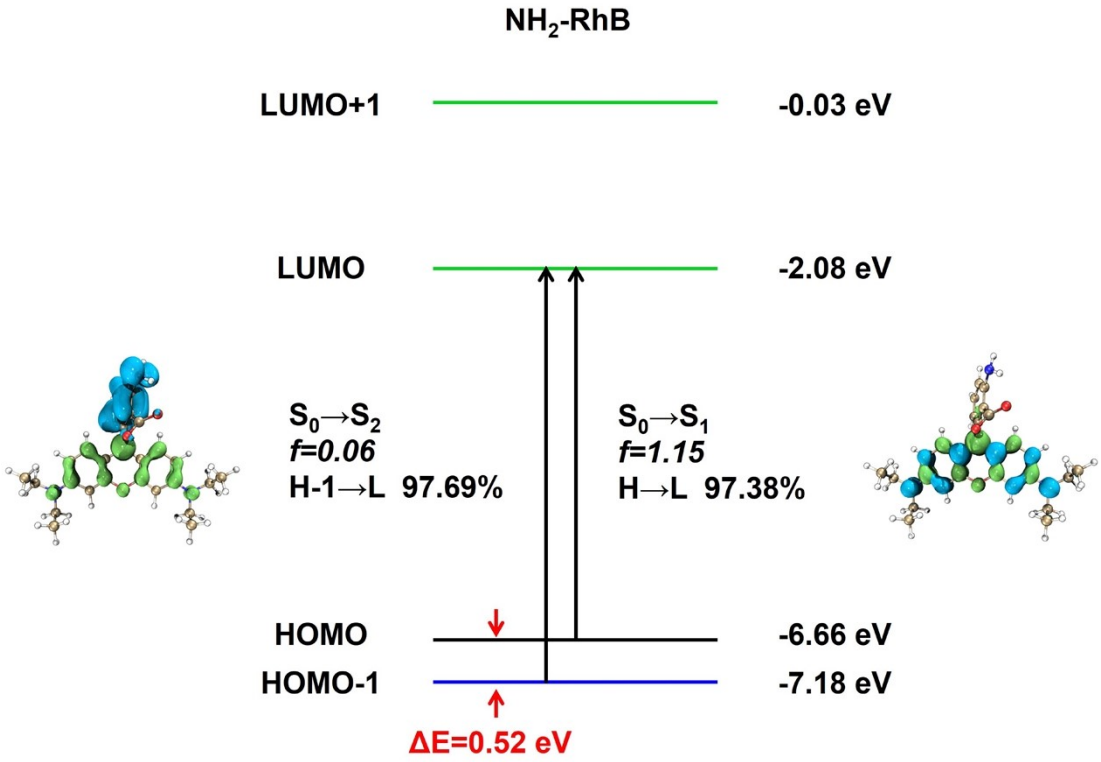


Figure S11. The absorption spectra oscillator strengths and orbital transition forms, as well as hole-electron distribution diagrams of **NH_2-RhB**. Green represents electron distribution, and blue represents hole distribution.

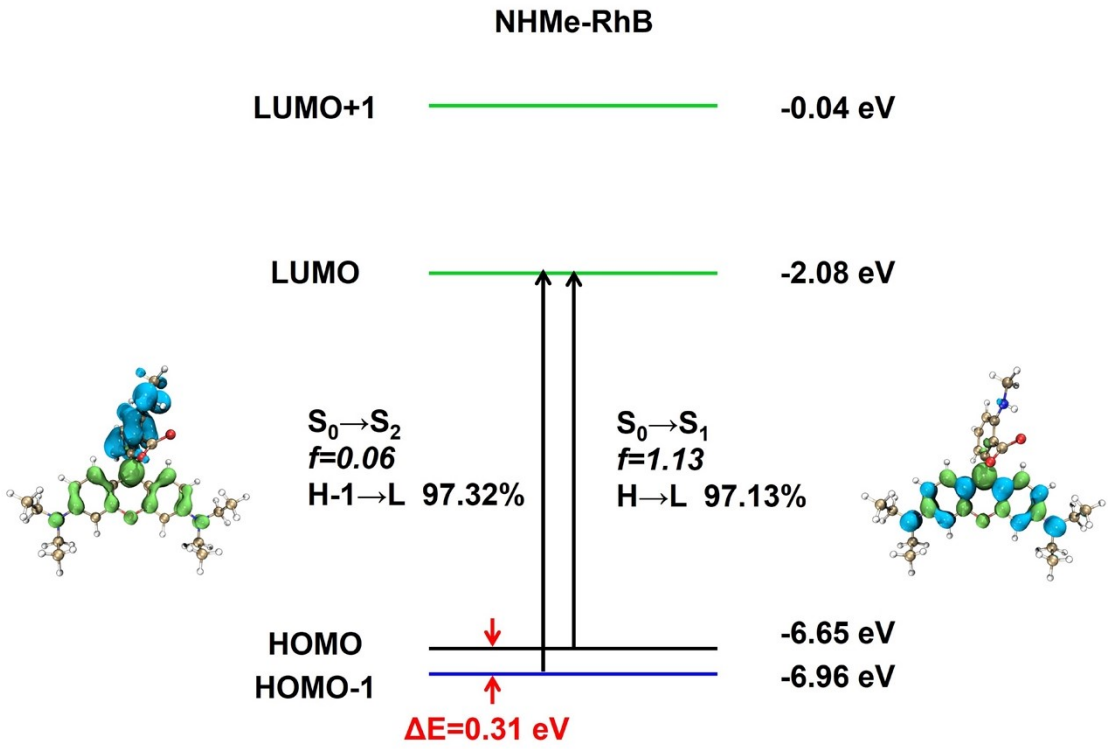


Figure S12. The absorption spectra oscillator strengths and orbital transition forms, as well as hole-electron distribution diagrams of **NHMe-RhB**. Green represents electron distribution, and blue represents hole distribution.

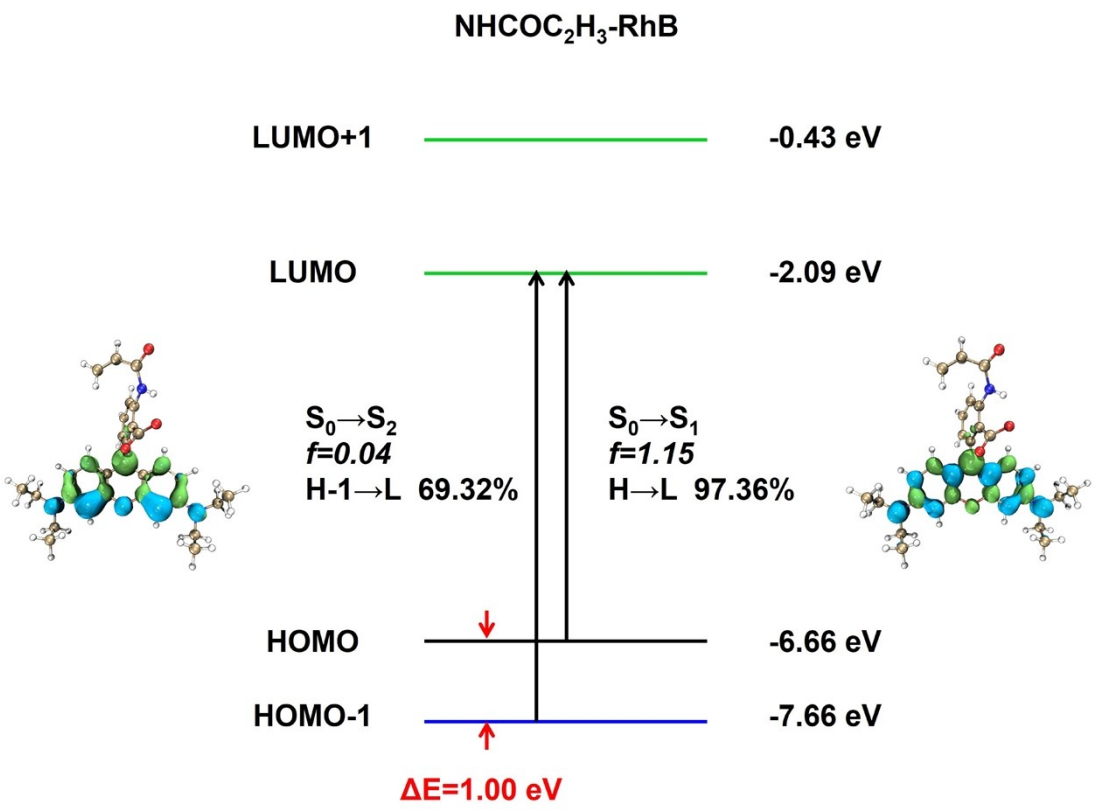


Figure S13. The absorption spectra oscillator strengths, and orbital transition forms, as well as hole-electron distribution diagrams of **$NHCOC_2H_3$-RhB**. Green represents electron distribution, and blue represents hole distribution.

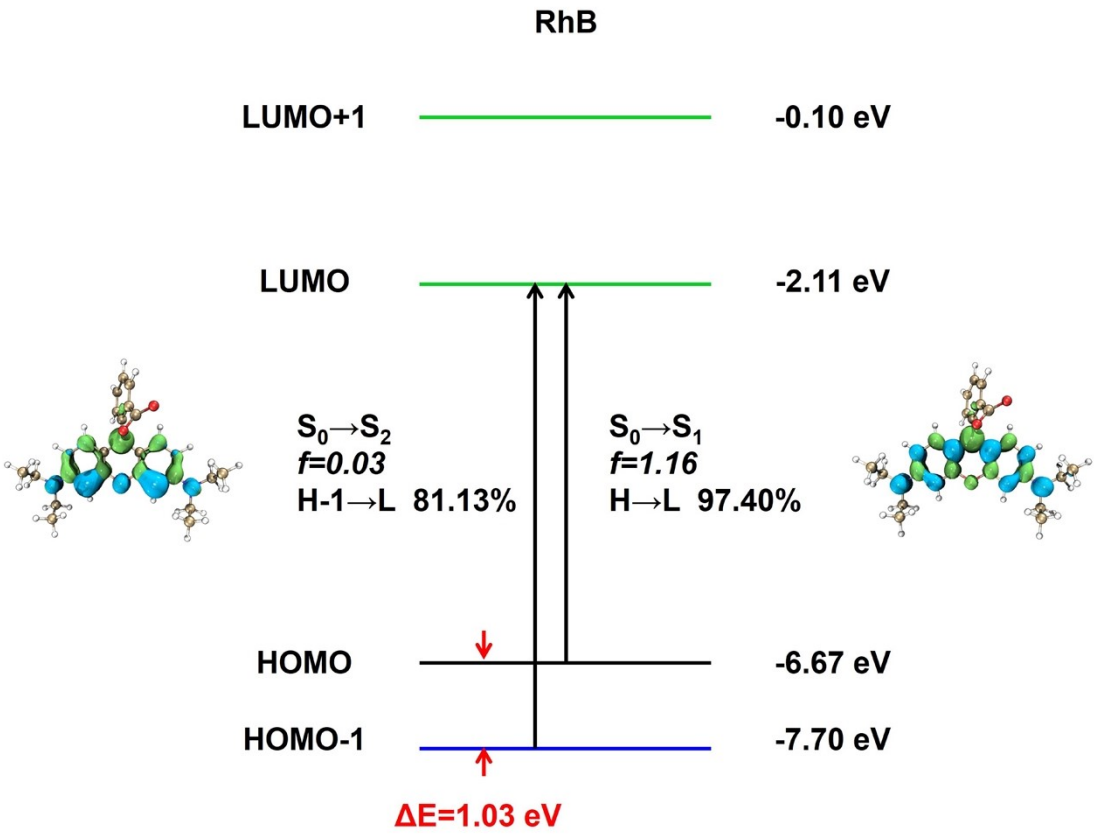


Figure S14. The absorption spectra oscillator strengths and orbital transition forms, as well as hole-electron distribution diagrams of **RhB**. Green represents electron distribution, and blue represents hole distribution.

7. Schematic illustration of water-jet printing

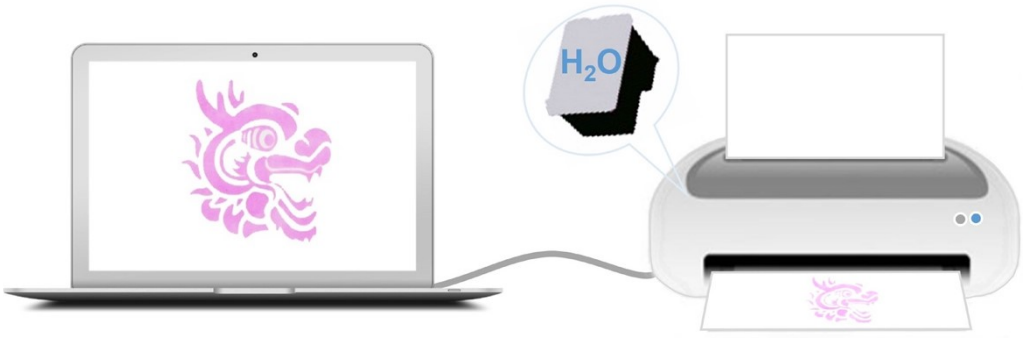


Figure S15. Schematic illustration of water-jet printing (WJP).

8. Cartesian Coordinates of Optimized Geometry

The minimum energy conformation of **NMe_2-RhB** in the S_0 state

C	1.26179800	1.96959900	1.37551900
C	0.92572100	2.69399300	0.07683400
C	1.25081400	4.04908300	-0.15188100
C	0.97132400	4.59367400	-1.41083900
H	1.20745200	5.62705300	-1.61864400
C	0.37727100	3.83557200	-2.41041900
H	0.17623400	4.28814500	-3.37338200
C	0.02613100	2.51838100	-2.17713500
H	-0.44651300	1.91986500	-2.94588200
C	0.30361700	1.95619600	-0.93152600
C	-0.03265700	0.52159800	-0.72923200
C	0.98008400	-0.44485800	-0.68414800
C	2.36691700	-0.16509900	-0.82703300
H	2.67589000	0.85672900	-1.00654800
C	3.30570100	-1.14284300	-0.75099000
H	4.34438300	-0.87600500	-0.87071600
C	2.93712400	-2.51437700	-0.52900400
C	1.56146900	-2.81255000	-0.40401700
H	1.20254700	-3.81451700	-0.22572100
C	0.63379100	-1.80503400	-0.48860700
C	-1.66654500	-1.25499500	-0.43535500
C	-2.94455000	-1.73655900	-0.29943500
H	-3.06923800	-2.79779900	-0.14828900
C	-4.04037500	-0.84518500	-0.34075400
C	-3.75401000	0.55659500	-0.48242000
H	-4.55872600	1.27533300	-0.48463500
C	-2.47890500	1.00440600	-0.61830900
H	-2.29527000	2.06588100	-0.72418200
C	-1.36943000	0.11698100	-0.62052800
C	3.50536700	-4.87553700	-0.24638500
H	4.31215200	-5.48719400	-0.64670000
H	2.61927800	-5.10499200	-0.83640700
C	3.27790400	-5.20375700	1.22311400
H	4.20510400	-5.11274900	1.78899500
H	2.91900900	-6.22960600	1.31811500
H	2.53529100	-4.53691600	1.66436500
C	5.30121100	-3.14228600	-0.36484200
H	5.58193900	-2.47402200	-1.17934400
H	5.84860700	-4.06969500	-0.52034200
C	5.67770200	-2.53760300	0.98149800
H	5.12045600	-1.62104700	1.17898800
H	6.74155900	-2.29577500	0.98503200
H	5.48188900	-3.23977900	1.79151700
C	-5.59676700	-2.71062500	-0.07751200
H	-6.61641100	-2.87770700	-0.41974200
H	-4.94867600	-3.28889200	-0.73545300
C	-5.44761800	-3.17010600	1.36700800
H	-4.45753400	-2.93078900	1.75785800
H	-5.58594200	-4.25088300	1.42245800
H	-6.19436400	-2.69740000	2.00464700
C	-6.43415600	-0.35372500	-0.13054800
H	-6.35623900	0.41788800	-0.89652500
H	-7.33633700	-0.92039800	-0.35131300
C	-6.53885800	0.27007700	1.25498200
H	-6.72489500	-0.49150800	2.01172100
H	-7.36684700	0.98037600	1.27188000
H	-5.62606800	0.80425500	1.52210300
N	1.86467400	4.81822100	0.85986400
N	3.87563200	-3.47742000	-0.48060500
N	-5.30989100	-1.28678900	-0.27279600
O	-0.66751300	-2.17243400	-0.36761000
O	0.30070000	1.45893100	2.00194800
O	2.46712000	1.90396100	1.70740300
C	2.32981800	6.13922900	0.46010500
H	2.88998500	6.56658100	1.29073700
H	2.99438800	6.06856100	-0.39963500
H	1.50502200	6.82276800	0.21811700
C	1.09499500	4.92709700	2.10227000
H	0.73106800	3.96366900	2.44542800
H	1.73444200	5.34226100	2.88062500
H	0.23167100	5.59251200	1.96922300

The minimum energy conformation of **NH_2-RhB** in the S_0 state

C	1.13276700	2.43586300	1.68043900	H	6.02768600	-2.43652800	1.62575700
C	0.72435500	3.13732700	0.39779000	C	-5.19920500	-2.97001400	-0.31378000
C	0.93168600	4.52031900	0.24300700	H	-6.18251800	-3.20707300	-0.71674700
C	0.50378100	5.14297700	-0.93736400	H	-4.47066800	-3.38770800	-1.00752900
H	0.65766000	6.21056500	-1.04661300	C	-5.04065900	-3.58119100	1.07211700
C	-0.09460000	4.41490300	-1.94778300	H	-4.09791100	-3.27868500	1.53088100
H	-0.40761700	4.91556800	-2.85557500	H	-5.05223600	-4.66943300	0.99567500
C	-0.29184700	3.04584400	-1.80931400	H	-5.85758200	-3.27657100	1.72633200
H	-0.74665200	2.46601700	-2.60239000	C	-6.29338600	-0.73897200	-0.04817100
C	0.11870200	2.41709100	-0.63729400	H	-6.35119400	0.10487900	-0.73630600
C	-0.04776000	0.94352100	-0.54924400	H	-7.13144800	-1.39146400	-0.28424500
C	1.07397100	0.10133500	-0.56747900	C	-6.39779100	-0.26406400	1.39533400
C	2.42021100	0.55201800	-0.63725400	H	-6.43176500	-1.10994700	2.08148100
H	2.61298100	1.61490200	-0.70639000	H	-7.31261600	0.31720000	1.52009700
C	3.46771900	-0.31277600	-0.62531500	H	-5.55319100	0.36825500	1.67142300
H	4.46874200	0.08624900	-0.67734900	N	1.47461700	5.28447900	1.26325200
C	3.26168800	-1.73296600	-0.55391400	H	1.82811100	6.18341400	0.96622200
C	1.92907500	-2.19798800	-0.49246800	H	2.10916900	4.77815700	1.86708500
H	1.68570500	-3.24735700	-0.42753000	N	4.30499400	-2.58352300	-0.58188100
C	0.88982600	-1.30115100	-0.50519900	N	-5.07527600	-1.51025400	-0.32790300
C	-1.45974100	-1.03469900	-0.45062000	O	-0.35975700	-1.83025000	-0.45370900
C	-2.67197100	-1.67516900	-0.37843000	O	0.31276400	1.63250800	2.18353600
H	-2.66848100	-2.75302800	-0.32493100	O	2.26436100	2.71498100	2.15387900
C	-3.86555200	-0.92024400	-0.34466600				
C	-3.74797300	0.51237500	-0.35176000				
H	-4.63375500	1.12633100	-0.30018600				
C	-2.53564200	1.11919700	-0.43049900				
H	-2.48108500	2.19991900	-0.43501500				
C	-1.32725900	0.37433900	-0.50230400				
C	4.09769700	-4.02657100	-0.43090200				
H	4.99023600	-4.51542400	-0.81637200				
H	3.27308600	-4.33075500	-1.07511100				
C	3.84572100	-4.45837000	1.00803400				
H	4.72530900	-4.28032700	1.62626100				
H	3.61884800	-5.52518800	1.03454500				
H	3.00296200	-3.91841600	1.44215100				
C	5.68552800	-2.09427000	-0.48575600				
H	5.83433800	-1.30155700	-1.21878800				
H	6.32872900	-2.91890300	-0.78606000				
C	6.06736500	-1.61662900	0.90905800				
H	5.40082500	-0.82509800	1.25438500				
H	7.08481300	-1.22302500	0.89334600				

The minimum energy conformation of **NHMe-RhB** in the S_0 state

C	1.33183000	2.13127900	1.58253100	H	5.53057700	-3.29037200	1.70070900
C	1.00291000	2.84080300	0.28118900	C	-5.59629600	-2.54862700	-0.19853200
C	1.37352800	4.19114300	0.08054300	H	-6.61591100	-2.68752800	-0.55353000
C	1.01231500	4.81456800	-1.12375200	H	-4.94856600	-3.07600100	-0.89805200
H	1.27765000	5.84895400	-1.29344600	C	-5.45010400	-3.11787500	1.20665800
C	0.32036100	4.12070400	-2.10299200	H	-4.46061100	-2.91030700	1.61678100
H	0.06017700	4.62360900	-3.02628900	H	-5.58947600	-4.19958600	1.17874000
C	-0.03525800	2.79359800	-1.91713600	H	-6.19782800	-2.69493200	1.87719700
H	-0.56242500	2.24302800	-2.68582600	C	-6.42771000	-0.19385000	-0.05619400
C	0.31066600	2.16273100	-0.72199500	H	-6.35741500	0.63519100	-0.76031800
C	-0.02648700	0.72208300	-0.58704600	H	-7.33345700	-0.74070400	-0.30972600
C	0.98777800	-0.24713700	-0.58930900	C	-6.51480300	0.32055800	1.37485200
C	2.37769100	0.03937400	-0.67155400	H	-6.69306000	-0.49699200	2.07286600
H	2.69432600	1.07040900	-0.76387800	H	-7.34128900	1.02812600	1.45660600
C	3.31534700	-0.94319500	-0.64479400	H	-5.59820900	0.83210900	1.67153700
H	4.35642300	-0.66756100	-0.71221600	N	2.02356200	4.89165700	1.07521700
C	2.94227600	-2.32713600	-0.54603900	H	2.54779900	4.29158900	1.69815000
C	1.56447000	-2.62984100	-0.47418800	N	3.87757700	-3.29563100	-0.56068000
H	1.20009800	-3.64162100	-0.38514600	N	-5.30709400	-1.11441400	-0.28418500
C	0.63856800	-1.61652200	-0.50160000	O	-0.66467900	-1.99281300	-0.43707300
C	-1.66256800	-1.07220000	-0.44162200	O	0.42436300	1.44675300	2.10967800
C	-2.94149700	-1.56239100	-0.34933700	O	2.49240300	2.28052700	2.04663100
H	-3.06675300	-2.63191200	-0.27870700	C	2.64834000	6.16654200	0.77479500
C	-4.03688200	-0.67040500	-0.32189300	H	1.89766800	6.93047900	0.56975500
C	-3.74959900	0.73772600	-0.35645300	H	3.21699300	6.48083500	1.64660200
H	-4.55377300	1.45518300	-0.30349300	H	3.32586000	6.11180800	-0.08409000
C	-2.47421000	1.19398100	-0.45562300				
H	-2.29070400	2.26027600	-0.47803900				
C	-1.36386200	0.30945700	-0.52129200				
C	3.49821100	-4.70425900	-0.42255000				
H	4.31766600	-5.29335700	-0.83024600				
H	2.63238900	-4.89605200	-1.05544400				
C	3.21841400	-5.12129600	1.01554400				
H	4.12454500	-5.06911400	1.61887700				
H	2.85457800	-6.14965600	1.03391700				
H	2.46129200	-4.48136400	1.47149500				
C	5.30440800	-2.97464000	-0.43074500				
H	5.57301900	-2.22753000	-1.17770400				
H	5.84951700	-3.88077300	-0.68732800				
C	5.70131800	-2.50660200	0.96328000				
H	5.13678200	-1.62282200	1.26339900				
H	6.76216000	-2.25185400	0.97201600				

The minimum energy conformation of **RhB** in the S_0 state

C	1.14031300	2.63447300	1.83771400	H	6.19682200	-2.04622500	1.57805300
C	0.65271300	3.32835100	0.57602400	C	-5.01464300	-3.01465900	-0.41884100
C	0.78236500	4.70993400	0.46951400	H	-5.98250800	-3.28175700	-0.83968900
C	0.30632800	5.38543100	-0.64577300	H	-4.26127800	-3.36875700	-1.12157800
H	0.40356000	6.46196800	-0.70764000	C	-4.83653700	-3.67243100	0.94303500
C	-0.29093300	4.67743700	-1.68095200	H	-3.91134700	-3.34605000	1.42070600
H	-0.65736600	5.19519600	-2.55817500	H	-4.79790200	-4.75614100	0.82343300
C	-0.41400800	3.29799200	-1.59332500	H	-5.67033500	-3.43150700	1.60234900
H	-0.86349900	2.73700600	-2.40418500	C	-6.21913700	-0.84719300	-0.09654800
C	0.05215400	2.61727200	-0.46880200	H	-6.29443900	0.02324700	-0.74876400
C	-0.04946400	1.13669000	-0.44943000	H	-7.02064500	-1.52337200	-0.38646300
C	1.10906200	0.34790400	-0.50741000	C	-6.38458100	-0.44226600	1.36242000
C	2.43382100	0.86056700	-0.56009200	H	-6.40720200	-1.31879000	2.00939200
H	2.58091100	1.93250100	-0.59283500	H	-7.32380800	0.09936900	1.48410200
C	3.51932000	0.04408000	-0.57903200	H	-5.57246000	0.20689100	1.69202100
H	4.50080100	0.49048300	-0.61689700	N	4.45684000	-2.18787400	-0.61600500
C	3.37754700	-1.38568000	-0.55729800	N	-4.96042300	-1.55097900	-0.37332500
C	2.06710400	-1.91186700	-0.51187900	O	-0.23575400	-1.64936600	-0.46379200
H	1.87170500	-2.97289700	-0.48313800	O	0.40551000	1.73963200	2.32065400
C	0.98869900	-1.06295800	-0.49475100	O	2.23368600	3.02551700	2.31196800
C	-1.37073000	-0.90550400	-0.43308600	H	1.25340900	5.25543600	1.27779100
C	-2.55242500	-1.60274300	-0.39860300				
H	-2.50025200	-2.68054600	-0.39430200				
C	-3.78011900	-0.90543200	-0.34573800				
C	-3.72788800	0.52977400	-0.28348800				
H	-4.64000100	1.10111600	-0.20909500				
C	-2.54409800	1.19407600	-0.32407400				
H	-2.54109000	2.27510500	-0.27577600				
C	-1.30214400	0.50941100	-0.42237000				
C	4.31288200	-3.64264600	-0.50920100				
H	5.22645000	-4.08041900	-0.90617400				
H	3.50356000	-3.96331000	-1.16486700				
C	4.07763800	-4.12780200	0.91546800				
H	4.94624900	-3.92646900	1.54206900				
H	3.90140200	-5.20445400	0.90981800				
H	3.20924300	-3.64149100	1.36221500				
C	5.81561500	-1.64195200	-0.51547900				
H	5.92083800	-0.81756000	-1.22041800				
H	6.49133500	-2.42534400	-0.85265400				
C	6.19242300	-1.19941700	0.89216800				
H	5.49610800	-0.45115600	1.27341600				
H	7.19161500	-0.76141800	0.88094300				

The minimum energy conformation of **$NHCOC_2H_3$-RhB** in the S_0 state

C	2.15771000	-0.39370000	-1.32335400
C	2.29457800	-1.08201100	0.03809300
C	3.44298100	-1.81232900	0.37395900
C	3.55401700	-2.41093500	1.62888000
H	4.46108900	-2.93783600	1.89096800
C	2.51273700	-2.32571900	2.53600700
H	2.60714800	-2.79325000	3.50734200
C	1.36107800	-1.62042000	2.21398900
H	0.55193800	-1.53222200	2.92839800
C	1.26047700	-0.99363600	0.97492300
C	0.04690200	-0.18109000	0.70661800
C	0.12931800	1.21818700	0.65490200
C	1.33384200	1.95914000	0.78684300
H	2.25723200	1.42411700	0.96703400
C	1.35502600	3.31438700	0.69618100
H	2.29854400	3.82533100	0.80613200
C	0.15095800	4.06624000	0.47542600
C	-1.05555100	3.34452600	0.35058200
H	-2.00177700	3.82837100	0.16647100
C	-1.04837600	1.97313900	0.44242900
C	-2.35469600	0.01140100	0.38390700
C	-3.61786300	-0.50727100	0.22963400
H	-4.42687000	0.18692900	0.06640300
C	-3.81691300	-1.90451400	0.26841900
C	-2.65639300	-2.73637200	0.43286700
H	-2.75564500	-3.81020600	0.43104300
C	-1.41947100	-2.19716800	0.58851300
H	-0.56404100	-2.84907800	0.70629700
C	-1.20836200	-0.79274600	0.59069800
C	-1.05145100	6.18223702	0.23559400
H	-0.87350200	7.17312701	0.64995700
H	-1.83759700	5.73319301	0.84181600
C	-1.48182200	6.29146099	-1.22340900
H	-0.74840000	6.85327600	-1.80130700
H	-2.43851600	6.81017002	-1.29041900
H	-1.59179100	5.30483702	-1.67514700
C	1.44718900	6.14650501	0.37104500
H	2.08462100	5.82075501	1.19390700
H	1.20978800	7.19118200	0.56084600
C	2.17239300	6.01598102	-0.96456700
H	2.39107100	4.97418500	-1.19996300
H	3.11526600	6.56217001	-0.92542600
H	1.56945600	6.42827198	-1.77286700
C	-6.22386601	-1.59660900	-0.02612600
H	-7.08784502	-2.17145100	0.30168100
H	-6.15117802	-0.73997500	0.64421400
C	-6.41356699	-1.14382300	-1.47050900
H	-5.52626302	-0.63135400	-1.84361200
H	-7.25898903	-0.45829400	-1.53495800
H	-6.61466698	-1.99565500	-2.11926300
C	-5.23863400	-3.89594300	0.09270700
H	-4.65855300	-4.37370400	0.88243800
H	-6.28504202	-4.08546700	0.32281200
C	-4.89135000	-4.48427000	-1.27104900
H	-5.54844798	-4.08549500	-2.04304400
H	-5.01002100	-5.56788101	-1.24599800
H	-3.86165200	-4.25884200	-1.54993800
N	0.17906300	5.41170102	0.41979000
N	-5.04600500	-2.44457400	0.16686800
O	-2.24664000	1.35775800	0.31577100
O	1.04074000	-0.45802900	-1.86600400
O	3.18645000	0.17840100	-1.75947800
N	4.49972400	-1.86490600	-0.55484400
H	4.56108200	-1.03482800	-1.14516600
C	5.38690600	-2.86073800	-0.82537900
O	6.38103900	-2.63799400	-1.50558400
C	5.11181600	-4.25663700	-0.37492900
H	5.99502502	-4.81794100	-0.09349800
C	3.92337200	-4.83428300	-0.47415600
H	3.04530300	-4.28156100	-0.78890900
H	3.79310300	-5.88546100	-0.25101200

The minimum energy conformation of **NMe_2-RhB** in the S_1 state

C	0.97177300	2.09734700	1.42097000	H	5.97344300	-2.52473300	1.90856900
C	0.58306900	2.78500900	0.11721800	C	-5.12510400	-3.43910100	-0.01688800
C	0.72109100	4.17761000	-0.07499200	H	-6.13797700	-3.75770400	-0.25224600
C	0.39887600	4.70912400	-1.32832200	H	-4.45303600	-4.01779100	-0.65195300
H	0.48878400	5.77074200	-1.50706000	C	-4.82681000	-3.69840300	1.45670900
C	-0.05005500	3.89603700	-2.36111600	H	-3.82899400	-3.35295400	1.72837000
H	-0.28855900	4.33816800	-3.32062900	H	-4.88219700	-4.77101300	1.64741400
C	-0.20133800	2.53537000	-2.16571000	H	-5.55357900	-3.19600400	2.09397300
H	-0.55338800	1.89393800	-2.96455600	C	-6.28906900	-1.27322100	-0.45475700
C	0.11520300	1.97841300	-0.92468400	H	-6.19642500	-0.50179000	-1.21737400
C	-0.02406600	0.51236600	-0.74816800	H	-7.05204200	-1.96868100	-0.79954500
C	1.10845200	-0.33228800	-0.66501400	C	-6.69984800	-0.66790100	0.88319300
C	2.45262500	0.12131500	-0.77806100	H	-6.92146700	-1.44805800	1.61097200
H	2.62620000	1.17512000	-0.95439800	H	-7.59705600	-0.06340000	0.74332200
C	3.52021300	-0.72226200	-0.67180000	H	-5.91034900	-0.02998300	1.28314800
H	4.51494400	-0.31466500	-0.77046500	N	1.19442800	5.00261500	0.97232100
C	3.33361300	-2.12181900	-0.44381100	N	4.38252800	-2.96373100	-0.34596200
C	1.99291900	-2.59810700	-0.35528100	N	-5.03296000	-2.02354400	-0.38715600
H	1.76723800	-3.64037700	-0.18575500	O	-0.30695000	-2.29132200	-0.37783000
C	0.94484200	-1.73240700	-0.46950600	O	0.05897700	1.51012700	2.05281100
C	-1.42142700	-1.49383900	-0.47180700	O	2.17755400	2.14251200	1.76115900
C	-2.62152900	-2.13392500	-0.37388800	C	1.49690100	6.37923800	0.60545100
H	-2.61089400	-3.20538100	-0.23974500	H	1.97508400	6.86033000	1.45784800
C	-3.84042600	-1.39710100	-0.44678400	H	2.18760500	6.40891700	-0.23598000
C	-3.74248500	0.02116700	-0.60220800	H	0.59835800	6.95669400	0.34925700
H	-4.63265900	0.63118700	-0.62414100	C	0.36202500	4.99219300	2.17850400
C	-2.52646500	0.63555400	-0.69597700	H	0.13412400	3.98351900	2.50895200
H	-2.48459600	1.71206200	-0.79927300	H	0.89653200	5.49769400	2.98227000
C	-1.30211400	-0.08791400	-0.65910400	H	-0.58533400	5.52017100	2.00503400
C	4.18748100	-4.39215700	-0.08936500				
H	5.08720400	-4.89926800	-0.43220800				
H	3.36581400	-4.75028000	-0.70786400				
C	3.93625800	-4.70942400	1.38099100				
H	4.81052400	-4.46813200	1.98487000				
H	3.72721100	-5.77476000	1.48761500				
H	3.08201100	-4.14865200	1.76289800				
C	5.75284500	-2.45135200	-0.24651700				
H	5.92926200	-1.74761400	-1.06033000				
H	6.41505100	-3.29857300	-0.40951200				
C	6.05804000	-1.80069100	1.09899400				
H	5.38000500	-0.97113600	1.30227000				
H	7.07825400	-1.41487300	1.08499700				

The minimum energy conformation of **NMe_2-RhB** in the S_2 state

C	1.35546400	1.96528000	1.27901300	H	5.41617200	-3.14813800	1.85310300
C	0.87961600	2.71442500	0.04119500	C	-5.60535600	-2.78038900	-0.05262400
C	1.18170800	4.10092200	-0.16548400	H	-6.61339800	-3.00911200	-0.39681600
C	0.91100100	4.67711800	-1.44384400	H	-4.92726400	-3.38064500	-0.65894200
H	1.13832300	5.71761500	-1.62075600	C	-5.46720200	-3.14461700	1.42220300
C	0.26940900	3.95250700	-2.41044500	H	-4.49899000	-2.83037500	1.81545900
H	0.02844700	4.41706000	-3.35767800	H	-5.55337600	-4.22573400	1.54341900
C	-0.09749800	2.62348400	-2.17378300	H	-6.25093400	-2.67207100	2.01429400
H	-0.61427400	2.05642300	-2.93782900	C	-6.49390100	-0.45414500	-0.17101800
C	0.23558100	1.99714200	-0.96427100	H	-6.48715600	0.27805300	-0.98047900
C	-0.07141500	0.56341000	-0.81185300	H	-7.39731400	-1.04831300	-0.29648500
C	0.96099800	-0.41404300	-0.72035600	C	-6.52601100	0.25458700	1.17965000
C	2.33701900	-0.15096900	-0.89083200	H	-6.63924600	-0.46123100	1.99339700
H	2.64911500	0.86280100	-1.10815700	H	-7.37158900	0.94382800	1.20807100
C	3.29424800	-1.13383900	-0.80089700	H	-5.61415900	0.82808300	1.35015400
H	4.32889300	-0.86114000	-0.94673400	N	1.67598100	4.89231200	0.80728800
C	2.94000300	-2.48037900	-0.53463000	N	3.88637400	-3.46758200	-0.48178600
C	1.56449800	-2.76488200	-0.37448800	N	-5.36497500	-1.36905200	-0.34038900
H	1.20734900	-3.76126600	-0.15942500	O	-0.68002200	-2.15291900	-0.30553600
C	0.62954400	-1.76276400	-0.47375600	O	0.48537300	1.39634200	1.97738600
C	-1.69698900	-1.24007000	-0.45925500	O	2.58919000	1.96674900	1.48849900
C	-2.96756800	-1.73832000	-0.31402600	C	2.25406400	6.19669100	0.50282400
H	-3.06837000	-2.79141000	-0.09630500	H	2.90598500	6.46970500	1.32930600
C	-4.09142500	-0.88473200	-0.42339100	H	2.84343700	6.15381800	-0.40883400
C	-3.83725800	0.49059900	-0.66715500	H	1.47357000	6.95571900	0.40541200
H	-4.65563700	1.18968100	-0.75398600	C	1.49596700	4.64515200	2.23135000
C	-2.55420100	0.96257500	-0.80842000	H	0.70072200	3.92750600	2.40582300
H	-2.40766000	2.01964600	-0.99114700	H	2.42247100	4.29882500	2.69096800
C	-1.42158500	0.12220300	-0.72198500	H	1.21042800	5.59189500	2.69093100
C	3.50413800	-4.84157200	-0.16979100				
H	4.30129600	-5.48537300	-0.54061900				
H	2.61249700	-5.09380700	-0.74326300				
C	3.27544500	-5.10628500	1.31485000				
H	4.20880800	-5.02736200	1.87241500				
H	2.88104700	-6.11441900	1.45345400				
H	2.56054000	-4.39662600	1.73490800				
C	5.29814400	-3.12087000	-0.31367400				
H	5.61073500	-2.46978300	-1.13215900				
H	5.85994500	-4.04729200	-0.42301000				
C	5.63036800	-2.47146200	1.02622700				
H	5.06003200	-1.55398100	1.17656700				
H	6.69174500	-2.21917200	1.05510900				

The minimum energy conformation of **NH_2-RhB** in the S_1 state

C	1.28412300	2.47081300	1.63498600	H	5.85365900	-2.46004400	1.73815200
C	0.78655000	3.16694500	0.36732100	C	-5.21759600	-2.95616600	-0.30076100
C	0.98321200	4.55309200	0.19876000	H	-6.20744700	-3.18561000	-0.69101600
C	0.46295800	5.18728400	-0.93728500	H	-4.49950900	-3.34644600	-1.02109000
H	0.60263300	6.25615500	-1.05205400	C	-5.02832300	-3.61032000	1.06644200
C	-0.20836000	4.46335700	-1.90614800	H	-4.06941500	-3.33219200	1.50474100
H	-0.59207700	4.96906100	-2.78366000	H	-5.05894400	-4.69482400	0.95859400
C	-0.37726300	3.09233000	-1.76496500	H	-5.82063600	-3.31221700	1.75196700
H	-0.87847200	2.51525900	-2.53236800	C	-6.32581800	-0.72904700	-0.04745200
C	0.11761400	2.44609200	-0.62980400	H	-6.33564700	0.12152500	-0.73025700
C	-0.05017700	0.97955100	-0.54037700	H	-7.15544500	-1.37137300	-0.33403400
C	1.06618200	0.10569700	-0.55157600	C	-6.50084800	-0.26625300	1.39792500
C	2.42057600	0.53672200	-0.62175400	H	-6.59313200	-1.11922500	2.06877600
H	2.61875100	1.59840800	-0.68259500	H	-7.40682200	0.33491300	1.47830400
C	3.46873800	-0.33813100	-0.61624500	H	-5.65561800	0.33881800	1.72551100
H	4.47176000	0.05536000	-0.67825600	N	1.61456600	5.30279400	1.17941500
C	3.25113200	-1.74881200	-0.54833900	H	1.96253500	6.19866300	0.87244400
C	1.90170300	-2.19936300	-0.49566100	H	2.27385200	4.76219500	1.72808600
H	1.65062300	-3.24706900	-0.43063800	N	4.28179400	-2.62091900	-0.55445900
C	0.87083800	-1.30242300	-0.50460800	N	-5.09928900	-1.49878400	-0.26252300
C	-1.47743300	-1.02191600	-0.42845800	O	-0.38441000	-1.84083500	-0.46508500
C	-2.68891100	-1.64985500	-0.35612300	O	0.52146800	1.63882800	2.16394600
H	-2.69056800	-2.72865200	-0.32825100	O	2.42408900	2.80698000	2.04640500
C	-3.89274700	-0.89263500	-0.29323800				
C	-3.76983000	0.53082400	-0.27117700				
H	-4.64788500	1.15274400	-0.19043600				
C	-2.54622400	1.13295500	-0.34721700				
H	-2.48363500	2.21258100	-0.32361100				
C	-1.33641700	0.39279500	-0.46112600				
C	4.05842700	-4.06594500	-0.56130800				
H	4.92612400	-4.52048800	-1.03697100				
H	3.20296200	-4.28504800	-1.19793000				
C	3.86229600	-4.64494800	0.83817800				
H	4.76597300	-4.52859200	1.43563100				
H	3.63576400	-5.70883900	0.76436700				
H	3.03965900	-4.14845700	1.35397500				
C	5.66300900	-2.15903400	-0.39993100				
H	5.86600200	-1.38294800	-1.13972000				
H	6.30460300	-3.00249000	-0.64455000				
C	5.97583900	-1.65975400	1.00951100				
H	5.32382800	-0.83373600	1.29263200				
H	7.00835300	-1.31198600	1.04768400				

The minimum energy conformation of **NH_2-RhB** in the S_2 state

C	1.56638900	2.38804400	1.57685200	H	4.54795500	-4.51426300	1.54429100
C	0.97264600	3.09982000	0.37077000	H	3.29710600	-5.62749600	0.98449200
C	1.22454500	4.50410400	0.20118300	H	2.87229300	-3.96354900	1.40624100
C	0.53565300	5.24740100	-0.81082200	C	5.56941700	-2.33768600	-0.48147700
H	0.72315700	6.31095300	-0.88561500	H	5.81369600	-1.55483000	-1.20136000
C	-0.30429500	4.59828100	-1.66355900	H	6.19860100	-3.19120500	-0.73027500
H	-0.81404900	5.14080800	-2.44846300	C	5.88329700	-1.86060100	0.93308100
C	-0.49270000	3.20963900	-1.54806100	H	5.22950800	-1.03936700	1.22999400
H	-1.12815300	2.69994600	-2.26059800	H	6.91440000	-1.50571300	0.97962400
C	0.14802200	2.45270900	-0.54135100	H	5.76770600	-2.66848300	1.65492400
C	-0.05620100	1.00499000	-0.52663000	C	-5.31810400	-2.84149100	-0.31121500
C	1.05157600	0.09778700	-0.55577000	H	-6.30842500	-3.07605100	-0.70056700
C	2.40720000	0.46842200	-0.66928200	H	-4.60153800	-3.26262900	-1.01638600
H	2.66279300	1.51679200	-0.75147400	C	-5.14350100	-3.47082100	1.06724300
C	3.43082300	-0.45139400	-0.69696400	H	-4.20095900	-3.16401800	1.52381000
H	4.44393400	-0.08806500	-0.78414200	H	-5.14416500	-4.55854200	0.97816600
C	3.17183300	-1.84092100	-0.62083100	H	-5.95864100	-3.18375200	1.73169200
C	1.82052900	-2.23231600	-0.52886000	C	-6.37608300	-0.60955700	0.02498900
H	1.52698400	-3.26988100	-0.46810500	H	-6.44421200	0.25874400	-0.63309500
C	0.81735700	-1.28914000	-0.50798900	H	-7.23625200	-1.23796300	-0.20031400
C	-1.54096500	-0.95014100	-0.43849400	C	-6.42810600	-0.16756400	1.48387600
C	-2.76802600	-1.56582400	-0.36418400	H	-6.46139500	-1.02818200	2.15152100
H	-2.77999000	-2.64505500	-0.32318000	H	-7.32443000	0.43201600	1.65134700
C	-3.95411600	-0.80053900	-0.31912600	H	-5.56052100	0.43829700	1.74784000
C	-3.80810900	0.61086600	-0.31025400	N	2.08016200	5.14363000	0.98081700
H	-4.67775500	1.24856400	-0.25415700	H	2.22934100	6.13792700	0.86560200
C	-2.56804200	1.19867800	-0.38556700	H	2.63753000	4.61582700	1.64740500
H	-2.51509000	2.27969100	-0.36324700	N	4.18531400	-2.76355500	-0.68794900
C	-1.37274800	0.45176500	-0.47969200	N	-5.18770700	-1.38745200	-0.32509300
C	3.89495800	-4.18222300	-0.49881400	O	-0.45974000	-1.79620800	-0.44152700
H	4.74695900	-4.73579400	-0.89237500	O	0.81449600	1.62716600	2.21841900
H	3.04196800	-4.44957400	-1.12308200	O	2.76350900	2.65547600	1.85811200
C	3.63860900	-4.59145300	0.94845500				

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