Electronic supplementary information

Gate-opening cooperative methanol binding to multi-bladed benzenes bearing 1,2-diboryl functionality

Yunyi Song, Hiromichi Yokoyama, Yoshiaki Shoji,* Hayato Sakai, Taku Hasobe and Takanori Fukushima*

*To whom correspondence should be addressed.
E-mail: yshoji@res.titech.ac.jp (Y.S.); fukushima@res.titech.ac.jp (T.F.)

Table of contents

1. Materials and methods

Handling of air- and/or moisture-sensitive compounds were performed either using standard Schlenk-line techniques or in a glove box under argon. Column chromatography was carried out using Silica Gel 60 N (spherical, neutral, particle size: 63–210 mm, Kanto Chemical Co., Inc.). Anhydrous CH_2Cl_2, hexane, toluene, and tetrahydrofuran (THF) were dried by passage through an activated alumina column and a Q-5 column (Nikko Hansen & Co., Ltd.). 1,2-Dichloroethane (1,2-DCE), deuterated chloroform ($CDCl_3$) and dichloromethane (CD_2Cl_2) were dried over CaH_2 and freshly distilled prior to use. Compounds **1**,[S1] $\mathbf{2_H}$,[S1] and 2,5-bis(4-bromophenyl)-3,4-diphenylcyclopenta-2,4-dienone[S2] were prepared according to reported procedures.

Fourier transform infrared (FT-IR) spectra were recorded at 25 °C with a JASCO model FT/IR-6600 Fourier transform infrared spectrometer. Nuclear magnetic resonance (NMR) spectroscopy measurements were carried out on a Bruker model AVANCE III HD-500 spectrometer (^{1}H: 500.0 MHz, ^{13}C: 125.7 MHz) or on Bruker model AVANCE-400 spectrometer (400.0 MHz for ^{1}H), where chemical shifts are expressed relative to the resonances of the residual non-deuterated solvent for ^{1}H ($CDCl_3$: ^{1}H(δ) = 7.26 ppm, and CD_2Cl_2: ^{1}H(δ) = 5.32 ppm), and the resonances of the residual solvent for ^{13}C ($CDCl_3$: ^{13}C(δ) = 77.16 ppm). The absolute values of the coupling constants are given in Hertz (Hz). Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), multiplet (m) and broad (br). Mass spectrometry measurements were carried out on a Bruker micrOTOF II mass spectrometer equipped with an atmospheric pressure chemical ionization (APCI) probe. Electronic absorption spectra were recorded using a quartz cell on a JASCO model V-670 UV/VIS spectrophotometer. Fluorescence spectra were measured using a quartz cell on a JASCO model FP-8500 spectrophotometer. Fluorescence lifetimes were measured on a Hamamatsu model Quantaurus-Tau C16361 fluorescence lifetime spectrometer. The absolute PLQY values were measured by a Hamamatsu Photonics model Quantaurus-QYC11347 absolute PLQY spectrometer.

2. Synthesis

Synthesis of carbazole-appended tetraarylcyclopentadienone $\mathbf{3_o}$. Under argon, a toluene solution (5.0 mL) of a mixture of 2,5-bis(4-bromophenyl)-3,4-diphenylcyclopenta-2,4-dienone[S2] (300 mg, 0.55 mmol), carbazole (204 mg, 1.22 mmol), palladium diacetate (3.0 mg, 14 μmol), tri-*tert*-butylphosphine (12 mg, 55 μmol), and sodium *tert*-butoxide (320 mg, 3.32 mmol) was heated at 110 °C for 8 h, allowed to cool to 25 °C, and then quenched by addition of water (5.0 ml). The reaction mixture was extracted with CH_2Cl_2. The combined organic layer was successively washed with water and brine, dried over anhydrous Na_2SO_4, and evaporated to dryness under reduced pressure. The obtained residue was thoroughly washed with cold ethanol and dried under reduced pressure to give $\mathbf{3_o}$ as a dark gray powder (334 mg, 0.47 mmol) in 84% yield: FT-IR (KBr): ν (cm^{-1}) 3050, 2359, 1706, 1604, 1516, 1478, 1449, 1333, 1223, 1173, 1120, 842, 746, 723, 623, 566, 530. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ (ppm) 8.14 (d, J = 7.7 Hz, 4H), 7.54–7.46 (m, 12H), 7.42 (t, J = 7.7 Hz, 4H), 7.35–7.27 (m, 10H), 7.07 (d, J =

8.3 Hz, 4H). ^{13}C NMR (125.7 MHz, $CDCl_3$, 25 °C): δ (ppm) 200.5, 155.4, 140.7, 137.1, 133.0, 131.7, 129.8, 129.5, 129.1, 128.4, 126.5, 126.1, 124.7, 123.6, 120.4, 120.2, 110.1. APCI-TOF mass: calculated for $C_{53}H_{34}N_2O$ $[M+H]^+$: m/z = 715.2754; found: 715.2744. ^{1}H, ^{13}C NMR spectra and high-resolution APCI-TOF mass spectra of **3*o*** are shown in Figs. S14, S15, and S16, respectively.

Synthesis of 2*o*. Under argon, a mixture of **1** (59 mg, 0.153 mmol), **3*o*** (100 mg, 0.140 mmol), and benzophenone (500 mg) was heated to 180 °C and stirred at this temperature for 24 h. After being allowed to cool to 25 °C, the reaction mixture was dissolved in $CHCl_3$ (1.0 mL). Hexane (3.0 mL) was added to the resulting mixture, and the white precipitate thus formed was collected by filtration, washed with hexane, and dried under reduced pressure. The residue was recrystallized from hexane to give **2*o*** (75.1 mg, 70.3 μmol) as a white powder in 50% yield: FT-IR (KBr): ν (cm^{-1}) 3054, 2365, 1604, 1576, 1550, 1517, 1491, 1476, 1362, 1334, 1315, 1232, 1184, 1152, 1120, 1099, 1071, 1018, 941, 911, 839, 810, 749, 724, 702, 677, 648, 625, 604, 549, 534. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.99 (d, J = 7.7 Hz, 4H), 7.92 (dd, J = 7.6, 1.6 Hz, 4H), 7.36 (ddd, J = 8.4, 7.1, 1.7 Hz, 4H), 7.24–7.07 (m, 26H), 6.80–6.77 (m, 8H), 6.58 (br, 4H). ^{13}C NMR (125.7 MHz, $CDCl_3$, 25 °C): δ (ppm) 158.4, 146.8. 143.5, 142.5, 141.0, 140.5, 139.2, 137.8, 135.1, 133.6, 133.1, 132.4, 127.3, 126.2, 125.9, 125.7, 124.5, 123.0, 121.2, 120.1, 120.0, 116.8, 109.7. A ^{11}B NMR signal of **2*o*** was not detected, presumably due to line broadening caused by rapid quadrupolar relaxation of the boron nuclei.[S3,S4] APCI-TOF mass: calculated for $C_{78}H_{50}B_2N_2O_2$ $[M+H]^+$: m/z = 1069.4138; found: 1069.4154. ^{1}H, ^{13}C NMR spectra and high-resolution APCI-TOF mass spectra of **3*o*** are shown in Figs. S17, S18, and S19, respectively.

3. Single-crystal X-ray diffraction analysis

A single crystal of **2*o***, obtained by recrystallization from a mixture of $CHCl_3$ and acetonitrile, was coated with an immersion oil (type B: Code 1248, Cargille Laboratories, Inc.) and mounted on a MicroMount (MiTeGen, LLC.). Diffraction data were collected at 93 K under a cold nitrogen gas stream on a RIGAKU model XtaLAB Synergy-DW diffractometer system equipped with a HyPix-6000 detector, using Cu-$K\alpha$ radiation (λ = 1.54184 Å).

Crystal data for $C_{78}H_{50}B_2N_2O_2 \cdot C_2H_3N$ (2*o*•MeCN): colorless prism, 0.37 x 0.15 x 0.11 mm^3, monoclinic, $P2_1/n$, a = 18.5760(2) Å, b = 13.6940(1) Å, c = 24.8877(3) Å, β = 111.155(1) °, V = 5904.27(11) $Å^3$, Z = 4, $density_{calcd}$ = 1.249 g cm^{-3}, T = 93 K, Cu-$K\alpha$ radiation, λ = 1.54184 Å, μ = 0.572mm^{-1}, 56950 reflections measured, 11823 unique reflections, 785 parameters, R_{int} = 0.0356, Completeness to theta = 67.68°: 99.93%, Absorption correction: multi-scan, GOF = 1.053, R_1 = 0.0539 ($I > 2\sigma(I)$), wR_2 = 0.1540 (all data), $\Delta\rho_{min, max}$ = –0.4689, 0.4731 e$Å^3$, CCDC-2498455.

4. The Hill fitting of the titration data

The absorbance changes at 360 nm upon titration of **2*o*** (Fig. 3c) or **2H** (Fig. S10a) with MeOH in 1,2-DCE at 25 °C were analyzed using the following nonlinear form of Hill equation[S5a,b]:

$$A_{\mathrm{obsd}} = A_0 + \Delta A_{max} \frac{[\mathrm{MeOH}]^n}{K_D^n + [\mathrm{MeOH}]^n}$$

where A_{obsd}: observed absorbance, A_0: initial absorbance. ΔA_{max}: the maximum change of absorbance, [MeOH]: total MeOH concentration, n: Hill coefficient, and K_{D}: apparent dissociation constant. The fitting was performed by nonlinear least-squares regression. The resulting fitting curves are shown in Fig. 3e and Fig. S10c. The Hill fitting for the fluorescence spectral changes of **2*o*** (Fig. 3d) was performed by replacing each absorbance-related parameter in the above equation with the corresponding fluorescence intensity parameter, and the resulting fitting curve is shown in Fig. 3f.

The ^{1}H NMR chemical shift changes of **2*o*** (Fig. S9a) upon titration with MeOH in CD_2Cl_2 at 25 °C were analyzed using the following equation[S5c]:

$$\delta_{\mathrm{obsd}} = \delta_0 + \Delta\delta_{max} \frac{[\mathrm{MeOH}]^n}{K_D^n + [\mathrm{MeOH}]^n}$$

where δ_{obsd}: observed chemical shift, δ_0: initial chemical shift. $\Delta\delta_{\mathrm{max}}$: the maximum change of chemical shift. The resulting fitting curve is shown in Fig. S9b.

5. Density functional theory (DFT) calculations

All calculations were carried out by the Gaussian 16 software package[S6]. Geometrical optimizations of **2*o*** and **2H** were performed at the ωB97X-D/6-31G(d,p) level of theory in vacuum.[S7] Vibrational frequency analyzes were carried out to confirm the stationary point and obtained thermochemistry corrections at the same level of theory. The obtained structure was subjected to single point energy calculation at the ωB97X-D/6-311G(d,p) level of theory in vacuum. The evaluation of the absorption properties of **2*o*** was performed by time-dependent (TD)-DFT calculations at the TD-ωB97X-D/6-311G(d,p) level of theory using the optimized ground-state geometry (Fig. S4b). The geometrical optimizations for 1:1 and 1:2 complexes of **2*o*** and **2H** with MeOH, as well as **2*o***, **2H**, and MeOH, in which the SMD method was employed to include the solvation effect by specifying 1,2-dichloroethane (1,2-DCE) as a solvent,[S8] were carried out using the SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) level of theory for C, H, B and N atoms and 6-31+G(d,p) level of theory for O atoms. Vibrational frequency analyses were carried out at the same level of theory to confirm the stationary point and to obtain thermochemistry correction values. Obtained structures were subjected to single point energy calculations at the SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) level of theory for C, H, B and N atoms and 6-311+G(d,p) level of theory for O atom to obtain the corresponding total electron energies. The Gibbs free energies at 298 K were obtained as the sums of the total electron

energies and the thermochemistry correction values. For the 1:1 and 1:2 complexes, the total electron energies were corrected taking the basis set superposition error (BSSE)[S9] into account, using the counterpoise method[S10] at the same level of theory. Thermal corrections were recomputed using the GoodVibes code (version 3.2).[S11] For this correction, the molecular volume of 1,2-dichloroethane was calculated at the B3LYP/6-31G(d) level of theory to supplement the missing solvent parameters in the GoodVibes code. The adopted values for the correction were 108.86 Å^3 for the molecular volume and 12.6 mol/L for the molar concentration of the pure solvent. To address the breakdown of the harmonic approximation for low-frequency modes, vibrational entropies were evaluated using Grimme's quasi-RRHO approximation[S12] with a frequency parameter of 100 cm^{-1}. Translational entropy was corrected to account for the reduced accessible volume in solution using the free volume model.[S13] A standard state correction was also applied to convert thermodynamic parameters from the gas phase (1 atm) to the solution phase (1 mol/L). The vibrational scaling factor for ZPE was taken as 0.975, adopted from the value for ωB97X-D/def2-TZVP, as scaling factors are known to be relatively insensitive to the basis set size.[S14] The obtained results were visualized using the GaussView program package.[S15] The non-covalent interactions (NCI) analysis was carried out using the NCIPLOT program (version 4.2.1),[S16] and the obtained plots were illustrated using the Visual Molecular Dynamics (VMD) program.[S17] Figures 1b, S4a, and S5 were prepared using the VESTA program (version 3).[S18] Figure 4a,b, in which the MeOH complexes of $\mathbf{2}_{\boldsymbol{o}}$ and $\mathbf{2}_{\mathbf{H}}$ are superimposed, was prepared using the PyMol program.[S19] The Cartesian coordinates and energies of the calculated structures are shown in Tables S1–S9.

6. Supplementary references

S1. T. Tsukada, Y. Shoji, K. Takenouchi, H. Taka and T. Fukushima, *Chem. Commun.*, 2022, **58**, 4973.

S2. S. Watanabe and J. Kido, *Chemistry Letters*, 2007, **36**, 590.

S3. B. Wrackmeyer, in Annual Reports on NMR Spectroscopy, Vol. 20, G. A. Webb (Ed.), Academic Press, London, 1988, pp. 1–124.

S4. H. Nöth, B. Wrackmeyer, Nuclear Magnetic Resonance Spectroscopy of Boron Compounds, Springer-Verlag, Berlin, 1978.

S5. (a) P. Chenprakhon, J. Sucharitakul, B. Panijpan and P. Chaiyen, *J. Chem. Educ.*, 2010, **87**, 829; (b) T.-P. Sheng, X.-X. Fan, G.-Z. Zheng, F.-R. Dai and Z.-N. *Chen, Molecules*, 2020, **25**, 2656; (c) W. Xue, K. Wu, N. Ouyang, T. Brotin and J. R. Nitschke, *Angew. Chem. Int. Ed.*, 2023, **62**, e202301319.

S6. Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,

H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

S7. J. D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys*., 2008, **10**, 6615.

S8. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B,* 2009, **113**, 6378.

S9. B. J. Ransil, *J. Chem. Phys.*, 1961, **34**, 2109.

S10. S. F. Boys and F. Bernardi, *Mol. Phys.*, 1970, **19**, 553.

S11. G. Luchini, J. V. Alegre-Requena, I. Funes-Ardoiz, R. S. Paton, F1000Research, 2020, **9**(Chem Inf Sci), 291.

S12. S. Grimme, *Chem. Eur. J.*, 2012, **18**, 9955.

S13. M. Mammen, E. I. Shakhnovich, J. M. Deutch and G. M. Whitesides, *J. Org. Chem*., 1998, **63**, 3821.

S14. I. M. Alecu, J. Zheng, Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput*., 2010, **6**, 2872.

S15. GaussView, Version 6.1, Roy Dennington, Todd A. Keith, and John M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.

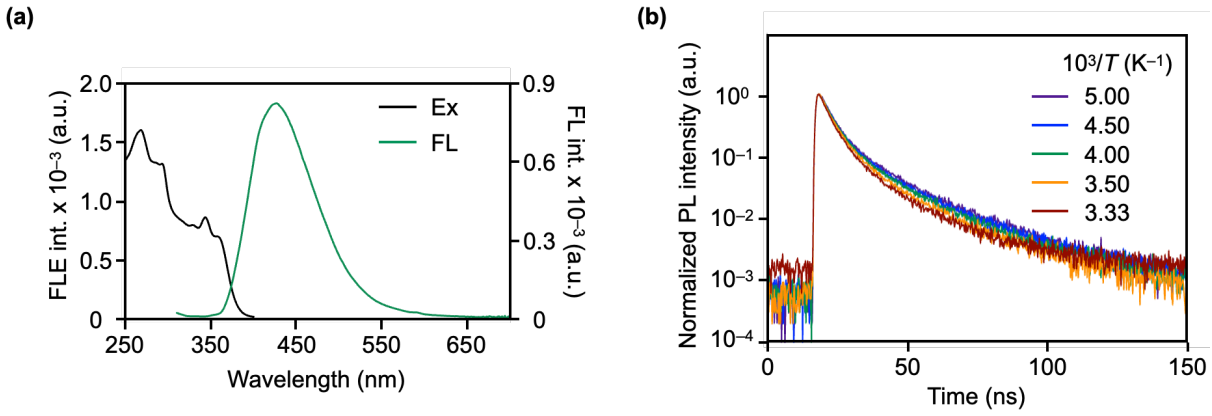
S16. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen and W. Yang, *J. Am. Chem. Soc.*, 2010, **132**, 6498.

S17. W. Humphrey, A. Dalke and K. Schulten, *J. Molec. Graphics*, 1996, **14**, 33.

S18. K. Momma and F. Izumi, *J. Appl. Crystallogr.*, 2011, **44**, 1272.

S19. The PyMOL Molecular Graphics System, Version 3.2.0 Schrödinger, LLC.

7. Supplementary figures



(c)

Temperature (°C)	CHI	τ_{all} (ns)	τ_1 (ns)	A_1 (%)	$\tau 2$ (ns)	A_2 (%)
200 K	1.28	10.47		85.5		14.5
222 K	1.15	9.76		88.1		11.9
250 K	1.10	9.74	5.1	88.1	19	11.9
286 K	1.12	10.20		86.6		13.4
300 K	1.17	9.44		89.1		10.9

Fig. S1. (a) Fluorescence (green) and excitation (black) spectra of a drop-cast film of **2*o*** (5 wt% in polystyrene) on a quartz substrate at 298 K (λ_{ex} = 294 nm, λ_{em} = 427 nm). (b) Emission decay profiles of the same sample at different temperatures (λ_{ex} = 280 nm, λ_{em} = 427 nm). (c) Emission lifetimes and proportions obtained by fitting the data in panel (b) at each temperature.

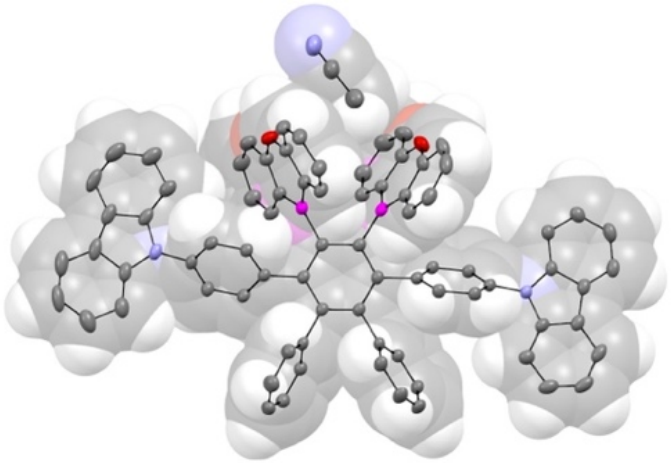


Fig. S2. X-ray crystal structure of **2*o***•MeCN with the atomic displacement parameters set at 50% probability. Color code: boron = pink, carbon = gray, nitrogen = blue, oxygen = red, and hydrogen = white.

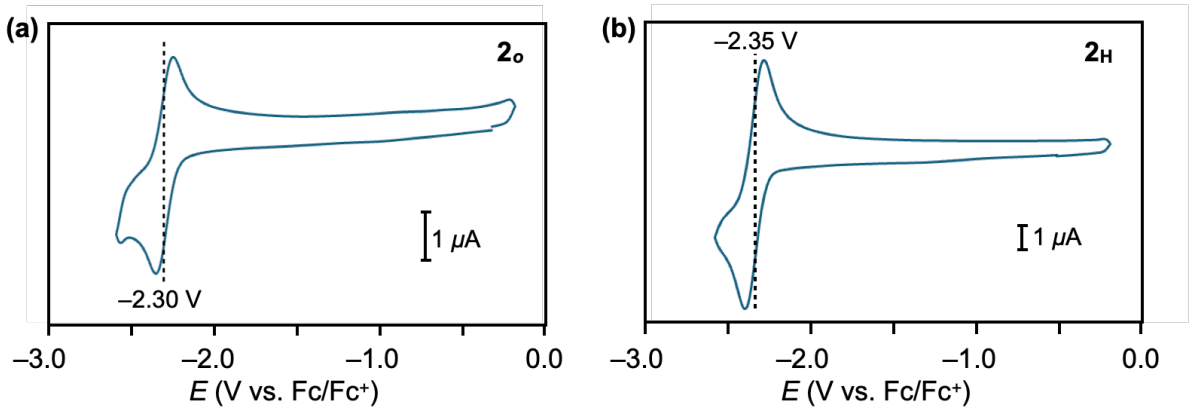
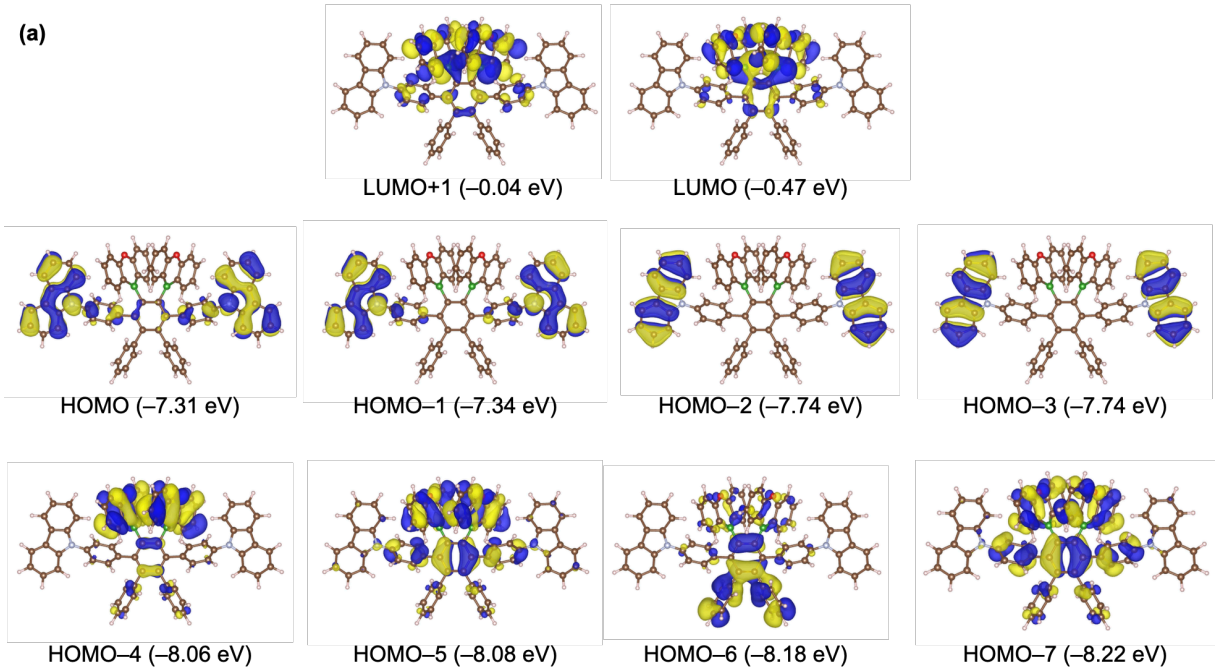


Fig. S3. Cyclic voltammograms of (a) $\mathbf{2}_o$ and (b) $\mathbf{2}_H$ in THF (5.0×10^{-4} M) at 298 K. Supporting electrolyte: 0.1 M tetrabutylammonium hexafluorophosphate, working electrode: glassy carbon, counter electrode: Pt rod, reference electrode: $Ag/AgNO_3$, scan rate: 100 mV sec^{-1}.



(b)

State	Configurations	Coefficient	Energy (eV)	λ (nm)	f
1	HOMO–7 →LUMO+1	–0.132	4.07	305	0.0344
	HOMO–6 →LUMO	–0.116			
	HOMO–5 →LUMO+1	0.244			
	HOMO–4 →LUMO	0.573			
	HOMO–1 →LUMO	0.110			

Fig. S4. (a) Selected Kohn-Sham orbitals and energies of $\mathbf{2}_o$ at the optimized ground-state geometry [the ωB97X-D/6-311G(d,p)//ωB97X-D/6-31G(d,p) level] and (b) Electronic configurations for the lowest-energy transition of $\mathbf{2}_o$ using the optimized ground-state geometry [the TD-ωB97X-D/6-311G(d,p) level].

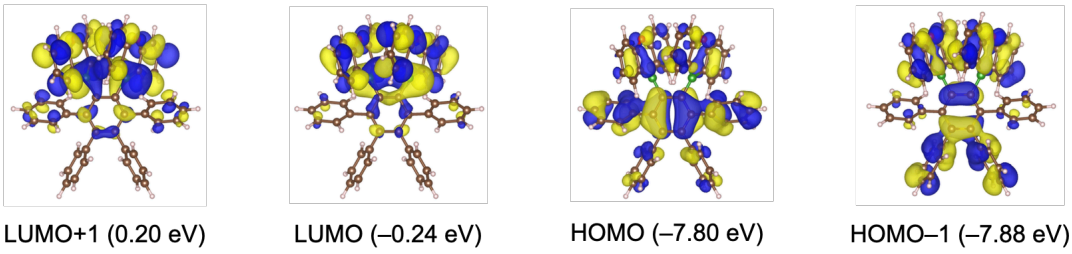


Fig. S5. Selected Kohn-Sham orbitals and energies of $\mathbf{2_H}$ at the optimized ground-state geometry [the ωB97X-D/6-311G(d,p)//ωB97X-D/6-31G(d,p) level].

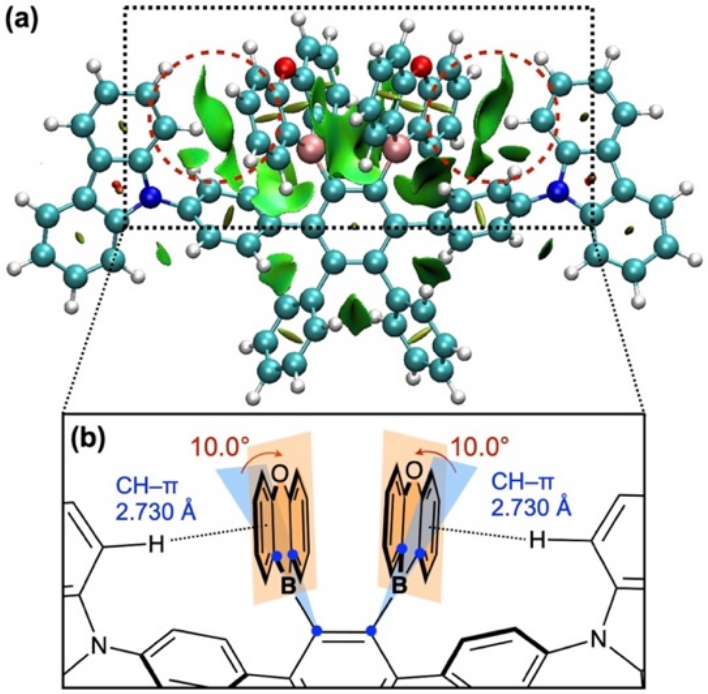


Fig. S6. (a) Non-covalent interaction (NCI) plot and (b) schematic representation of $\mathbf{2}_o$ for the optimized geometry [the ωB97X-D/6-311G(d,p)//ωB97X-D/6-31G(d,p) level of theory]. As shown in panel(a), $\mathbf{2}_o$ exhibits van der Waals interactions between the windmill-arranged blade units (green areas). Moreover, additional CH–π interactions occur between the carbazole and the adjacent OBAn units (red dotted circles). In panel (b), the bending angles are defined as the dihedral angles between the OBAn mean planes (orange) and the trigonal boron planes (blue). The distances between the carbazole protons and the centroids of the phenylene rings in the OBAn units fall within the range of CH–π interactions.

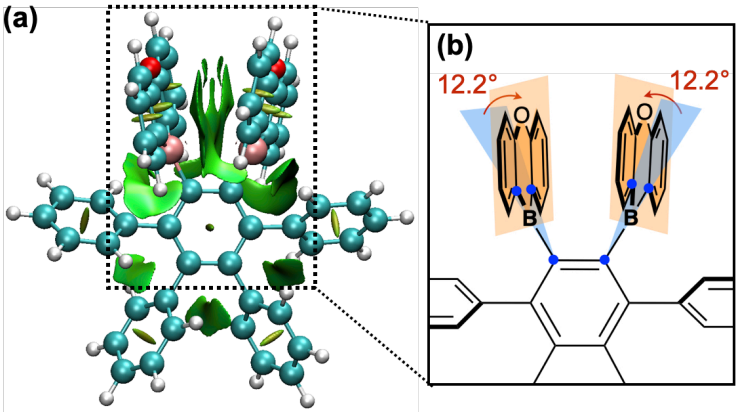


Fig. S7. (a) Non-covalent interaction (NCI) plot and (b) schematic representation of $\mathbf{2_H}$ for the optimized geometry [the ωB97X-D/6-311G(d,p)//ωB97X-D/6-31G(d,p) level of theory]. As shown in panel(a), $\mathbf{2_H}$ exhibits van der Waals interactions between the windmill-arranged blade units (green areas). In panel (b), the bending angles are defined as the dihedral angles between the OBAn mean planes (orange) and the trigonal boron planes (blue).

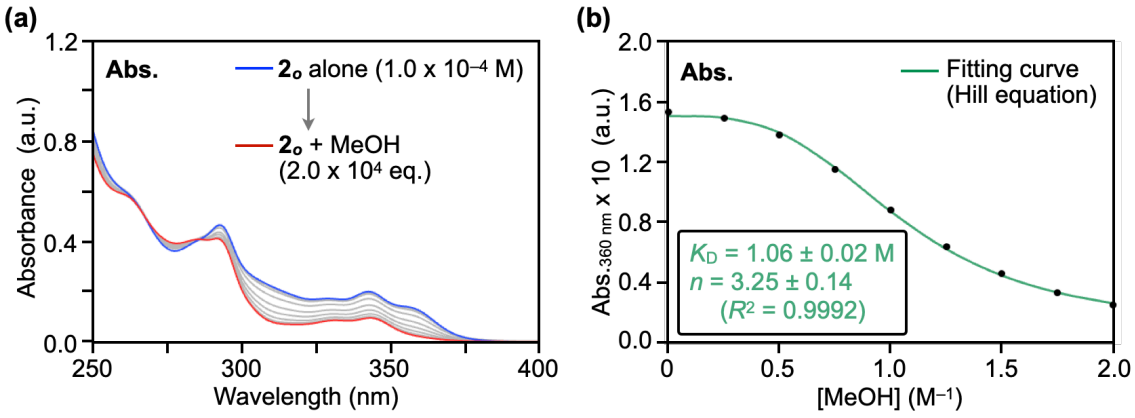


Fig. S8. (a) Absorption spectra of $\mathbf{2_o}$ (1.0×10^{-4} M in 1,2-DCE at 298 K) upon titration with MeOH ($0.0–2.0 \times 10^4$ eq.). (b) Hill fittings of the absorbance change at 360 nm using the data in panel (a).

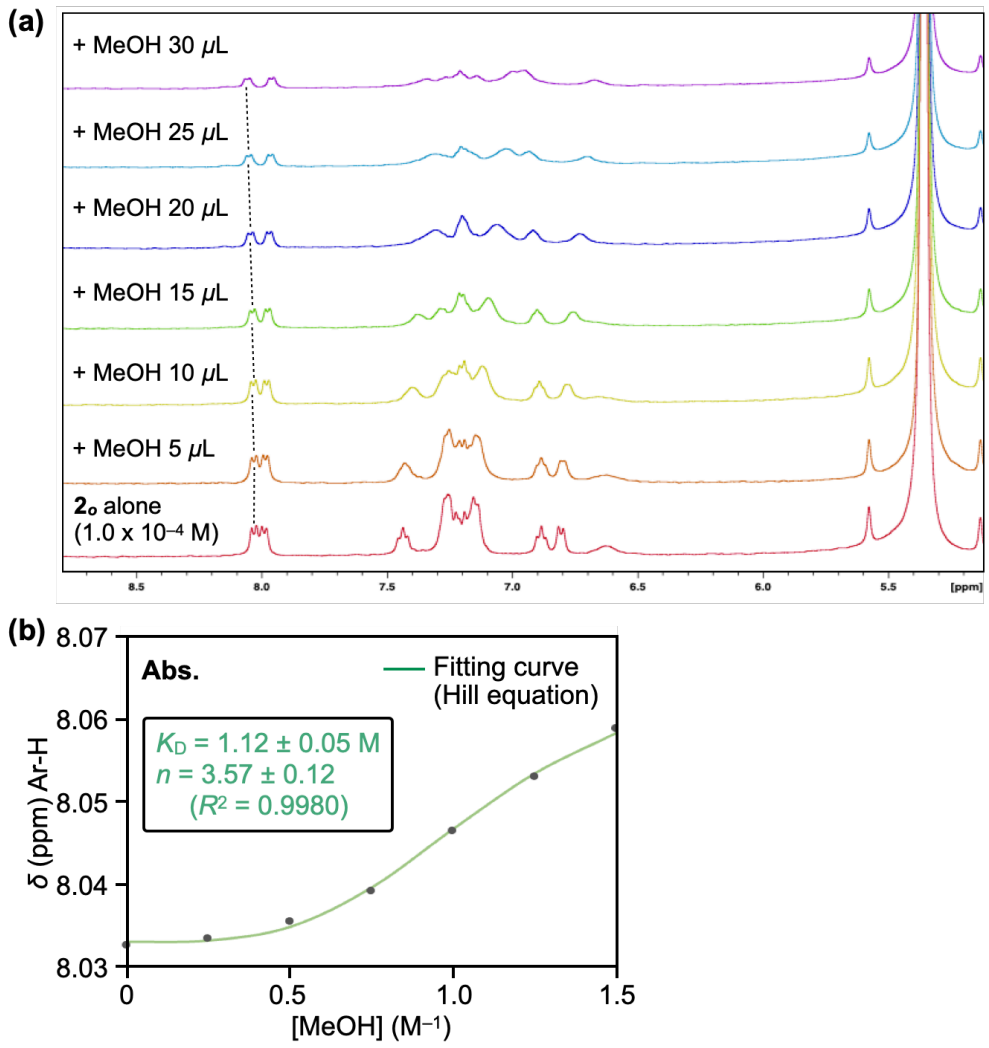


Fig. S9. (a) ^{1}H NMR spectra (400 MHz, aromatic region) of $\mathbf{2_o}$ (1.0×10^{-4} M) in CD_2Cl_2 at 298 K upon titration with MeOH ($0.0–1.5 \times 10^{4}$ eq.). (b) Hill fittings of the chemical change of an aromatic signal using the data in panel (a).

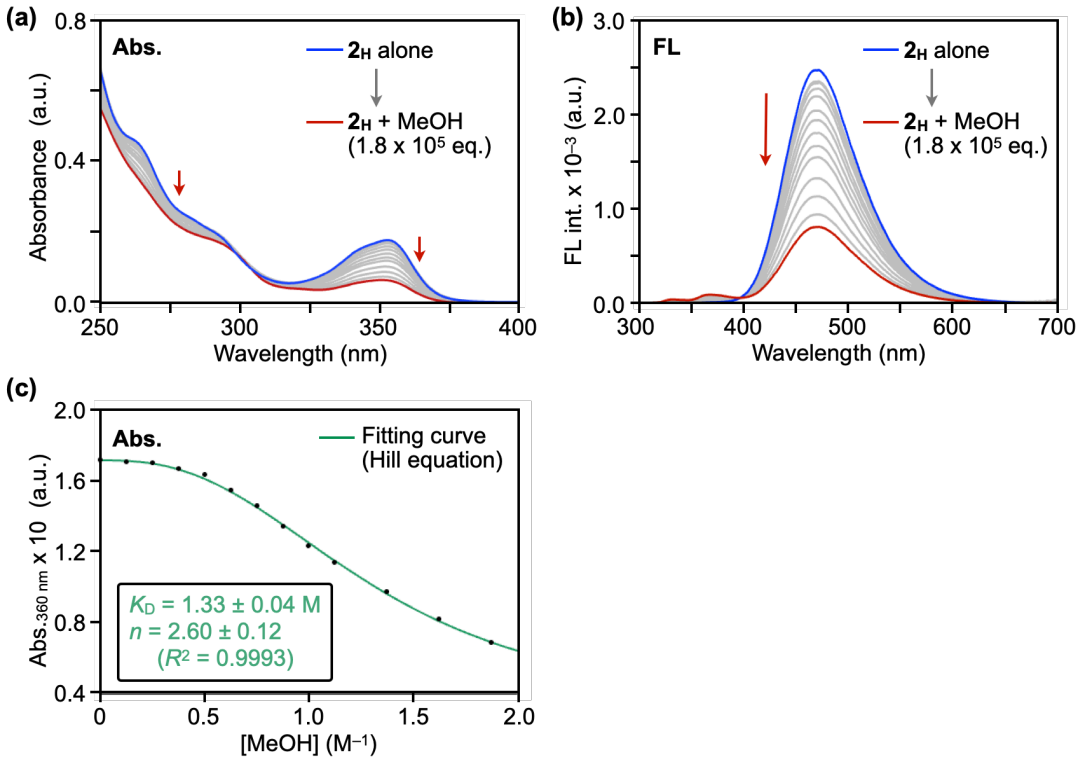


Fig. S10. Absorption and fluorescence spectra of $\mathbf{2_H}$ (1.0×10^{-5} M in 1,2-DCE at 298 K) upon titration with MeOH (0.0–1.8×10^5 eq.). (c) Hill fittings of the absorbance change at 360 nm using the data in panel (a).

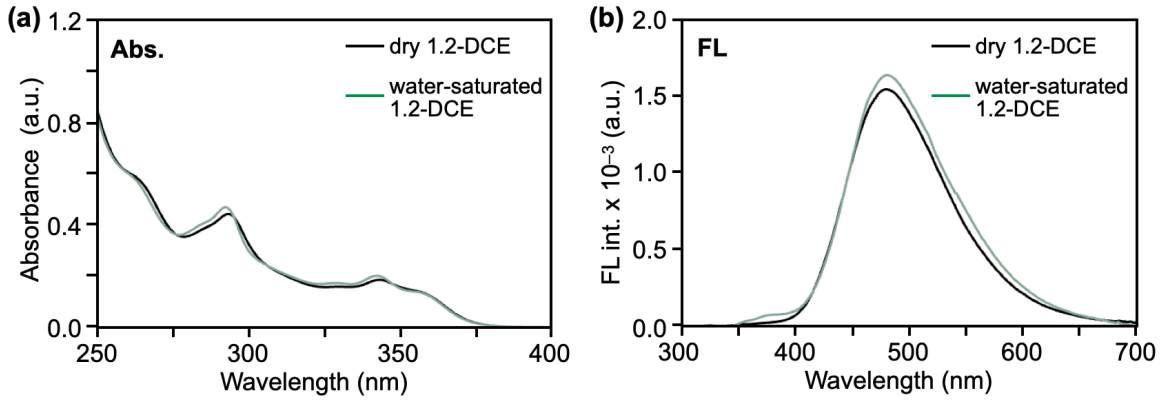


Fig. S11. (a) Absorption and (b) fluorescence spectra of $\mathbf{2}_o$ (1.0×10^{-5} M) in dry 1,2-DCE (black) and in water-saturated 1,2-DCE (green).

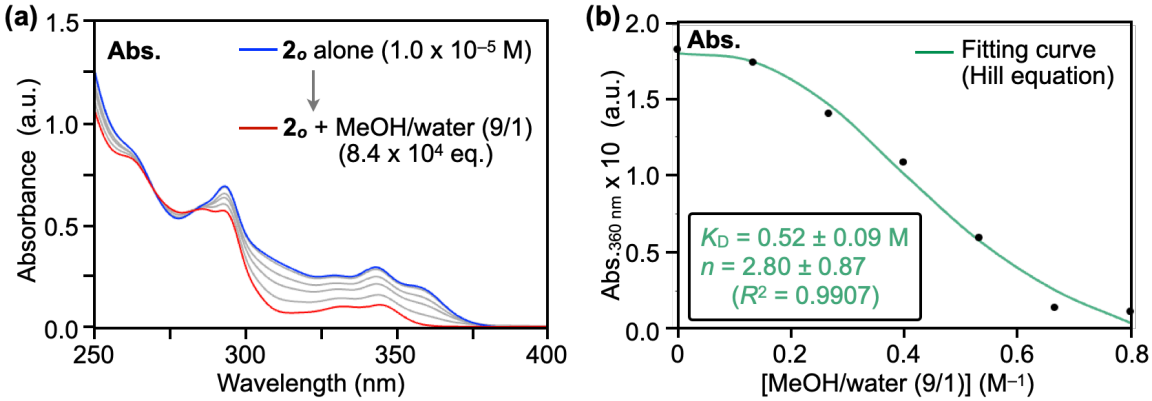


Fig. S12. (a) Absorption spectra of $\mathbf{2}_o$ (1.0×10^{-5} M in 1,2-DCE at 298 K) upon titration with MeOH/water (9/1 v/v, 0.0–8.4×10^4 eq.). (b) Hill fittings of the absorbance change at 360 nm using the data in panel (a). As shown in panel (a), significant absorption spectral changes are observed at relatively low total guest concentrations compared to those observed for titration using MeOH alone (Fig. 3c,e). Hill fitting of these spectral changes gave a smaller apparent dissociation constant (K_D = 0.52±0.09 M) and reduced cooperativity (apparent n = 2.80 ± 0.87) relative to the values obtained using MeOH alone (Fig. 3e). Interestingly, ESI-TOF mass spectrometric analysis of the titrated solution displayed only ion peaks corresponding to the 1:1 complex of $\mathbf{2}_o$ and MeOH (Fig. S13).

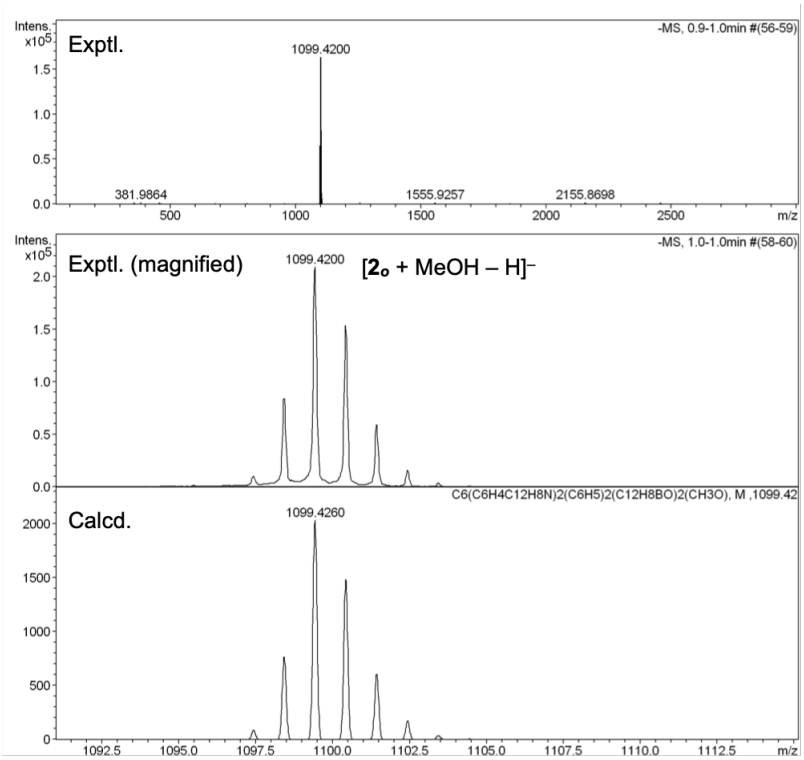


Fig. S13. High-resolution ESI-TOF mass spectrum (negative mode) of a 1,2-DCE solution containing $\mathbf{2}_o$ (1.0×10^{-5} M) and MeOH/water (9/1 v/v, 0.8 M).

8. Analytical data

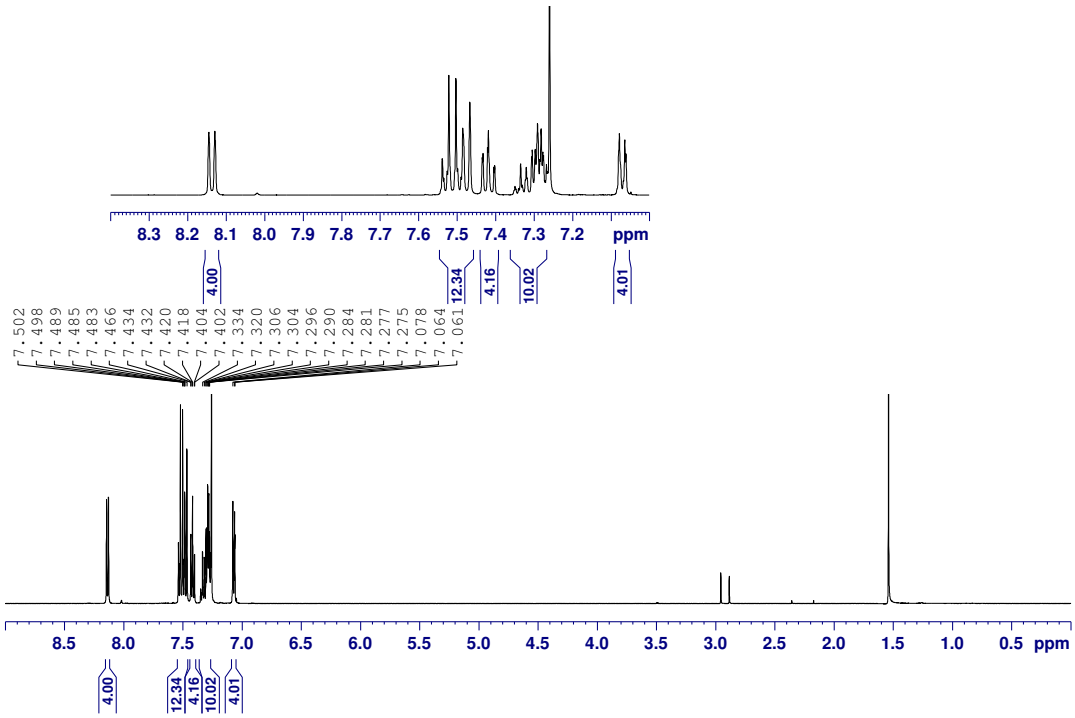


Fig. S14. ^{1}H NMR spectrum (500 MHz) of **3*o*** in $CDCl_3$ at 25 °C.

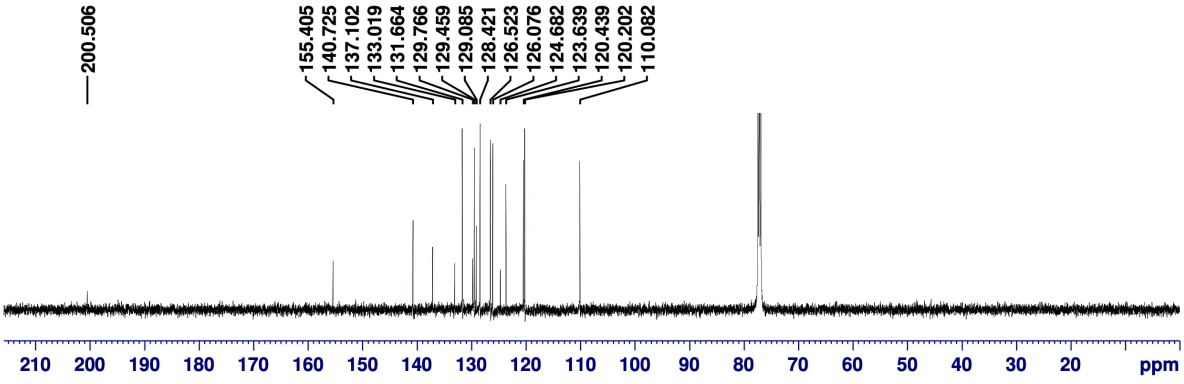


Fig. S15. ^{13}C NMR spectrum (125.7 MHz) of **3*o*** in $CDCl_3$ at 25 °C.

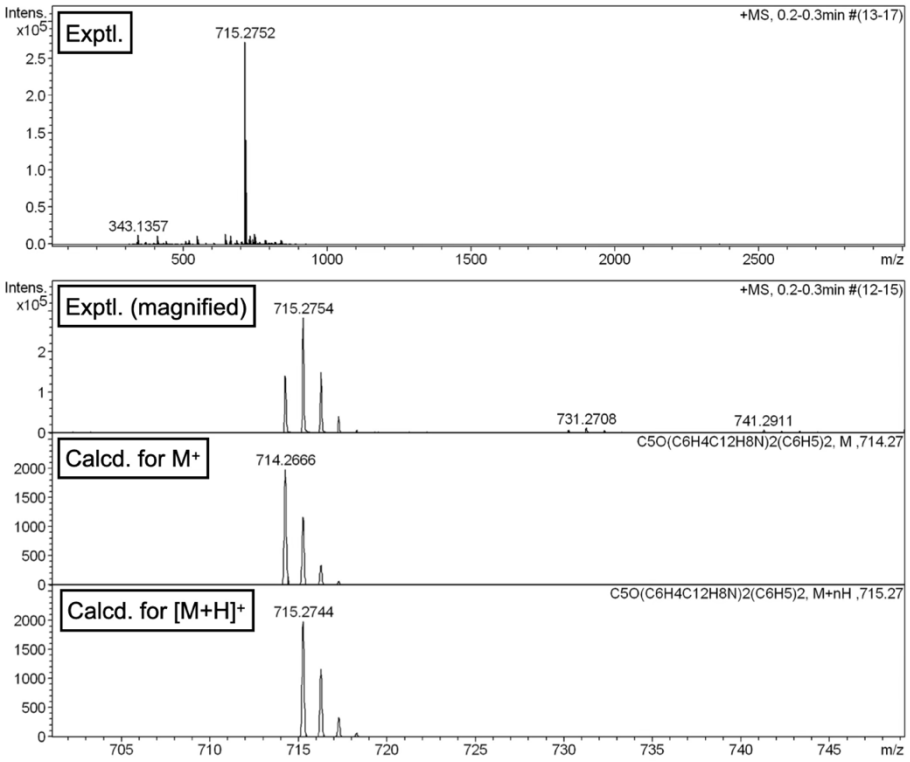


Fig. S16. High-resolution APCI-TOF mass spectrum of **3*o***.

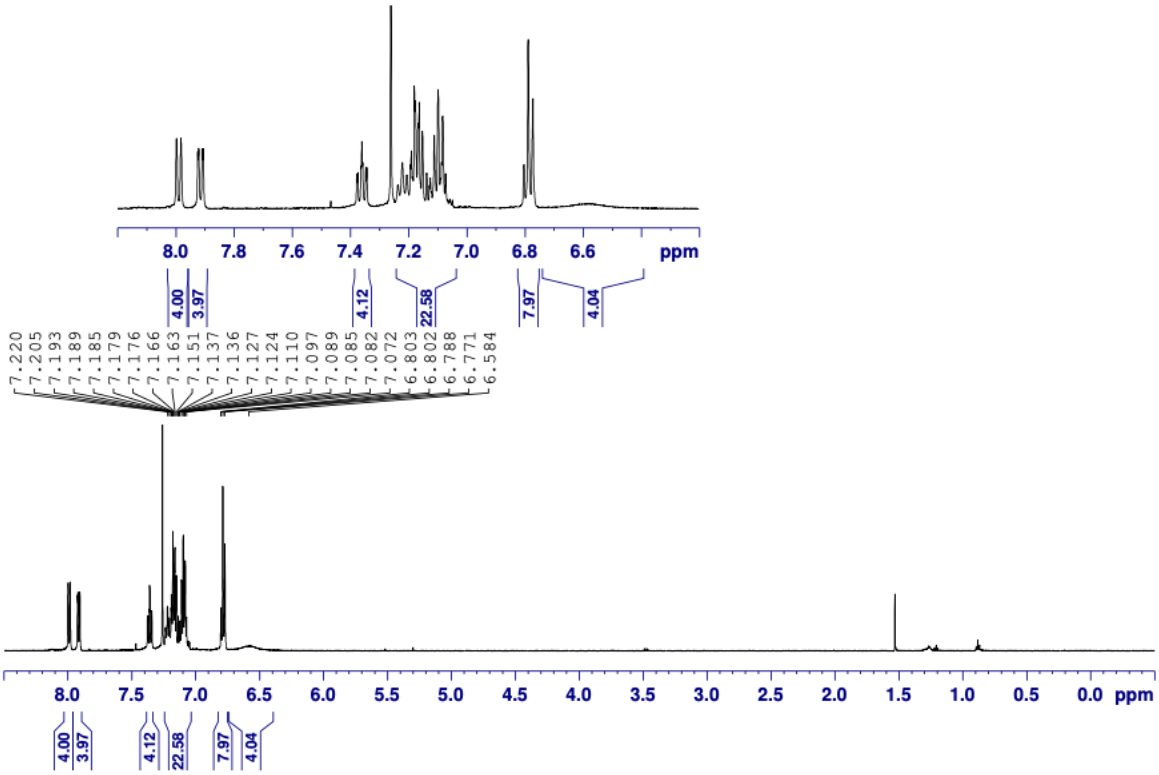


Fig. S17. ^{1}H NMR spectrum (500 MHz) of **2*o*** in $CDCl_3$ at 25 °C.

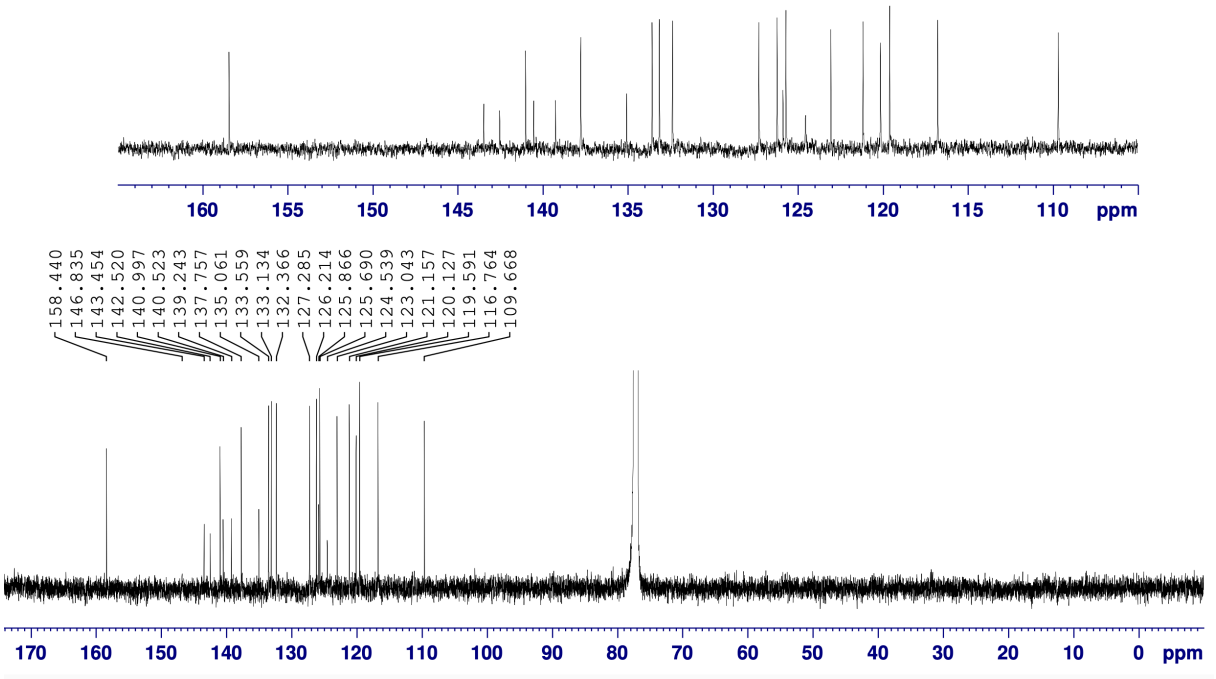


Fig. S18. ^{13}C NMR spectrum (125.7 MHz) of **2**$_o$ in $CDCl_3$ at 25 °C.

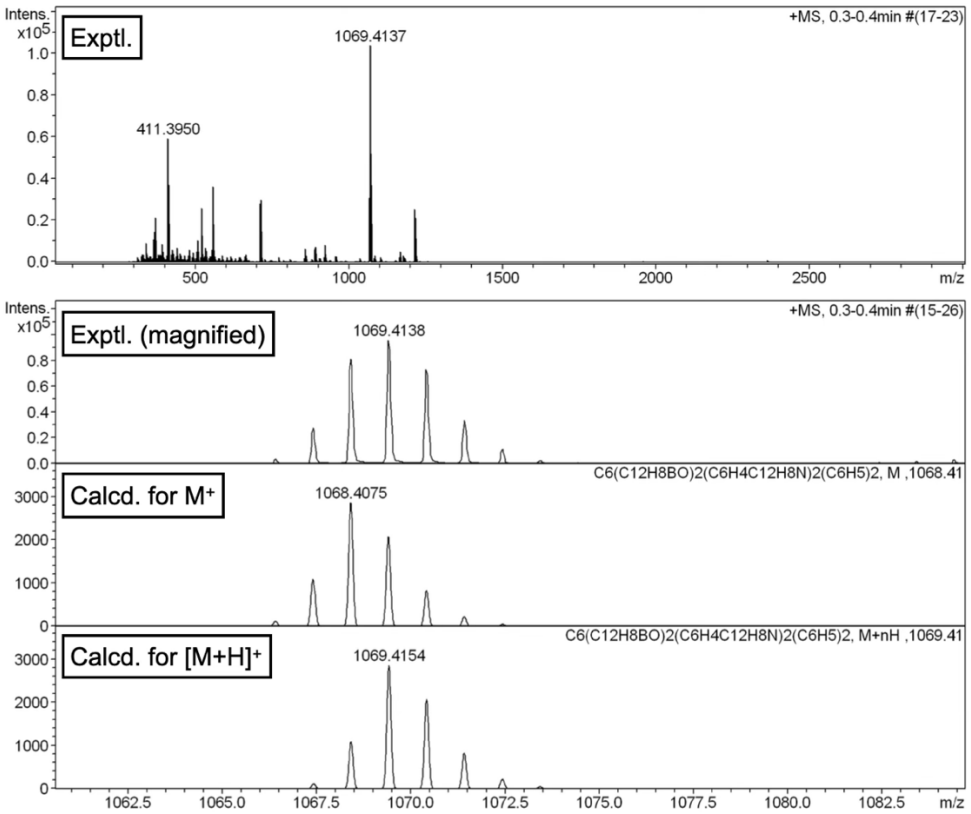


Fig. S19. High-resolution APCI-TOF mass spectrum of **2**$_o$.

9. Cartesian coordinates and energies

Table S1. Cartesian coordinates for the optimized geometry of **2*o*** (–3311.872841 hartree) calculated at the ωB97X-D/6-311G(d,p)//ωB97X-D/6-31G(d,p) level in vacuum.

C	0.69800000	0.17700000	-0.10700000
C	1.37900000	1.40000000	-0.22600000
C	0.69300000	2.62300000	-0.11600000
C	-0.69300000	2.62300000	0.11600000
C	-1.37900000	1.40000000	0.22600000
C	-0.69800000	0.17700000	0.10700000
C	2.85900000	1.32900000	-0.39400000
C	1.44100000	3.90900000	-0.24200000
C	-1.44100000	3.90900000	0.24200000
C	-2.85900000	1.32900000	0.39400000
C	-3.40800000	0.50200000	1.37700000
C	-4.76600000	0.21000000	1.38700000
C	-5.59400000	0.74800000	0.40800000
C	-5.07600000	1.64400000	-0.52800000
C	-3.72200000	1.93800000	-0.52400000
C	-1.48100000	4.82200000	-0.81500000
C	-2.19500000	6.00900000	-0.69700000
C	-2.87500000	6.30300000	0.48100000
C	-2.83900000	5.40100000	1.54100000
C	-2.12800000	4.21100000	1.42000000
C	2.12800000	4.21100000	-1.42000000
C	2.83900000	5.40100000	-1.54100000
C	2.87500000	6.30300000	-0.48200000
C	2.19500000	6.00900000	0.69700000
C	1.48200000	4.82200000	0.81400000
C	3.72200000	1.93800000	0.52400000
C	5.07600000	1.64400000	0.52800000
C	5.59400000	0.74800000	-0.40800000
C	4.76600000	0.21000000	-1.38700000
C	3.40800000	0.50200000	-1.37700000
N	6.94300000	0.32700000	-0.32300000
N	-6.94300000	0.32700000	0.32300000
B	1.43800000	-1.22300000	-0.21400000
C	2.39400000	-1.80500000	0.84800000
C	2.73800000	-3.16100000	0.76100000
O	2.29900000	-3.98300000	-0.23100000
C	1.54100000	-3.52900000	-1.26200000
C	1.10900000	-2.19900000	-1.36200000
C	1.20700000	-4.49300000	-2.21800000
C	0.44200000	-4.11900000	-3.30800000
C	0.01700000	-2.79300000	-3.46300000
C	0.35100000	-1.86100000	-2.50200000
C	2.90700000	-1.09200000	1.95000000
C	3.72300000	-1.68500000	2.89200000
C	4.04300000	-3.04400000	2.77000000
C	3.55000000	-3.78700000	1.71400000
B	-1.43800000	-1.22300000	0.21400000
C	-1.10900000	-2.19900000	1.36200000
C	-1.54100000	-3.52800000	1.26200000
O	-2.29900000	-3.98300000	0.23100000
C	-2.73800000	-3.16100000	-0.76100000
C	-2.39400000	-1.80500000	-0.84800000
C	-3.55000000	-3.78700000	-1.71400000
C	-4.04300000	-3.04400000	-2.77000000
C	-3.72400000	-1.68500000	-2.89200000
C	-2.90700000	-1.09200000	-1.95000000
C	-0.35100000	-1.86100000	2.50200000
C	-0.01700000	-2.79300000	3.46300000
C	-0.44200000	-4.11900000	3.30800000
C	-1.20700000	-4.49300000	2.21800000
C	-8.07700000	1.11500000	0.46200000
C	-9.21900000	0.32200000	0.22000000
C	-8.74100000	-1.00900000	-0.09900000
C	-7.33400000	-0.95900000	-0.03200000
C	-9.36700000	-2.20700000	-0.44800000
C	-8.58400000	-3.31700000	-0.73400000
C	-7.18400000	-3.23900000	-0.67900000
C	-6.53600000	-2.06300000	-0.32900000
C	-8.17200000	2.46400000	0.79900000

C	-9.44400000	3.01300000	0.88500000
C	-10.59100000	2.24200000	0.64800000
C	-10.48600000	0.89800000	0.31700000
C	8.07700000	1.11500000	-0.46200000
C	9.21900000	0.32200000	-0.22000000
C	8.74100000	-1.00900000	0.09900000
C	7.33400000	-0.95900000	0.03200000
C	8.17200000	2.46400000	-0.79900000
C	9.44400000	3.01300000	-0.88500000
C	10.59100000	2.24200000	-0.64700000
C	10.48600000	0.89800000	-0.31700000
C	9.36700000	-2.20700000	0.44800000
C	8.58400000	-3.31700000	0.73300000
C	7.18400000	-3.23900000	0.67900000
C	6.53600000	-2.06300000	0.32900000
H	-2.76200000	0.05700000	2.12800000
H	-5.18600000	-0.46200000	2.12900000
H	-5.73400000	2.06500000	-1.28100000
H	-3.31500000	2.60200000	-1.27900000
H	-0.94300000	4.60000000	-1.73000000
H	-2.21800000	6.70800000	-1.52800000
H	-3.43100000	7.23000000	0.57400000
H	-3.36600000	5.62200000	2.46300000
H	-2.10900000	3.50400000	2.24300000
H	2.10900000	3.50300000	-2.24300000
H	3.36600000	5.62200000	-2.46300000
H	3.43100000	7.23000000	-0.57400000
H	2.21800000	6.70800000	1.52700000
H	0.94300000	4.60000000	1.73000000
H	3.31500000	2.60200000	1.27900000
H	5.73400000	2.06500000	1.28100000
H	5.18600000	-0.46200000	-2.12900000
H	2.76200000	0.05700000	-2.12800000
H	1.55200000	-5.51200000	-2.08400000
H	0.17400000	-4.86400000	-4.05000000
H	-0.58800000	-2.51000000	-4.31700000
H	0.00300000	-0.83600000	-2.59900000
H	2.64500000	-0.04400000	2.05000000
H	4.11700000	-1.10700000	3.72200000
H	4.68500000	-3.51900000	3.50400000
H	3.77600000	-4.84100000	1.60100000
H	-3.77600000	-4.84100000	-1.60100000
H	-4.68500000	-3.51900000	-3.50400000
H	-4.11700000	-1.10800000	-3.72200000
H	-2.64500000	-0.04400000	-2.05000000
H	-0.00300000	-0.83600000	2.59900000
H	0.58800000	-2.51000000	4.31700000
H	-0.17400000	-4.86400000	4.05000000
H	-1.55200000	-5.51200000	2.08400000
H	-10.45000000	-2.26600000	-0.50300000
H	-9.05700000	-4.25400000	-1.00800000
H	-6.58600000	-4.11200000	-0.92000000
H	-5.45300000	-2.00200000	-0.30300000
H	-7.28400000	3.05800000	0.98600000
H	-9.55100000	4.06200000	1.14400000
H	-11.57000000	2.70300000	0.72500000
H	-11.37500000	0.30300000	0.13600000
H	7.28400000	3.05800000	-0.98600000
H	9.55100000	4.06200000	-1.14400000
H	11.57000000	2.70300000	-0.72500000
H	11.37500000	0.30300000	-0.13500000
H	10.45000000	-2.26600000	0.50300000
H	9.05700000	-4.25400000	1.00800000
H	6.58600000	-4.11300000	0.92000000
H	5.45300000	-2.00200000	0.30300000

Table S2. Cartesian coordinates for the optimized geometry of $\mathbf{2_H}$ (–2279.440024 hartree) calculated at the ωB97X-D/6-311G(d,p)//ωB97X-D/6-31G(d,p) level in vacuum.

O	4.11150200	-2.22884800	0.08952900
O	4.11150500	2.22873000	-0.08940000

C	4.34679600	0.49359500	-3.23179500
C	-2.49335400	0.68545500	-0.15544800
C	-1.27168300	-1.36770800	0.30112100
C	-3.78325500	1.41877900	-0.32846300
C	-3.78312900	-1.41895900	0.32834300
C	-2.49330700	-0.68550300	0.15530200
C	-1.27176800	1.36774000	-0.30128200
C	-0.05297300	-0.69107900	0.14333600
C	-1.21917800	2.82788800	-0.60738000
C	-4.68888700	1.53476700	0.72879500
H	-4.45510700	1.07036000	1.68180000
C	-0.05301900	0.69116500	-0.14360300
C	-1.21900300	-2.82780200	0.60746600
C	2.35620600	-1.12843200	1.34985700
C	-5.88440600	2.22486400	0.56532700
H	-6.57735600	2.30541000	1.39696600
C	1.88905100	-2.33442800	-0.88939800
C	-4.10117200	-2.00922100	1.55361700
H	-3.39739700	-1.93410200	2.37701900
C	-4.68873100	-1.53510300	-0.72892300
H	-4.45500700	-1.07068500	-1.68193500
C	3.25813000	-2.62955600	-0.89258800
C	3.08623400	3.77239600	2.99153400
H	5.11866800	-0.23664500	3.95053700
C	-4.10136700	2.00902900	-1.55372200
H	-3.39756800	1.93403800	-2.37711600
C	-0.49431800	3.28238300	-1.71268300
H	-0.02824600	2.56207200	-2.37866000
C	2.05477700	0.41226900	-2.52617800
H	1.03054500	0.08127800	-2.67409100
C	3.68717900	-1.52935500	1.17411000
C	2.35626800	1.12842000	-1.34988600
C	-0.49394900	-3.28206400	1.71273500
H	-0.02777200	-2.56160700	2.37848000
C	-0.36965400	4.64445600	-1.97258600
H	0.19883400	4.97710600	-2.83526600
C	-1.82722600	-3.77132800	-0.22692000
H	-2.40119600	-3.43214200	-1.08346200
C	-6.19334400	2.80741200	-0.66048300
H	-7.12737900	3.34516800	-0.78909600
C	-5.88415300	-2.22537000	-0.56545100
H	-6.57708200	-2.30603800	-1.39709500
C	-0.97118000	5.57198600	-1.13036100
H	1.10733300	3.85133200	3.85437300
C	-1.82728100	3.77125600	0.22728400
H	-2.40107000	3.43190300	1.08388000
C	1.13565700	-2.79342800	-1.98777500
H	0.07416600	-2.56568800	-2.01177100
C	1.71036200	3.50546600	3.02140900
C	1.88893500	2.33458700	0.88923800
C	3.25803400	2.62964500	0.89254700
C	-0.97083000	-5.57179100	1.13089400
C	3.86414100	-3.33812200	-1.93559700
H	4.93066900	-3.52835100	-1.89430700
C	-1.70227300	-5.12994200	0.03045200
H	-2.17490300	-5.84803100	-0.63219300
C	4.34664100	-0.49359000	3.23186400
H	5.11885200	0.23668100	-3.95044900
C	-5.29781700	-2.69704100	1.72012300
H	-5.52978600	-3.14955200	2.67913900
C	2.05467000	-0.41222200	2.52610000
H	1.03044300	-0.08118400	2.67392900
C	3.68723500	1.52932200	-1.17405700
C	3.02221700	0.09552900	-3.45803300
H	2.76757200	-0.47865700	-4.34192800
C	4.68598900	-1.21203000	2.10072400
H	5.70455100	-1.53058700	1.90989900
C	-6.19302000	-2.80793300	0.66036900
H	-7.12697300	-3.34582900	0.78898400
C	3.08647600	-3.77216100	-2.99166700
H	3.54973400	-4.32359700	-3.80415400
B	1.34195400	-1.43164000	0.23153000
C	-1.70241400	5.12991700	-0.02986800
H	-2.17494900	5.84787500	0.63298700
C	1.13545600	2.79371900	1.98750200
H	0.07393600	2.56609200	2.01138400
C	1.71062300	-3.50513500	-3.02167400

H	1.10766700	-3.85091100	-3.85472800
H	5.70465300	1.53052900	-1.90972900
C	-0.36919500	-4.64408500	1.97285600
H	0.19946000	-4.97657300	2.83548900
C	3.02206500	-0.09546600	3.45800100
H	2.76738100	0.47877000	4.34185400
B	1.34193400	1.43169800	-0.23163900
C	4.68609800	1.21198700	-2.10061100
C	-5.29811100	2.69668000	-1.72022700
H	-5.53012900	3.14918300	-2.67923500
H	4.93052700	3.52838400	1.89437400
H	3.54944100	4.32386300	3.80402900
C	3.86398100	3.33823600	1.93557200
H	-0.87289800	6.63451100	-1.32863900
H	-0.87244800	-6.63427500	1.32933500

Table S3. Cartesian coordinates and energies for the optimized geometry of **2*o*** in 1,2-DCE.

Energies [SMD(1,2-DCE)-*ω*B97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–3311.287807	Hartree
Zero-point Energy Correction	1.068686	Hartree
Thermal Correction (298 K) to Energy	1.131147	Hartree
Thermal Correction (298 K) to Enthalpy	1.132091	Hartree
Thermal Correction (298 K) to Free Energy	0.962732	Hartree

Single-point energy

[SMD(1,2-DCE)-*ω*B97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–3311.955689	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	1.041969	Hartree
Enthalpy including thermal corrections: H_SPC	-3310.848802	Hartree
Entropic term (RRHO): T.S.	0.163457	Hartree
Entropic term (quasi-RRHO): T.qh-S	0.144087	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-3311.01226	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-3310.992889	Hartree

O	-2.70516200	-3.84438200	-0.11742700
O	2.70499100	-3.84446300	0.11755800
N	6.97129000	0.33973300	-0.13523700
N	-6.97128700	0.33990100	0.13513500
C	0.69966500	2.59565600	-0.07173700
C	-1.38794600	1.37328100	0.12810900
C	1.45979300	3.87829400	-0.15510600
C	-1.45964500	3.87838300	0.15509900
C	-0.69959700	2.59569700	0.07171300
C	1.38794400	1.37320200	-0.12812700
C	-0.70298000	0.14771800	0.04888600
C	2.87495900	1.29673200	-0.22693300
C	1.48632100	4.76655200	0.92425200
H	0.93650600	4.52393200	1.82892200
C	0.70290800	0.14768000	-0.04890200
C	-2.87496600	1.29689600	0.22693000
C	-1.41641800	-2.24400900	1.17364000
C	2.20700000	5.95453500	0.84564800
H	2.22020500	6.63317400	1.69320600
C	-2.32015300	-1.69837600	-1.18982200
C	-2.16974400	4.20309700	1.31489500
H	-2.15693200	3.51826000	2.15802800
C	-1.48614700	4.76664200	-0.92425900
H	-0.93637400	4.52398600	-1.82894500
C	-2.85518100	-2.99337200	-1.17120400
C	9.19185600	0.07263200	-0.57756600
C	8.01386600	0.75987900	-0.94736200

C	2.16994500	4.20296200	-1.31488300
H	2.15711400	3.51812300	-2.15801400
C	3.46306200	0.60115200	-1.28808200
H	2.84444300	0.24947700	-2.10802100
C	0.76025700	-2.01130400	-2.40106300
H	0.29664400	-1.04201500	-2.55924700
C	-2.01860100	-3.49906900	1.00620600
C	1.41628700	-2.24411300	-1.17358000
C	-3.46309700	0.60133900	1.28807800
H	-2.84449300	0.24964700	2.10802100
C	4.82380100	0.31279500	-1.28426800
H	5.27114400	-0.26490400	-2.08673800
C	-3.69122800	1.77093300	-0.80499100
H	-3.25013100	2.32699400	-1.62608000
C	2.90944100	6.27156300	-0.31530600
H	3.47085100	7.19884300	-0.37699500
C	-2.20675400	5.95466800	-0.84563800
H	-2.21994200	6.63330500	-1.69319800
C	5.60927200	0.73456500	-0.21588100
C	8.82866400	-0.81901600	0.50664100
C	3.69124200	1.77073700	0.80498500
H	3.25016600	2.32681100	1.62607800
C	-8.82851600	-0.81913600	-0.50664500
C	-2.52815400	-0.94533400	-2.36516300
H	-2.10789200	0.05487700	-2.41635300
C	-7.45029400	-0.62522600	-0.74030500
C	7.45044000	-0.62518400	0.74035500
C	2.32001000	-1.69841100	1.18986900
C	2.85502300	-2.99341300	1.17130400
C	-5.60928500	0.73477900	0.21584000
C	-3.57127600	-3.52441800	-2.25066500
H	-3.96429000	-4.53356700	-2.18611300
C	-5.05040100	1.49057800	-0.81490200
H	-5.67962200	1.82394000	-1.63391000
C	8.00209300	1.70507200	-1.97424800
H	7.08987400	2.22625700	-2.24613900
C	-2.88767300	5.39299900	1.39614600
H	-3.43122800	5.63325800	2.30497500
C	-0.76038500	-2.01116200	2.40111400
H	-0.29675300	-1.04187600	2.55925500
C	2.01842400	-3.49918600	-1.00608600
C	0.68403000	-2.97837800	-3.38507800
H	0.16166500	-2.77781600	-4.31477600
C	-1.95454700	-4.49426500	1.98748500
H	-2.42929700	-5.45337400	1.80883600
C	-2.90914400	6.27174000	0.31533500
H	-3.47049600	7.19905400	0.37703800
C	-3.75272800	-2.74857200	-3.38075600
H	-4.30164600	-3.15496200	-4.22486300
C	9.52982300	-1.75581100	1.27133000
H	10.59110600	-1.91719000	1.10597000
C	5.05041000	1.49036400	0.81487500
H	5.67964800	1.82372700	1.63386900
C	2.52804100	-0.94531500	2.36517000
H	2.10779900	0.05490700	2.41632100
C	-3.22987400	-1.44772500	-3.44444200
H	-3.37355300	-0.84705300	-4.33661200
C	10.38518900	0.33882800	-1.25420600
H	11.29899800	-0.18119800	-0.98176000
C	-4.82384100	0.31300600	1.28424500
H	-5.27120500	-0.26469000	2.08670400
C	-0.68419700	-2.97818900	3.38517700
H	-0.16182800	-2.77759900	4.31486800
C	-6.75105800	-1.35427200	-1.70365700
H	-5.68775000	-1.20420700	-1.86338400
C	2.88794700	5.39282100	-1.39611600
H	3.43154200	5.63304500	-2.30493000
C	-9.52954000	-1.75613300	-1.27121100
H	-10.59081900	-1.91757700	-1.10589400
C	6.75133500	-1.35411900	1.70388900
H	5.68802500	-1.20412000	1.86366200
C	-9.19185400	0.07267700	0.57737900
C	1.28214000	-4.22834500	-3.16727700
H	1.22388100	-4.99744800	-3.93150500
C	-1.28235700	-4.22814300	3.16743900
H	-1.22413400	-4.99720600	3.93170900
C	9.20066600	1.94948300	-2.63200000

H	9.22336500	2.67837200	-3.43663600
C	1.95432400	-4.49443200	-1.98731100
H	2.42903600	-5.45355000	-1.80861300
C	-7.46977000	-2.28169700	-2.44586900
H	-6.95253000	-2.86676400	-3.20066200
C	3.57112800	-3.52441800	2.25077700
H	3.96413700	-4.53357200	2.18626500
C	10.38181500	1.27569500	-2.27952200
H	11.30047700	1.49218700	-2.81568300
C	-8.84509600	-2.48079800	-2.23855400
H	-9.37528100	-3.21367800	-2.83866700
C	3.75259600	-2.74852600	3.38083500
H	4.30151900	-3.15488500	4.22495300
C	3.22975900	-1.44767100	3.44446800
H	3.37345000	-0.84696000	4.33661000
C	8.84551000	-2.48036000	2.23885100
H	9.37580200	-3.21308300	2.83906400
C	7.47018200	-2.28134300	2.44622300
H	6.95304700	-2.86631700	3.20116000
B	-1.49697300	-1.22195100	0.02540200
C	-8.01394600	0.76009100	0.94712800
B	1.49683200	-1.22202400	-0.02537100
C	-10.38525100	0.33888900	1.25390100
H	-11.29900000	-0.18126100	0.98148900
C	-10.38201900	1.27593000	2.27905800
H	-11.30073100	1.49243500	2.81512600
C	-8.00231500	1.70545800	1.97385500
H	-7.09015500	2.22676500	2.24571200
C	-9.20094800	1.94987700	2.63149500
H	-9.22375800	2.67889900	3.43600700

Table S4. Cartesian coordinates and energies for the optimized geometry of MeOH in 1,2-DCE.

Energies [SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–115.798780	Hartree
Zero-point Energy Correction	0.051867	Hartree
Thermal Correction (298 K) to Energy	0.055193	Hartree
Thermal Correction (298 K) to Enthalpy	1.190623	Hartree
Thermal Correction (298 K) to Free Energy	0.056137	Hartree

Single-point energy

[SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–115.728696	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	0.050571	Hartree
Enthalpy including thermal corrections: H_SPC	-115.673834	Hartree
Entropic term (RRHO): T.S.	0.018113	Hartree
Entropic term (quasi-RRHO): T.qh-S	0.018115	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-115.691947	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-115.691949	Hartree

C	0.66609100	-0.02000000	0.00000000
H	1.08891100	0.98676700	-0.00000100
H	1.02203000	-0.54822500	-0.89296300
H	1.02203000	-0.54822300	0.89296400
O	-0.74835700	0.12315500	0.00000000
H	-1.14265900	-0.75555600	0.00000000

Table S5. Cartesian coordinates and energies for the optimized geometry of **2_o•MeOH** (1:1 complex) in 1,2-DCE.

Energies [SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–3426.992996	Hartree
Zero-point Energy Correction	1.123780	Hartree
Thermal Correction (298 K) to Energy	1.189679	Hartree
Thermal Correction (298 K) to Enthalpy	1.190623	Hartree
Thermal Correction (298 K) to Free Energy	1.016355	Hartree
BSSE Energy	0.004317	Hartree

Single-point energy

[SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–3427.690875	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	1.095685	Hartree
Enthalpy including thermal corrections: H_SPC	-3426.526765	Hartree
Entropic term (RRHO): T.S.	0.168522	Hartree
Entropic term (quasi-RRHO): T.qh-S	0.149641	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-3426.695287	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-3426.676405	Hartree

O	-3.80906000	-3.33531000	0.58548300
O	3.88583300	-3.54632800	-0.54241700
N	7.09678600	0.78426200	0.11706000
N	-7.06181300	0.50871400	-0.03286900
C	0.62330900	2.16568700	-0.12155600
C	-1.35120900	0.75143100	-0.04274400
C	1.26350400	3.51455900	-0.11889900
C	-1.64399800	3.24672300	-0.08453900
C	-0.77364500	2.03078600	-0.07498400
C	1.41447000	1.01283700	-0.16354700
C	-0.56129800	-0.42025500	-0.06807600
C	2.90756600	1.10927300	-0.14383600
C	1.17643500	4.34156800	1.00517500
H	0.62796200	3.99929100	1.87795500
C	0.83975200	-0.27524300	-0.15081200
C	-2.84729700	0.66463500	-0.02664400
C	-1.88075400	-2.18023600	1.52604800
C	1.78504500	5.59346600	1.01305900
H	1.71079500	6.22298600	1.89475600
C	-2.33675400	-2.28674100	-1.04789500
C	-2.36096600	3.62634700	1.05403000
H	-2.27093500	3.03691900	1.96168600
C	-1.76459000	4.01688300	-1.24447700
H	-1.20779100	3.73272800	-2.13291900
C	-3.48222400	-3.00933800	-0.70536300
C	9.34366800	0.94688000	-0.24124400
C	8.07878200	1.47916000	-0.57585800
C	1.97168900	3.96811700	-1.23591100
H	2.04364600	3.33380500	-2.11470900
C	3.66776000	0.83374700	-1.28305000
H	3.16914900	0.64358700	-2.22760200
C	1.71012500	-1.70942600	-2.86492900
H	0.96008800	-0.92239100	-2.86561100
C	-3.07887700	-2.88589000	1.65563500
C	2.26978900	-2.09307100	-1.62950700
C	-3.55527800	0.48175300	1.16263600
H	-3.01639500	0.37871600	2.09825900
C	5.05392300	0.74767300	-1.21145800
H	5.63790600	0.48947100	-2.08910000
C	-3.56416600	0.80346300	-1.21804300
H	-3.02740700	0.95596900	-2.14905600
C	2.48826400	6.03683200	-0.10509600
H	2.96268200	7.01347100	-0.09938800

C	-2.59166400	5.13677500	-1.26959300
H	-2.67780300	5.72246500	-2.17996700
C	5.69329500	0.96147600	0.00746800
C	9.10453600	-0.13541500	0.69291400
C	3.56898600	1.37374400	1.05901200
H	2.99007100	1.60970900	1.94648800
C	-9.20503500	-0.16143800	-0.44270700
C	-2.15289000	-2.01237900	-2.41312000
H	-1.28186800	-1.43151900	-2.70881100
C	-7.84406300	-0.40579500	-0.72701000
C	7.70754700	-0.20223000	0.88167300
C	2.67886100	-2.03417600	0.93105000
C	3.62665800	-3.03881600	0.69813300
C	-5.64333800	0.55625900	-0.03368300
C	-4.40023000	-3.45055900	-1.66265800
H	-5.27796500	-4.00346800	-1.34268300
C	-4.95190600	0.75504400	-1.22819800
H	-5.50268700	0.87737900	-2.15525700
C	7.94183000	2.55193900	-1.45873200
H	6.96551700	2.95718100	-1.70352000
C	-3.18770700	4.74595600	1.03140700
H	-3.73850900	5.02727800	1.92413100
C	-1.26577500	-1.76548900	2.71763300
H	-0.34400300	-1.19458100	2.64706400
C	3.25377800	-3.08886100	-1.66231500
C	2.10094200	-2.29052200	-4.05901200
H	1.65484000	-1.97620000	-4.99699200
C	-3.64430700	-3.17612200	2.90035900
H	-4.58377000	-3.71819600	2.94384900
C	-3.30743500	5.50334200	-0.13214700
H	-3.95422100	6.37525700	-0.15156800
C	-4.17899300	-3.16332500	-3.00185700
H	-4.89333600	-3.50126000	-3.74674600
C	9.93406800	-1.04340600	1.35696200
H	11.01107500	-1.00395200	1.22217600
C	4.95299600	1.30540700	1.13835000
H	5.46440100	1.49097900	2.07741300
C	2.53545400	-1.59360800	2.26133000
H	1.82644000	-0.79531500	2.46240000
C	-3.04807600	-2.43793000	-3.38563800
H	-2.87539600	-2.20594000	-4.43198100
C	10.49623200	1.49748300	-0.80780200
H	11.47515700	1.09818800	-0.55888200
C	-4.94379700	0.41425700	1.16343000
H	-5.48683000	0.25316100	2.08923600
C	-1.79932000	-2.04631700	3.96823700
H	-1.29455600	-1.71235200	4.86951400
C	-7.44373900	-1.44375000	-1.57008600
H	-6.39508500	-1.62737800	-1.77722200
C	2.57906100	5.22075300	-1.23057400
H	3.12327500	5.55940100	-2.10718200
C	-10.18759000	-0.96964700	-1.02136000
H	-11.23836700	-0.79237500	-0.81115200
C	7.11872400	-1.16385100	1.70493300
H	6.04261200	-1.21498400	1.83486500
C	-9.24142500	0.96420300	0.46909800
C	3.08544300	-3.28765300	-4.04718500
H	3.40245400	-3.74931400	-4.97729600
C	-2.99959000	-2.75738300	4.05444700
H	-3.43703300	-2.97922400	5.02327500
C	9.10234700	3.08031900	-2.00907200
H	9.02703800	3.91483500	-2.69978800
C	3.66661900	-3.68921100	-2.85643200
H	4.43561000	-4.45452400	-2.83173600
C	-8.43819100	-2.23426400	-2.13047100
H	-8.15451100	-3.04988500	-2.78934000
C	4.38422800	-3.60455800	1.72964300
H	5.10642000	-4.38078600	1.49907900
C	10.36825900	2.56148600	-1.69095800
H	11.25375400	2.99962500	-2.14053500
C	-9.79781300	-2.00247800	-1.86394000
H	-10.54893300	-2.63921800	-2.32078800
C	4.19982700	-3.15122000	3.02464100
H	4.78376900	-3.58594600	3.83025900
C	3.27484400	-2.13412100	3.29843500
H	3.14366800	-1.77603000	4.31433100
C	9.35787300	-1.99913400	2.18375400

H	9.98855700	-2.71237200	2.70513800
C	7.96408700	-2.05711100	2.34934200
H	7.53329200	-2.81760100	2.99411500
B	-1.30442300	-1.84889200	0.08229800
C	-7.90019800	1.34409400	0.69507200
B	1.85525300	-1.48767200	-0.26066400
C	-10.27467100	1.67057100	1.09058600
H	-11.31020200	1.38747600	0.92548600
C	-9.95515500	2.73979100	1.91680800
H	-10.74593500	3.29818100	2.40783000
C	-7.57125000	2.42520500	1.51586400
H	-6.53875300	2.72105100	1.67004100
C	-8.61600900	3.11121600	2.12115500
H	-8.38976500	3.95591300	2.76494600
O	-0.01372900	-2.98091400	-0.15079900
H	-0.00685100	-3.23539600	-1.08798900
C	0.13601200	-4.17234300	0.65573500
H	0.97567800	-4.74186300	0.25591900
H	0.35055700	-3.84715600	1.67082100
H	-0.78301000	-4.76036400	0.62495000

Table S6. Cartesian coordinates and energies for the optimized geometry of **2_o•(MeOH)$_2$** (1:2 complex) in 1,2-DCE.

Energies [SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–3542.716188	Hartree
Zero-point Energy Correction	1.178297	Hartree
Thermal Correction (298 K) to Energy	1.248085	Hartree
Thermal Correction (298 K) to Enthalpy	1.249030	Hartree
Thermal Correction (298 K) to Free Energy	1.066547	Hartree
BSSE Energy	0.007461	Hartree

Single-point energy

[SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–3543.442871	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	1.14884	Hartree
Enthalpy including thermal corrections: H_SPC	-3542.221664	Hartree
Entropic term (RRHO): T.S.	0.176893	Hartree
Entropic term (quasi-RRHO): T.qh-S	0.157313	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-3542.398557	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-3542.378976	Hartree

O	-3.77835300	-3.16786700	0.86025600
O	3.88200100	-3.45816200	-0.22864400
N	7.12439600	0.91713200	0.08426600
N	-7.04159900	0.68256500	-0.01906900
C	0.65090000	2.28623400	-0.19578100
C	-1.32667300	0.88444900	0.00041100
C	1.29357800	3.63050500	-0.29341100
C	-1.61176700	3.37199300	-0.23451600
C	-0.74632400	2.15671500	-0.13194500
C	1.43973600	1.13196300	-0.16107500
C	-0.53765200	-0.28789300	0.05930200
C	2.93287800	1.22594700	-0.16138700
C	1.21084600	4.53790700	0.76725700
H	0.66301600	4.26165600	1.66350800
C	0.86131600	-0.14957900	-0.04975300
C	-2.82420700	0.80752900	0.01603700
C	-1.90480500	-1.89686000	1.75936200
C	1.82274800	5.78540600	0.68276500
H	1.75142800	6.47784800	1.51625600

C	-2.29075500	-2.20333100	-0.80891000
C	-2.33063900	3.84017200	0.86924800
H	-2.24774200	3.31970400	1.81871700
C	-1.72224900	4.05583200	-1.44852600
H	-1.16389500	3.70330200	-2.31114000
C	-3.44472500	-2.89794500	-0.44302100
C	9.36939900	1.06915100	-0.28952900
C	8.10094500	1.57562300	-0.65011200
C	2.00090700	3.99973900	-1.44169800
H	2.06982100	3.30287500	-2.27203700
C	3.68252500	0.86905700	-1.28493000
H	3.17509100	0.61415000	-2.20934200
C	1.69745900	-1.78531900	-2.66027800
H	0.96214800	-0.98685200	-2.71601100
C	-3.09984700	-2.60141400	1.91127000
C	2.26778700	-2.07743000	-1.40615300
C	-3.54543900	0.72433300	1.20838000
H	-3.01756500	0.69202400	2.15501600
C	5.06935200	0.78768700	-1.21998900
H	5.64600900	0.46859300	-2.08237000
C	-3.53070400	0.86120200	-1.18857100
H	-2.98490300	0.93899500	-2.12341400
C	2.52493000	6.14414100	-0.46599400
H	3.00181800	7.11733700	-0.53256600
C	-2.54036200	5.17693900	-1.56024900
H	-2.61831200	5.69448100	-2.51173800
C	5.71967800	1.08680200	-0.02504100
C	9.13786700	0.04096000	0.70574600
C	3.60526000	1.57416300	1.01372000
H	3.03422100	1.87214700	1.88751800
C	-9.18525400	-0.00046800	-0.40614200
C	-2.11178400	-1.97110900	-2.18147600
H	-1.23668600	-1.40800100	-2.49650800
C	-7.82304400	-0.27246100	-0.65720600
C	7.74168800	-0.02074700	0.90245000
C	2.70011000	-1.83170000	1.13856600
C	3.64191400	-2.85394900	0.97253900
C	-5.62260100	0.72086200	-0.00957200
C	-4.36686500	-3.36700700	-1.38381900
H	-5.24994800	-3.89899500	-1.04347200
C	-4.91864900	0.82336600	-1.20882900
H	-5.45966400	0.87927100	-2.14795500
C	7.95587300	2.59514200	-1.59269600
H	6.97660700	2.98045100	-1.85722900
C	-3.14883500	4.96103700	0.76017700
H	-3.70087900	5.31142200	1.62736800
C	-1.34192600	-1.36110000	2.92763000
H	-0.41935800	-0.79208200	2.83841100
C	3.23576600	-3.08726600	-1.37121900
C	2.05001900	-2.47862000	-3.80713600
H	1.59430100	-2.23450400	-4.76136400
C	-3.71284100	-2.77701000	3.15463900
H	-4.64847400	-3.32438200	3.21390200
C	-3.25816800	5.63162700	-0.45637900
H	-3.89825100	6.50442900	-0.54282800
C	-4.14801400	-3.12448500	-2.73244800
H	-4.86735500	-3.47929100	-3.46465300
C	9.97294400	-0.82401300	1.41856900
H	11.04940700	-0.78816300	1.27851000
C	4.98990100	1.50988100	1.08550000
H	5.50998000	1.75994000	2.00463700
C	2.56405300	-1.29676300	2.43430200
H	1.85048100	-0.49064600	2.58295800
C	-3.01332200	-2.41672100	-3.13978500
H	-2.84308900	-2.21394500	-4.19276400
C	10.51760000	1.59278500	-0.88971500
H	11.49932000	1.21358400	-0.62114200
C	-4.93442000	0.66721300	1.20111700
H	-5.48620000	0.58194200	2.13174500
C	-1.92381300	-1.52392600	4.17838700
H	-1.45847200	-1.09750700	5.06184400
C	-7.42100600	-1.36852500	-1.42229800
H	-6.37138400	-1.57219600	-1.60376500
C	2.61161300	5.24770500	-1.52896500
H	3.15513600	5.52001400	-2.42882100
C	-10.16708700	-0.84037100	-0.93915000
H	-11.21882800	-0.64246100	-0.75362000

C	7.15908100	-0.93501700	1.78209600
H	6.08359100	-0.98217700	1.91849000
C	-9.22348800	1.18553500	0.42548300
C	3.01445900	-3.49437500	-3.72571600
H	3.30222800	-4.04289200	-4.61732600
C	-3.12018600	-2.23794400	4.28717500
H	-3.59462100	-2.36940500	5.25512900
C	9.11216100	3.09742400	-2.17543300
H	9.03058200	3.89073800	-2.91244100
C	3.61437300	-3.79821300	-2.51570200
H	4.36894900	-4.57403800	-2.43723300
C	-8.41469700	-2.18932600	-1.93860500
H	-8.12964500	-3.04999200	-2.53683500
C	4.40806000	-3.34351300	2.03600000
H	5.12620700	-4.13711900	1.85761300
C	10.38160500	2.60420700	-1.83156900
H	11.26367800	3.02091000	-2.30751600
C	-9.77551100	-1.93104600	-1.70442300
H	-10.52606800	-2.59286000	-2.12514300
C	4.23466500	-2.79570400	3.29576200
H	4.82485000	-3.17089700	4.12639200
C	3.31117600	-1.76149300	3.50239300
H	3.18607500	-1.33277000	4.49138500
C	9.40301300	-1.73268300	2.30084900
H	10.03815100	-2.41200500	2.86070600
C	8.00995100	-1.78622900	2.47434300
H	7.58429400	-2.50966500	3.16362100
B	-1.25717100	-1.71915500	0.31089200
C	-7.88202700	1.57162200	0.63982500
B	1.86319500	-1.37510300	-0.08165600
C	-10.25867800	1.93932700	0.98500400
H	-11.29422400	1.65172700	0.82795400
C	-9.94095400	3.06089200	1.73936300
H	-10.73310800	3.65665700	2.18186300
C	-7.55501600	2.70488700	1.38796500
H	-6.52237000	3.00454900	1.53326000
C	-8.60156000	3.43732300	1.93266200
H	-8.37643100	4.32295400	2.51933800
O	-0.01272400	-2.83977200	0.23307900
H	-0.01912700	-3.34228500	-0.63861500
C	0.18966000	-3.83192000	1.26095700
H	1.00495300	-4.47958100	0.93610200
H	0.46591600	-3.32130300	2.18047300
H	-0.72432400	-4.41069300	1.41015200
H	-1.27984700	-5.66011300	-0.91369900
C	-1.02959600	-5.31123400	-1.91701400
H	-1.88983600	-4.78868900	-2.34370200
H	-0.76683200	-6.17143000	-2.53943100
O	0.09438700	-4.43748300	-1.78111800
H	0.32317300	-4.04853500	-2.63584100

Table S7. Cartesian coordinates and energies for the optimized geometry of $\mathbf{2_H}$ in 1,2-DCE.

Energies [SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–2279.035818	Hartree
Zero-point Energy Correction	0.751042	Hartree
Thermal Correction (298 K) to Energy	0.795088	Hartree
Thermal Correction (298 K) to Enthalpy	0.796032	Hartree
Thermal Correction (298 K) to Free Energy	0.669787	Hartree

Single-point energy

[SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–2279.496965	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	0.732266	Hartree
Enthalpy including thermal corrections: H_SPC	-2278.718666	Hartree
Entropic term (RRHO): T.S.	0.119399	Hartree

Entropic term (quasi-RRHO): T.qh-S	0.10703	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-2278.838066	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-2278.825697	Hartree

---

O	-4.07652525	2.40599836	0.05850699
O	-4.07612749	-2.40657898	-0.05812102
C	-4.39348643	-0.73103085	-3.22955025
C	2.47226907	-0.68606218	-0.15315202
C	1.25084508	1.37031702	0.29059401
C	3.76381712	-1.41595130	-0.33306104
C	3.76341526	1.41667090	0.33332201
C	2.47208713	0.68640991	0.15328500
C	1.25120694	-1.37025517	-0.29066903
C	0.03051496	0.69278004	0.13409400
C	1.20281487	-2.83240528	-0.59205805
C	4.64680718	-1.58551135	0.73749604
H	4.39052818	-1.17680631	1.71058411
C	0.03070789	-0.69302007	-0.13426402
C	1.20206715	2.83251113	0.59173203
C	-2.38290619	1.20892219	1.31783108
C	5.84708125	-2.26834346	0.56427003
H	6.52196227	-2.39315351	1.40579109
C	-1.86128510	2.35980825	-0.94066208
C	4.10573331	1.94565993	1.58113310
H	3.42359026	1.82302895	2.41757316
C	4.64648133	1.58642087	-0.73714407
H	4.39043530	1.17757586	-1.71023413
C	-3.20753618	2.74814434	-0.93511208
C	-2.97661248	-3.87491314	3.03845221
H	-5.17205943	0.53831128	3.96173827
C	4.10643412	-1.94476635	-1.58086213
H	3.42434908	-1.82229231	-2.41737319
C	0.51343480	-3.28819528	-1.72077414
H	0.07419780	-2.56893520	-2.40624318
C	-2.11361626	-0.49860994	-2.50644719
H	-1.10634216	-0.12241997	-2.66189221
C	-3.68963726	1.68755729	1.14813007
C	-2.38278931	-1.20941498	-1.31774111
C	0.51266412	3.28838320	1.72038911
H	0.07372005	2.56916917	2.40609416
C	0.39395272	-4.65231037	-1.98045516
H	-0.14422033	-4.98666137	-2.86225622
C	1.77774423	3.77477717	-0.26880603
H	2.31457826	3.43611512	-1.14972209
C	6.18203124	-2.78921052	-0.68401906
H	7.11917827	-3.32043160	-0.82010807
C	5.84654446	2.26959886	-0.56382005
H	6.52148950	2.39455084	-1.40527012
C	0.96431572	-5.57963846	-1.11397509
H	-1.00718334	-3.80411724	3.92585627
C	1.77885987	-3.77475037	0.26814701
H	2.31564792	-3.43620237	1.14913507
C	-1.08937502	2.75999224	-2.05139616
H	-0.04732496	2.45590217	-2.09073216
C	-1.62323937	-3.50794618	3.08298621
C	-1.86071133	-2.36033009	0.94063205
C	-3.20695445	-2.74868105	0.93535106
C	0.96271727	5.57979636	1.11284506
C	-3.77399818	3.49786943	-1.97214715
H	-4.82398924	3.76720250	-1.92519515
C	1.65739129	5.13580027	-0.01207701
H	2.10242336	5.85315832	-0.69499606
C	-4.39330236	0.73024126	3.22988522
H	-5.17235248	-0.53923780	-3.96132230
C	5.30698544	2.62671992	1.75678012
H	5.56006948	3.02948893	2.73297018
C	-2.11349521	0.49812713	2.50649017
H	-1.10615115	0.12208405	2.66181918
C	-3.68945142	-1.68817495	-1.14784110
C	-3.09166431	-0.25861988	-3.45262426
H	-2.86151227	0.30097515	-4.35325632
C	-4.69944735	1.44752432	2.08657413
H	-5.70007539	1.82602440	1.90565512
C	6.18119853	2.79063288	0.68447803

H	7.11818062	3.32212288	0.82065105
C	-2.97761010	3.87449141	-3.03820423
H	-3.40941110	4.45612348	-3.84702029
B	-1.35455510	1.45261416	0.19754400
C	1.65893679	-5.13573647	0.01101699
H	2.10428279	-5.85314155	0.69368304
C	-1.08857229	-2.76045016	2.05123613
H	-0.04653120	-2.45630719	2.09036114
C	-1.62424502	3.50752832	-3.08301323
H	-1.00833696	3.80375131	-3.92597230
H	-5.69996955	-1.82691186	-1.90511915
C	0.39276018	4.65254130	1.97967013
H	-0.14542584	4.98698636	2.86142719
C	-3.09139529	0.25797916	3.45277923
H	-2.86105530	-0.30159489	4.35337730
B	-1.35424825	-1.45304305	-0.19761803
C	-4.69940949	-1.44829289	-2.08616517
C	5.30789816	-2.62548046	-1.75641414
H	5.56120515	-3.02811950	-2.73260021
H	-4.82321861	-3.76767705	1.92582213
H	-3.40825654	-4.45649016	3.84739226
C	-3.77321652	-3.49834808	1.97253713
H	0.87011066	-6.64294055	-1.31236611
H	0.86814231	6.64312444	1.31093708

Table S8. Cartesian coordinates and energies for the optimized geometry of **2_H•MeOH** (1:1 complex) in 1,2-DCE.

Energies [SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–2394.738257	Hartree
Zero-point Energy Correction	0.805677	Hartree
Thermal Correction (298 K) to Energy	0.853285	Hartree
Thermal Correction (298 K) to Enthalpy	0.854229	Hartree
Thermal Correction (298 K) to Free Energy	0.721269	Hartree
BSSE Energy	0.007456	Hartree

Single-point energy

[SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–2395.229892	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	0.785535	Hartree
Enthalpy including thermal corrections: H_SPC	-2394.394696	Hartree
Entropic term (RRHO): T.S.	0.126272	Hartree
Entropic term (quasi-RRHO): T.qh-S	0.113537	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-2394.520968	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-2394.508233	Hartree

O	-3.54786126	-3.45309125	0.46843603
O	4.16348230	-3.02689022	-0.35745803
C	3.49218125	-2.81257020	-3.89297128
C	0.40626103	2.39161417	-0.03041200
C	-1.43140310	0.79946806	-0.04216000
C	0.90799306	3.79815727	0.00901100
C	-1.94389714	3.26309924	-0.07823601
C	-0.97319607	2.12610615	-0.04207300
C	1.30790710	1.32074109	-0.05353000
C	-0.53059504	-0.29077102	-0.04579600
C	2.78141720	1.58332712	0.00679100
C	0.70799205	4.59209233	1.14235508
H	0.17753001	4.17877330	1.99528414
C	0.85317606	-0.01400200	-0.07684601
C	-2.91203821	0.56244804	-0.08905301

C	-1.73332712	-2.18544716	1.48753411
C	1.18080509	5.90063642	1.18467809
H	1.01850107	6.50349446	2.07324615
C	-2.08227115	-2.30566217	-1.10334608
C	-2.71751020	3.58591826	1.04025307
H	-2.61431519	2.99765222	1.94730514
C	-2.08412015	4.03002129	-1.23829109
H	-1.48418611	3.78919427	-2.11133815
C	-3.19735423	-3.09274522	-0.80750206
C	4.31238431	-2.60256319	3.21807523
H	-3.31534224	-3.18343223	4.92181636
C	1.59260012	4.34212331	-1.08169808
H	1.75415013	3.73368427	-1.96676614
C	3.59627226	1.40951710	-1.11523408
H	3.14906823	1.11912008	-2.06062615
C	1.96110514	-1.33993509	-2.76739320
H	1.15682808	-0.60895004	-2.79773720
C	-2.87851321	-2.98074122	1.56778111
C	2.49505018	-1.68763512	-1.51030111
C	-3.64784926	0.30174502	1.06910108
H	-3.14190823	0.27432102	2.02894815
C	4.97373336	1.60217311	-1.03033708
H	5.59206142	1.46039410	-1.91169114
C	-3.58421026	0.60737504	-1.31424109
H	-3.02306222	0.81737206	-2.21998716
C	1.86020614	6.43456145	0.09167901
H	2.22850316	7.45552556	0.12353601
C	-2.97942421	5.09535337	-1.28116709
H	-3.07753022	5.68057838	-2.19068416
C	5.55339640	1.97657614	0.17889601
H	3.10481122	-1.31320610	4.46217532
C	3.37276224	1.97369614	1.21302309
H	2.74720620	2.11854415	2.08909515
C	-1.85413013	-2.02534815	-2.46046818
H	-1.00413207	-1.39865010	-2.72194320
C	3.30177624	-1.66062112	3.45316225
C	2.79309120	-1.60792712	1.06506707
C	3.82178428	-2.53803518	0.87169007
C	-5.67361743	0.08505401	-0.22698702
C	-4.05795929	-3.57020726	-1.79973313
H	-4.91926735	-4.16625830	-1.51452711
C	-4.95192836	0.36392203	-1.38655310
H	-5.45387737	0.38831703	-2.34918817
C	-2.87134221	-2.90515521	3.97063929
H	3.87884928	-3.24768523	-4.80944935
C	-3.61147426	4.65227734	1.00058807
H	-4.20336530	4.89203335	1.87896814
C	-1.18377408	-1.75376413	2.70454119
H	-0.30394702	-1.11699808	2.67248119
C	3.54827326	-2.61052119	-1.50282811
C	2.44127218	-1.88721114	-3.94492428
H	2.01305314	-1.60176512	-4.90032835
C	-3.45155225	-3.34363224	2.78979220
H	-4.34752431	-3.95654128	2.79537420
C	-3.74569127	5.40991840	-0.16103001
H	-4.44305332	6.24166047	-0.19267701
C	-3.79663228	-3.27253123	-3.12894223
H	-4.46389132	-3.64193126	-3.90192928
B	-1.13882208	-1.78560913	0.06849700
C	4.74743934	2.16699715	1.30034009
H	5.19129137	2.46266918	2.24625116
C	2.56467919	-1.17769209	2.38647617
H	1.79051013	-0.43422403	2.55605818
C	-2.68434319	-2.49794818	-3.46821725
H	-2.47866618	-2.26038817	-4.50739632
H	4.86991435	-3.88616428	-2.62371719
C	-5.01893536	0.06342500	1.00219207
H	-5.57293442	-0.14461201	1.91284014
C	-1.72736913	-2.10309315	3.93356228
H	-1.27328109	-1.75321613	4.85554435
B	1.97584214	-1.12736208	-0.15766101
C	4.05086329	-3.17639023	-2.67936519
C	2.06439615	5.65130139	-1.04227308
H	2.59174918	6.05994841	-1.89915014
H	5.36597838	-3.76402727	1.73397313
H	4.89777135	-2.98940022	4.04670129
C	4.58039733	-3.04237622	1.93306814

H	6.62701348	2.12351615	0.24745002
H	-6.74083146	-0.10826901	-0.28096502
H	0.66061805	-3.64490926	1.69676812
C	0.48234203	-3.97477329	0.67615905
H	1.36449010	-4.48140432	0.28332802
H	-0.39284103	-4.62529733	0.62791405
O	0.26022202	-2.78935120	-0.12287601
H	0.31961802	-3.03201322	-1.06122508

Table S9. Cartesian coordinates and energies for the optimized geometry of $\mathbf{2_H{\bullet}(MeOH)_2}$ (1:2 complex) in 1,2-DCE.

Energies [SMD(1,2-DCE)-ωB97X-D/6-31G(d,p) for C, H, B, N, 6-31+G(d,p) for O]

Electronic Energy (EE)	–2510.461318	Hartree
Zero-point Energy Correction	0.860441	Hartree
Thermal Correction (298 K) to Energy	0.911820	Hartree
Thermal Correction (298 K) to Enthalpy	0.912764	Hartree
Thermal Correction (298 K) to Free Energy	0.772683	Hartree
BSSE Energy	0.007456	Hartree

Single-point energy

[SMD(1,2-DCE)-ωB97X-D/6-311G(d,p) for C, H, B, N, 6-311+G(d,p) for O]

Electronic Energy (EE)	–2510.981798	Hartree

Energy values obtained by the GoodVibes corrections

Zero-point energy	0.83893	Hartree
Enthalpy including thermal corrections: H_SPC	-2510.08938	Hartree
Entropic term (RRHO): T.S.	0.133545	Hartree
Entropic term (quasi-RRHO): T.qh-S	0.120769	Hartree
Gibbs free energy (RRHO): G(T)_SPC	-2510.222925	Hartree
Gibbs free energy (quasi-RRHO): qh-G(T)_SPC	-2510.210149	Hartree

O	-3.30050624	3.48213879	0.70258793
O	-2.79034641	-4.21229977	0.00420902
C	2.57934660	-0.38098490	-0.11993292
C	0.96343430	1.43318825	0.00345098
C	3.99212516	-0.85998562	-0.20124349
C	3.41087008	1.98038884	-0.21710031
C	2.29257575	0.99404974	-0.10220211
C	1.52429081	-1.29876254	-0.06159173
C	-0.11114252	0.51556307	0.08327060
C	1.81561665	-2.76786733	-0.03089449
C	4.86343458	-0.69113764	0.87896943
H	4.50555919	-0.20213572	1.78043863
C	0.18585523	-0.86230777	0.02371512
C	0.71047517	2.91201266	-0.03280987
C	-1.89507644	1.76347243	1.70599866
C	6.17881945	-1.14104332	0.80662423
H	6.84297939	-1.00332308	1.65471672
C	-2.18859853	2.00527185	-0.88287882
C	3.81515682	2.73968408	0.88458838
H	3.30286404	2.61479367	1.83406402
C	4.08004459	2.14875434	-1.43255587
H	3.77606863	1.56025709	-2.29361009
C	-2.97801049	3.11534530	-0.58032013
C	4.46505764	-1.49045409	-1.35576448
H	3.79552861	-1.62716693	-2.20007465
C	1.58388278	-3.57825285	-1.14566310
H	1.21978156	-3.13061158	-2.06500974
C	-1.32498053	-2.01802142	-2.55006834
H	-0.60183148	-1.21230738	-2.64728283
C	-2.71110199	2.89237270	1.79335682
C	-1.56734175	-2.54133737	-1.26532720

C	0.53158492	3.65760841	1.13426307
H	0.57781414	3.16147921	2.09813273
C	1.81180545	-4.95159350	-1.08656993
H	1.62368337	-5.56624456	-1.96182548
C	0.66430812	3.57551235	-1.26284101
H	0.81251056	3.00830359	-2.17690067
C	6.64169138	-1.76602407	-0.34943872
H	7.66789031	-2.11623594	-0.40707877
C	5.12833806	3.05799183	-1.54617375
H	5.63665789	3.17840783	-2.49827364
C	2.28046547	-5.53206892	0.08903421
C	2.29966300	-3.35989802	1.14061233
H	2.48978371	-2.73811176	2.01070746
C	-1.92979953	1.77632783	-2.24306172
H	-1.29546479	0.93459483	-2.51030296
C	-1.28399163	-2.80896843	1.29768823
C	-2.20835511	-3.85422393	1.18770548
C	0.20690208	5.67115495	-0.15896206
C	-3.49699532	3.95752525	-1.56844321
H	-4.09650792	4.81399006	-1.27576774
C	0.40725554	4.94099903	-1.32928247
H	0.35988905	5.43432316	-2.29557260
C	4.86449403	3.64770617	0.77420151
H	5.16741173	4.22874485	1.64025014
C	-1.34397889	1.29656366	2.90873100
H	-0.68874327	0.42953538	2.87040365
C	-2.47728881	-3.60055572	-1.17456208
C	-1.96973448	-2.50561172	-3.67540249
H	-1.76379307	-2.08563478	-4.65472339
C	-2.98206096	3.52808808	3.00792437
H	-3.61657128	4.40899598	3.01716413
C	5.52408458	3.81014821	-0.44231442
H	6.34225384	4.51877137	-0.52937845
C	-3.22600424	3.69065983	-2.90240297
H	-3.62353607	4.34521854	-3.67234228
C	2.52842137	-4.73062725	1.20235383
H	2.89756944	-5.17468140	2.12199318
C	-0.75874113	-2.55454934	2.57916491
H	-0.02494144	-1.75963423	2.68323582
C	-2.43558679	2.59060395	-3.24823139
H	-2.21185512	2.38296479	-4.29029186
C	0.27842776	5.02626776	1.07338970
H	0.13291038	5.58618142	1.99253008
C	-1.59814298	1.90387540	4.13196408
H	-1.15643103	1.51227397	5.04326169
C	5.78073359	-1.93935808	-1.43099224
H	6.13372890	-2.42468350	-2.33610027
C	-2.88615844	-3.55899848	-3.53876275
H	-3.39592896	-3.95225835	-4.41297575
C	-2.42564611	3.02891397	4.17660614
H	-2.63154633	3.52179116	5.12218690
C	-3.13990927	-4.11309103	-2.29575956
H	-3.83900409	-4.93415752	-2.17473879
C	-2.61419170	-4.60992296	2.29243624
H	-3.33575993	-5.40931816	2.15868221
C	-2.08068917	-4.31916713	3.53648349
H	-2.39091537	-4.90160457	4.39877656
C	-1.14388463	-3.28786885	3.68773422
H	-0.72517972	-3.07146868	4.66524410
B	-1.61816344	1.07986042	0.28962238
B	-0.91752995	-1.99464965	0.03408158
O	-2.59702407	-0.28166713	0.24910217
H	-3.08107658	-0.36135493	-0.62855139
C	-3.58085978	-0.55130447	1.26887147
H	-4.13737072	-1.43813707	0.96232855
H	-3.06140040	-0.74488601	2.20444177
H	-4.25209077	0.30303305	1.37987331
H	-5.52639328	0.61665841	-0.94583546
C	-5.14006268	0.39455440	-1.94203138
H	-4.71366733	1.30310648	-2.37558785
H	-5.95791584	0.02840968	-2.56932896
O	-4.14659682	-0.62159129	-1.78198527
H	-3.72542755	-0.81424068	-2.63002278
H	2.45549180	-6.60253940	0.13745940
H	0.00226847	6.73649771	-0.20746622