Electronic Supplementary Material (ESI) for Dalton Transactions.

A molecular boron cluster-based chromophore with dual emission

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Supporting Information (SI)

Contents

General Considerations

Decaborane (Alfa Aesar), aluminum chloride (Sigma-Aldrich), bromine (Oakwood), poly(methyl methacrylate) (PMMA) (Acros Organics), methylcyclohexane (Aldrich), cyclohexane (Alfa Aesar), MilliQ water (Fisher), methanol (Sigma, ACS Reagent Grade, ≥99.8%), TFA (EMD Millipore, 99%), Water Optima™ (Fisher, LC/MS grade), and Acetonitrile Optima™ (Fisher, LC/MS grade) were used as received. *Anti*-$B_{18}H_{22}$ (Boron Specialties) was purified from *syn*-$B_{18}H_{22}$ by repeated recrystallizations in cyclohexane, or was synthesized according to literature procedures.[1] Deuterated solvents were purchased from Cambridge Isotope Laboratories and used as received. All experiments were performed air and moisture free under an atmosphere of nitrogen using standard Schlenk techniques. Anhydrous dichloromethane used for reactions was purified on a JC Meyer Glass Contour Solvent Drying System. All post-Schlenk work-up and characterization was conducted under ambient conditions.

Instrumentation

^{1}H NMR and ^{11}B NMR spectra were obtained on a Bruker DRX500 spectrometer; MestreNova software was used to process the NMR data. ^{1}H NMR spectra were referenced to residual proteo solvent resonances in deuterated solvents ($CDCl_3$: δ 7.26 ppm). ^{11}B NMR spectra were referenced to $BF_3{\cdot}Et_2O$ (δ 0 ppm) standard. Mass spectra were obtained using a direct inject method on a Waters LCT Premier Mass Spectrometer with a Waters ACQUITY UPLC System and autosampler. UV−Vis spectra were recorded on an Ocean Optics DH-2000 spectrometer. Photoluminescence spectra were measured using a QuantaMaster Photon Technology International phosphorescence/fluorescence spectrofluorimeter. Quantum yield measurements were carried out using a Hamamatsu C9920 system equipped with a xenon lamp, calibrated integrating sphere, and model C10027 photonic multichannel analyzer (PMA). Photoluminescence lifetimes were measured by time-correlated single-photon counting using an IBH Fluorocube instrument equipped with an LED excitation source. For the oxygen sensing studies,

nitrogen/oxygen gas mixtures were regulated using a flow-meter (GMR2-010123, G-METER 2-TUBE 150mm ALUMINUM MFV, AALBORG Instruments), and the subsequent emission spectra were measured with a Horiba Fluorometer PTI QM-400.

Experimental

Synthesis of 4-Br-*anti*-$B_{18}H_{21}$: *Anti*-$B_{18}H_{22}$ (100 mg, 0.461 mmol, 1.00 equiv) and $AlCl_3$ (9 mg, 0.07 mmol, 15 mol%) were added to a dry 10 mL reaction tube equipped with a stir bar. Dry dichloromethane (6 mL) was added, and the slurry was stirred and sonicated for approx. 5 min until most of the solid was dissolved. Br_2 (52 mg, 0.32 mmol, 0.70 equiv) was added under a flow of N_2 and the reaction mixture was stirred at ambient temperature for 30 min, or until the reaction was pale orange in color. The presence of $B_{18}H_{21}Br$, $B_{18}H_{20}Br_2$, and *anti*-$B_{18}H_{22}$ was detected by ESI mass spectrometry. The reaction mixture was quenched through the addition of water (5 mL) and then transferred into a separatory funnel. An aqueous solution of saturated sodium bicarbonate (2 mL) was added, and the organic phase was extracted from the biphasic solution with DCM (3 x 5 mL). The DCM solution was then dried over $MgSO_4$ and vacuum filtered through a filter frit packed with Celite. The solvent was removed under reduced pressure to yield a yellow-white solid. Crystals of suitable quality for a single crystal X-ray diffraction study were grown by dissolution of 4-Br-*anti*-$B_{18}H_{21}$ in hot benzene followed by cooling the solution to room temperature and its storage at ~5 °C for 1-2 days. Purification of the bulk material was conducted *via* HPLC. 4-Br-*anti*-$B_{18}H_{21}$ was isolated with >95% purity in 22% yield (29.9 mg), and >99% purity in 8% yield (10.8 mg). **$^1H\{^{11}B\}$ NMR (400 MHz, $CDCl_3$):** δ 4.52 (1H, s), 4.26 (1H, s), 4.10 (1H, s), 3.91 (1H, s), 3.83 (1H, s), 3.47 (3H, s), 3.04 (3H, s), 0.53 (1H, s), 0.23 (1H, s), 0.12 (2H, m), -0.14 (1H, s), -0.46 (1H, s), -0.89 (1H, s), -0.94 (1H, s), -2.13 (1H, s), -2.86 (1H, s) ppm. **$^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$):** δ 15.65 (1B, s), 14.54 (1B, s), 9.28 (2B, s), 3.60 (4B, m), 1.80 (1B, s), 0.18 (1B, s), -3.71 (2B, s), -11.24 (1B, s), -12.36 (1B, s), -31.32 (2B, s), -32.17 (1B, s), -39.85 (1B, s) ppm. **ESI(-)-MS** *m/z*: 294.2565 (calc. 294.2647).

Purification of Brominated Compounds:

An Agilent Technologies Infinity II 1260 HPLC instrument with dual wave detection at 254 nm and 280 nm was utilized to separate $B_{18}H_{21}Br$ from $B_{18}H_{22}$ and $B_{18}H_{20}Br_2$ impurities formed during the synthetic procedure described on pg. S3. A mixture of $B_{18}H_{22}$, $B_{18}H_{21}Br$, and $B_{18}H_{20}Br_2$ (10-15 mg) was dissolved in methanol (1 mL) and manually loaded (through a 1 mL injection loop) onto a Zorbax SB-C18 (5 μm pore size, 9.4 x 250 mm) column. A gradient from 65% methanol, 35% water to 72% methanol, 28% water across 125 min resulted in elution of $B_{18}H_{22}$ first, $B_{18}H_{21}Br$ second and $B_{18}H_{20}Br_2$ last. All HPLC solvents were spiked with TFA (0.1%). All fractions were collected from detection at 254 nm. Pure fractions of $B_{18}H_{21}Br$ were combined and the solvent was removed *in vacuo*.

In order to ensure purity of $B_{18}H_{21}Br$ (as determined by LCMS analysis), a second HPLC purification was performed using a gradient from 65% methanol, 35% water to 68% methanol, 32% water across 225 min. This procedure was reproduced four times with the same result.

Characterization

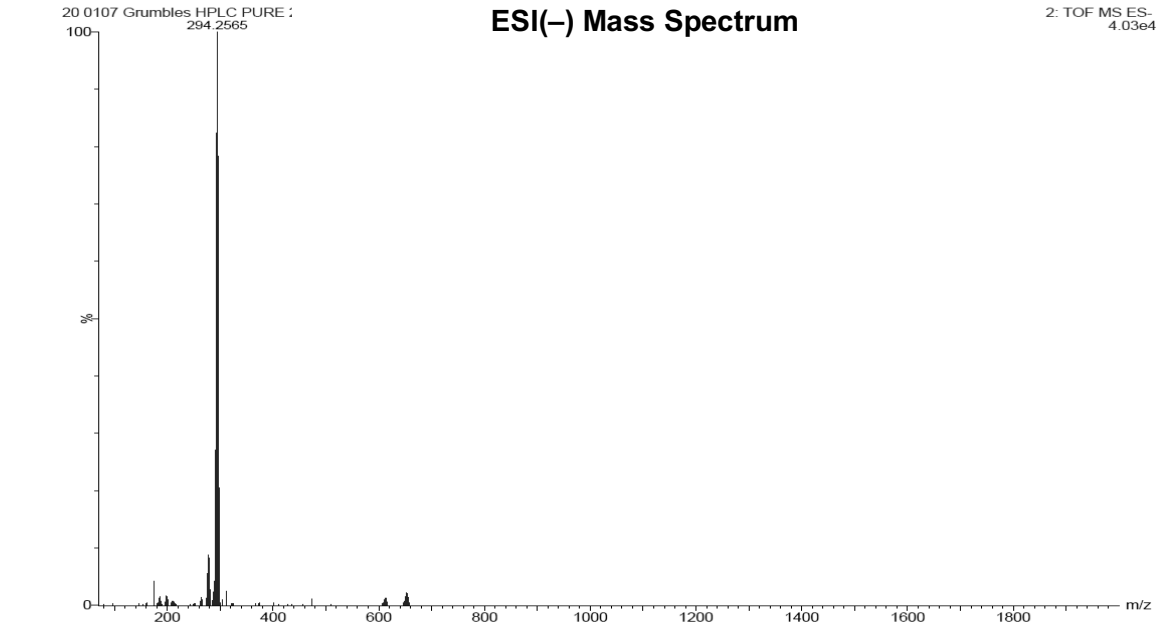


Figure S1 ESI mass spectrum of 4-Br-*anti*-$B_{18}H_{21}$ observed in negative mode.

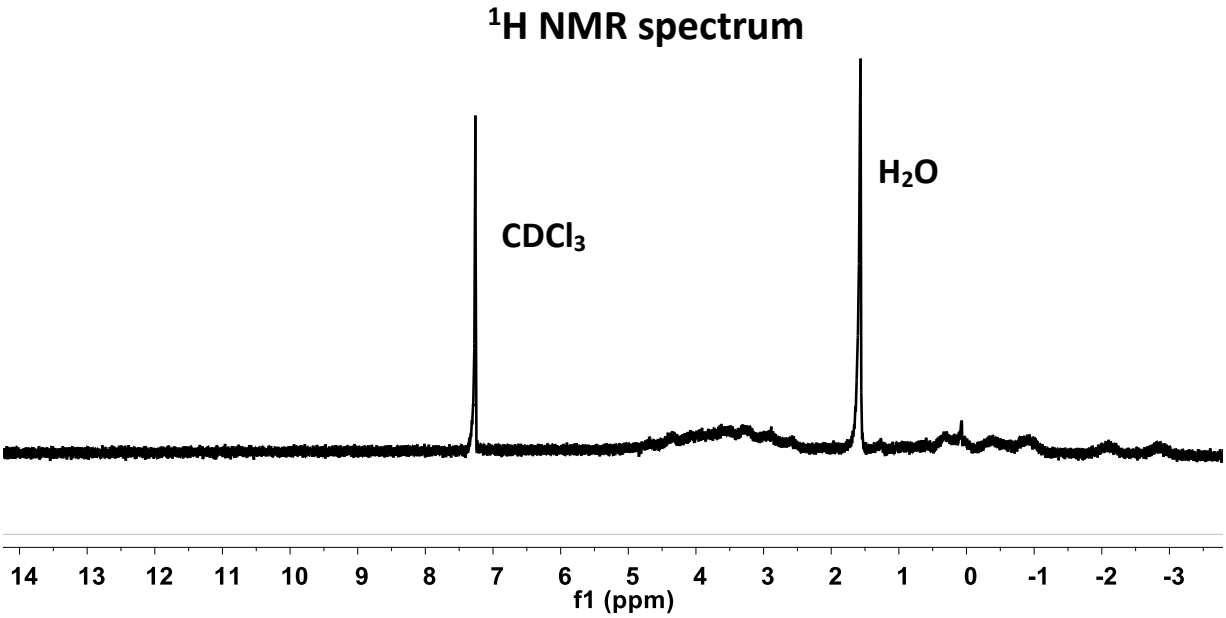


Figure S2 ^{1}H NMR spectrum of 4-Br-*anti*-$B_{18}H_{21}$ in $CDCl_3$.

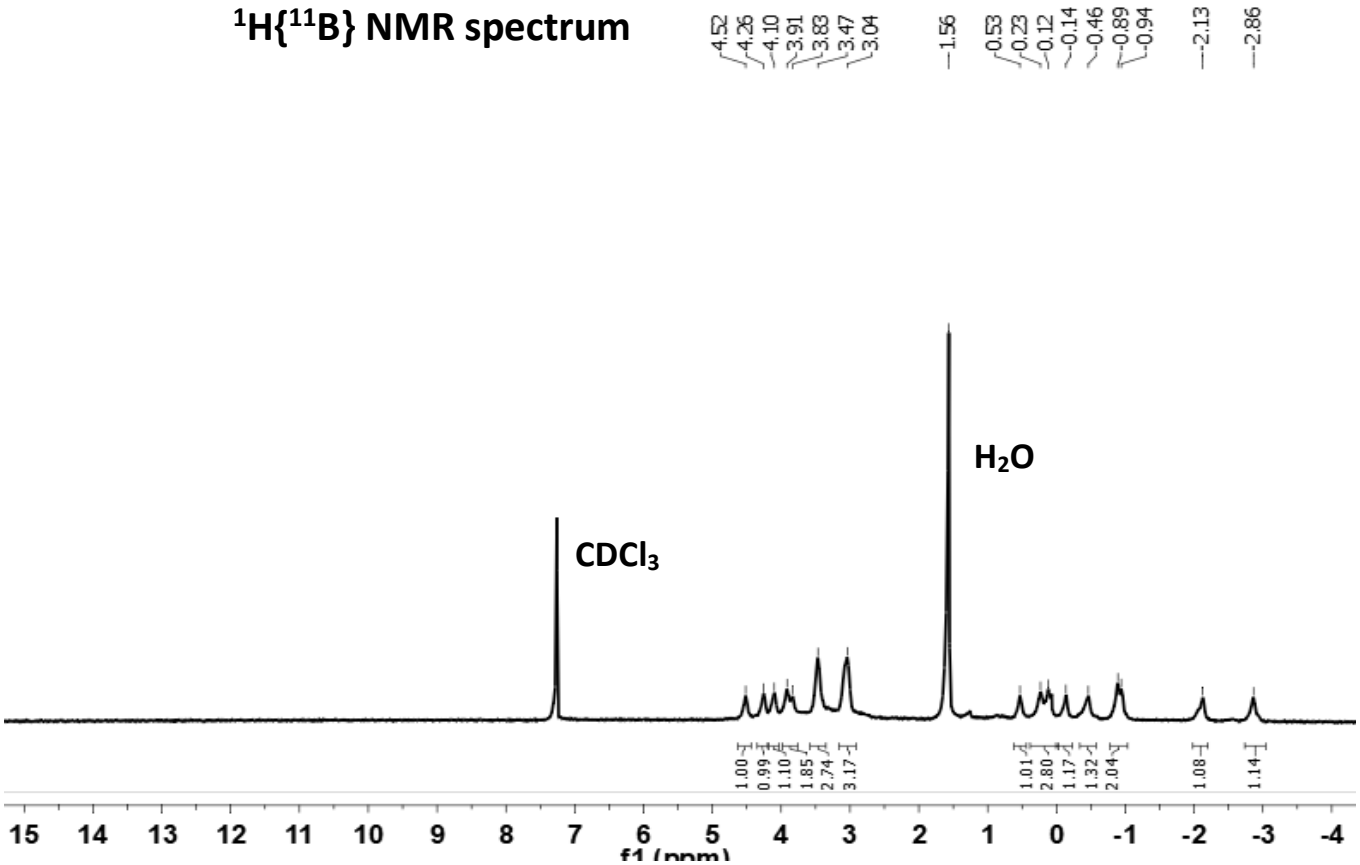


Figure S3 $^{1}H\{^{11}B\}$ NMR spectrum of 4-Br-*anti*-$B_{18}H_{21}$ in $CDCl_3$.

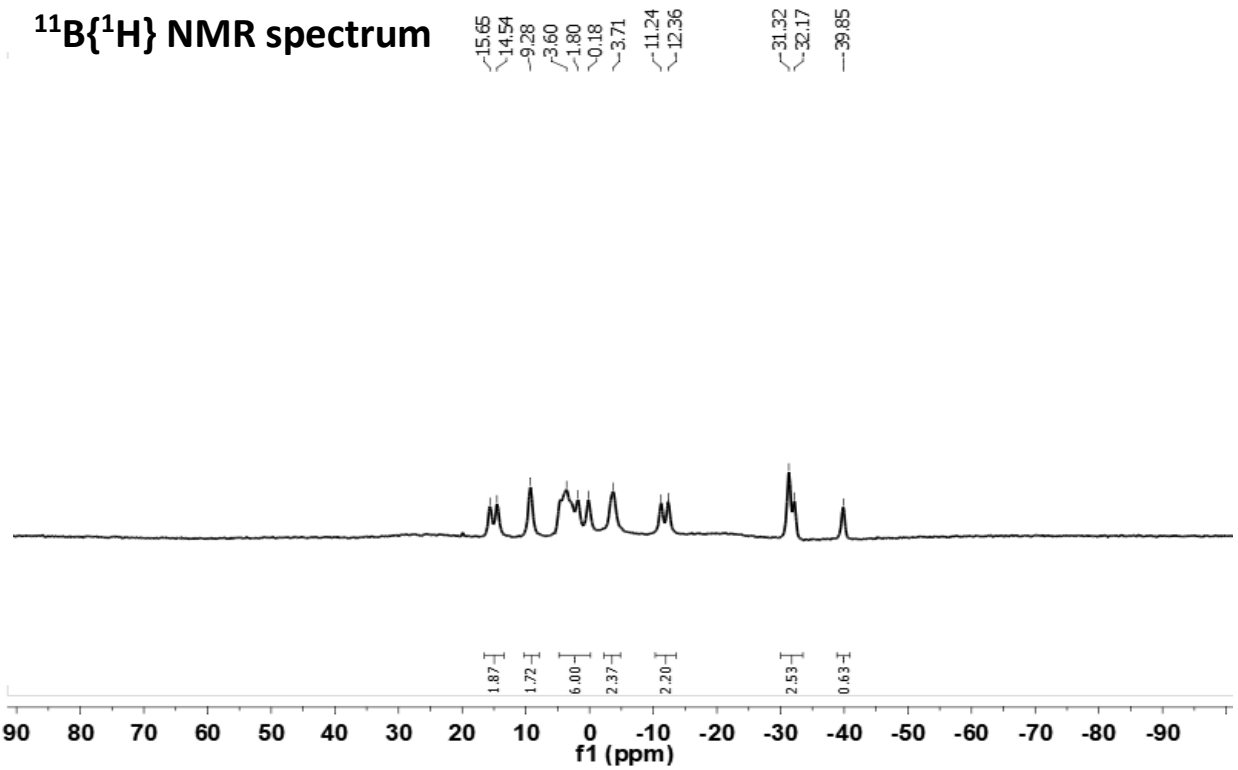


Figure S4 $^{11}B\{^{1}H\}$ NMR spectrum of 4-Br-*anti*-$B_{18}H_{21}$ in $CDCl_3$.

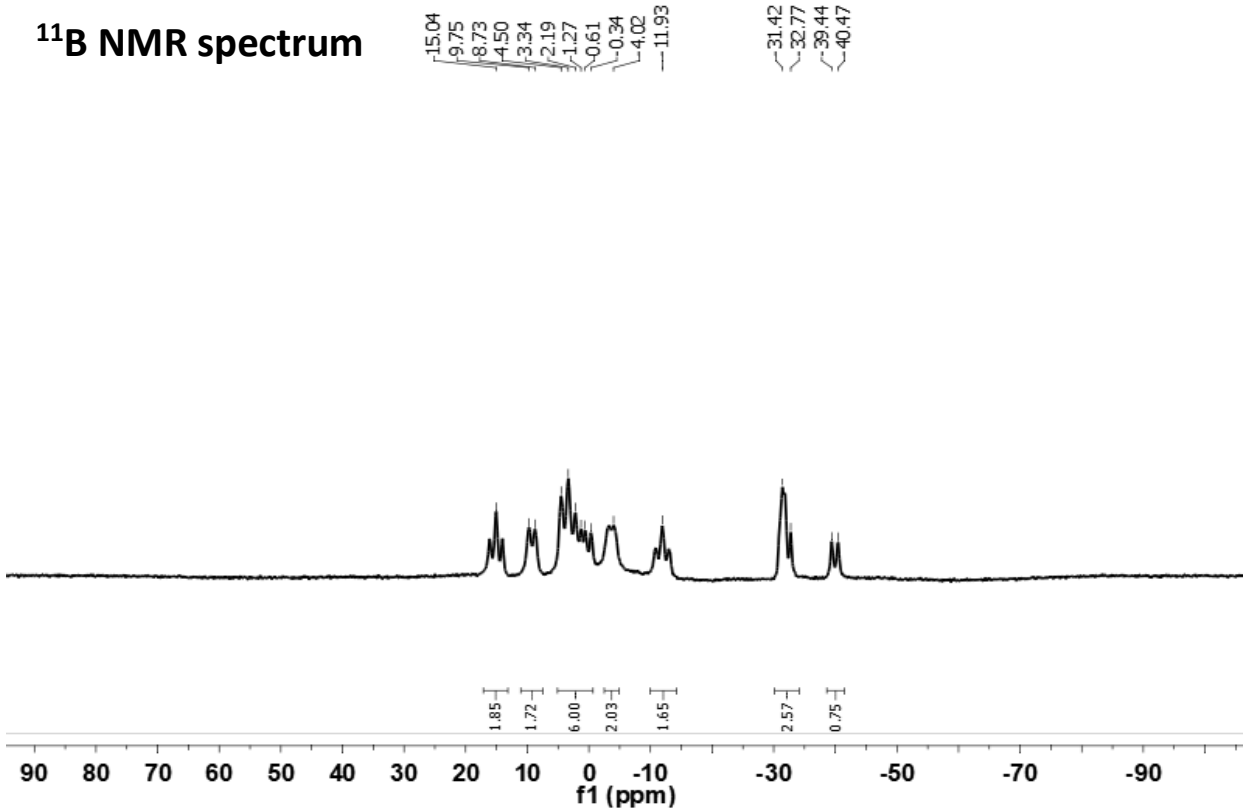


Figure S5 ^{11}B NMR spectrum of 4-Br-*anti*-$B_{18}H_{21}$ in $CDCl_3$.

LCMS Quantification of $B_{18}H_{21}Br$ and $B_{18}H_{20}Br_2$ Content:

LC-MS quantification was performed using an Agilent 6530 ESI-Q-TOF instrument with an Agilent ZORBAX 300SB C18 column (5 µm, 2.1 × 150 mm). Water and acetonitrile acidified with formic acid (0.1%) were used as the mobile phase solvents. Negative mode ionization was used to detect all species: $B_{18}H_{21}Br$ and $B_{18}H_{20}Br_2$. Stock solutions were prepared by dissolution of the isolated material from a single HPLC purification in MeOH (1.75 mg in 2 mL), and isolated material from the second HPLC purification in MeOH (0.67 mg in 1 mL). Samples were then prepared from 50 µL of stock B_{18} material. An injection of 0.2 µL of each sample was made. The following method was utilized: 0-2 min gradient 99% water, 1% acetonitrile to 50% water, 50% acetonitrile; 2-17 min 50% water, 50% acetonitrile to 10% water, 90% acetonitrile.

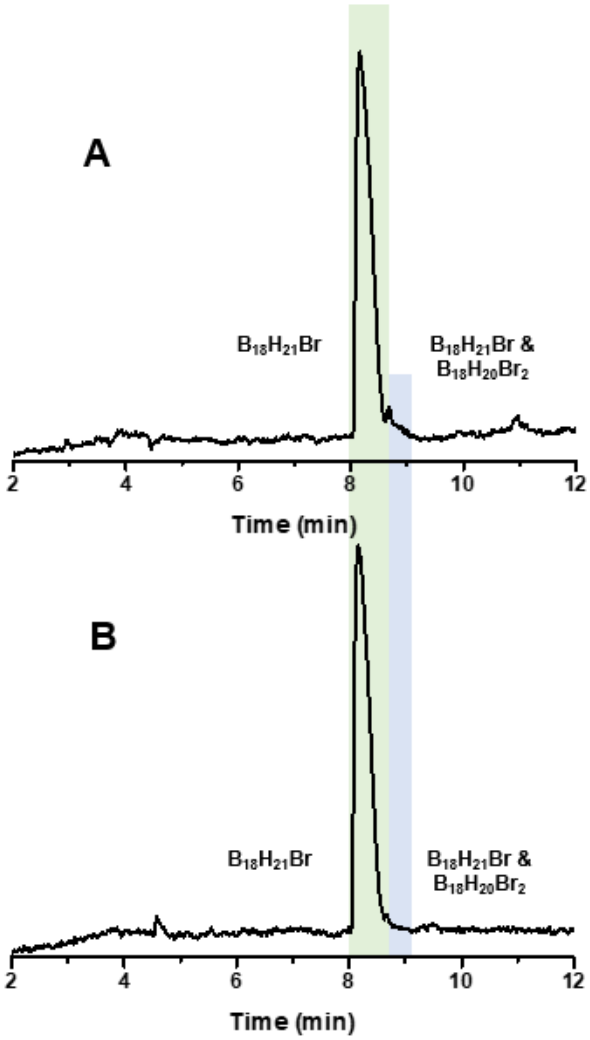


Figure S6 A) LC trace of the material isolated from a single HPLC purification. B) LC trace of the material isolated after a second HPLC purification. The peak highlighted in green represents $B_{18}H_{21}Br$, and the peak highlighted in blue represents a mixture of $B_{18}H_{21}Br$ and $B_{18}H_{20}Br_2$.

Table S1 Summary of the species present in the LC traces in Figure S6.

Spectrum	Peak Retention Time (min)	Identity	Observed Masses (*m/z*)	Area by Integration	Percent Area	Percent $B_{18}H_{21}Br$
A	8.165	$B_{18}H_{21}Br$	295.2560	1794584244.57	95%	>95%
	8.681	$B_{18}H_{21}Br$; $B_{18}H_{20}Br_2$	295.2553; 373.1694	91235119.35	5%	
B	8.163	$B_{18}H_{21}Br$	295.2560	1557733457.77	99%	>99%
	8.663	$B_{18}H_{21}Br$; $B_{18}H_{20}Br_2$	295.2504; 373.1632	15986494.6	1%	

Crystal Structure Data

Experimental Summary

The single crystal X-ray diffraction studies were carried out on a Bruker APEX II Ultra CCD diffractometer equipped with Mo K_α radiation (λ = 0.71073 Å). Crystals of the subject compound were grown from benzene at 4.5 °C using the yellow powder sample. A 0.12 x 0.090 x 0.040 mm colorless block crystal was mounted on a Cryoloop with Fomblin Y oil.

Data were collected in a nitrogen gas stream at 100(2) K using ϖ scans. Crystal-to-detector distance was 40 mm using an exposure time of 8 seconds with a scan width of 0.65°. Data collection was 99.9 % complete to 25.242° in θ. A total of 7816 reflections were collected. 4624 reflections were found to be symmetry independent, with a R_{int} of 0.0262. Indexing and unit cell refinement indicated a Primitive Triclinic lattice. The space group was found to be *P*1**.** The data were integrated using the Bruker SAINT Software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model consistent with the proposed structure.

All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. The positions of all terminal, boron bonded hydrogen atoms were located in the electron density map, and their displacement parameters fixed at 1.2 x the U(eq) of the boron atom to which they were attached. The terminal B-H distances were restrained at 1.12 Å . The positions of all bridging hydrogen atoms were located in the electron density map, and their displacement parameters fixed at 1.2 x the average U(eq) values of the boron atoms to which they were attached.

Notes: There is one molecule per asymmetric unit. The molecule co-crystallizes with two benzene solvent molecules per formula unit. The electron density data support a structural model with a Br atom that is disordered across two positions with a partial substitution of Cl. However, the occupancy of the Br atoms is 38/56, not the expected 50/50. This could indicate the presence of

the unsubstituted borane as an impurity that co-crystallized with the mono-brominated product or possibly the presence of a small amount of di-brominated product. The check cif report indicates a possibility of the higher symmetry space group *P*-1. However due to the substitutional pattern of the Br atoms, the *P*1 space group was indicated and also gave a better fit of the model to the observed data.

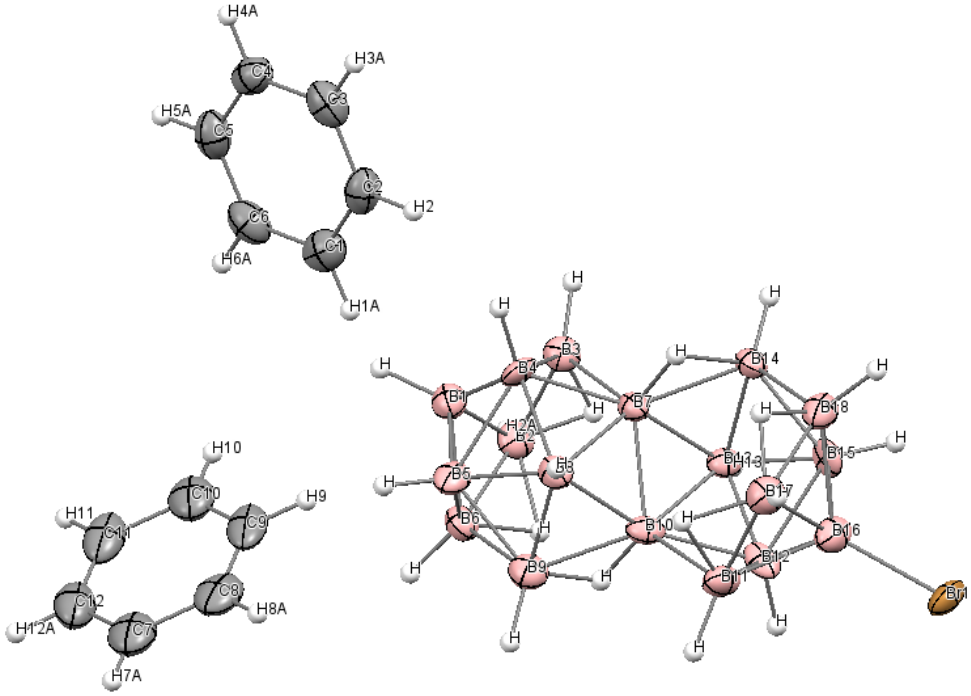


Figure S7 4-Br-*anti*-$B_{18}H_{21}$ single crystal X-ray structure with two co-crystallized benzene solvent molecules.

Table S2: Selected bond lengths for 4-Br-*anti*-$B_{18}H_{21}$•($2C_6H_6$) and anti-$B_{18}H_{22}$•$(C_6H_6)^2$ with bond length differences calculated. Highlighted rows indicate that the length difference exceeds three standard uncertainties and is therefore significant.

Connectivity	4-Br-*anti*-$B_{18}H_{21}$ Length (Å)	*anti*-$B_{18}H_{22}$ Length (Å)	Difference (Å)
Br-B4	1.906(5)	-	-
B4-B8	1.811(7)	1.789(5)	+0.022
B4-B9	1.735(7)	1.702(5)	+0.033
B4-B10	1.768(7)	1.775(5)	-0.007
B4-B1	1.804(6)	1.786(5)	+0.018
B8-B9	1.806(8)	1.795(5)	+0.011
B9-B10	1.789(7)	1.783(5)	+0.006
B1-B10	1.766(7)	1.740(5)	+0.026
B1-B2	1.750(7)	1.786(5)	-0.036
B1-B3	1.767(7)	1.778(5)	-0.011
B1-B5	1.753(7)	1.746(5)	+0.007
B2-B3	1.760(7)	1.746(5)	+0.014
B2-B5	1.816(7)	1.802(4)	+0.014
B2-B7	1.793(6)	1.774(5)	+0.019
B3-B4	1.772(7)	1.774(5)	-0.002
B3-B7	1.763(7)	1.746(5)	+0.017
B3-B8	1.758(7)	1.723(6)	+0.035
B5-B10	1.990(7)	1.968(5)	+0.022
B7-B6	1.824(6)	1.815(5)	+0.009
B7-B8	1.973(7)	1.946(5)	+0.027

Table S3. Crystal data and structure refinement parameters for 4-Br-*anti*-$B_{18}H_{21}$•($2C_6H_6$), CSD #1984161.

Report date	2019-10-22
Identification code	Spok145R
Empirical formula	C_{12} H_{34} B_{18} $Br_{0.94}$ $Cl_{0.20}$
Formula weight	455.18
Temperature	100.0 K
Wavelength	0.71073 Å

Crystal system	Triclinic	
Space group	*P*1	
Unit cell dimensions	a = 8.4707(19) Å	α = 114.351(7)°
	b = 8.912(2) Å	β = 106.910(7)°
	c = 9.494(2) Å	γ = 90.302(7)°
Volume	617.44(5) Å^3	
Z	1	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	1.589 mm^{-1}	
F(000)	232	
Crystal size	0.12 x 0.09 x 0.04 mm^3	
Theta range for data collection	2.488 to 26.022°	
Index ranges	-10<=h<=10, -10<=k<=10, -11<=l<=11	
Reflections collected	7816	
Independent reflections	4624 [R(int) = 0.0262]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6765	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4624 / 19 / 362	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2Σ(I)]	R1 = 0.0330, wR2 = 0.0804	
R indices (all data)	R1 = 0.0362, wR2 = 0.0817	
Absolute structure parameter	0.078(14)	
Extinction coefficient	n/a	

Largest diff. peak and hole	0.398 and -0.159 e.Å^{-3}

Photoluminescence Data

Preparation of PMMA films A solution of PMMA (0.100 g, 35 kDa) in 1,2- difluorobenzene (1 mL) was thermally sonicated for 1 h at 40 °C, or until the PMMA was completely dissolved. Next, 4-Br-*anti*-$B_{18}H_{21}$ (0.002 g, 2 wt. %) was added to the solution and sonicated for an additional 5-10 min. The solution was spin coated on a quartz substrate (800-1,000 RPM, 30 sec), and this process was repeated (~4-6 times) until the film was thick enough to emit light under λ = 365 nm excitation in a dark room under ambient conditions.

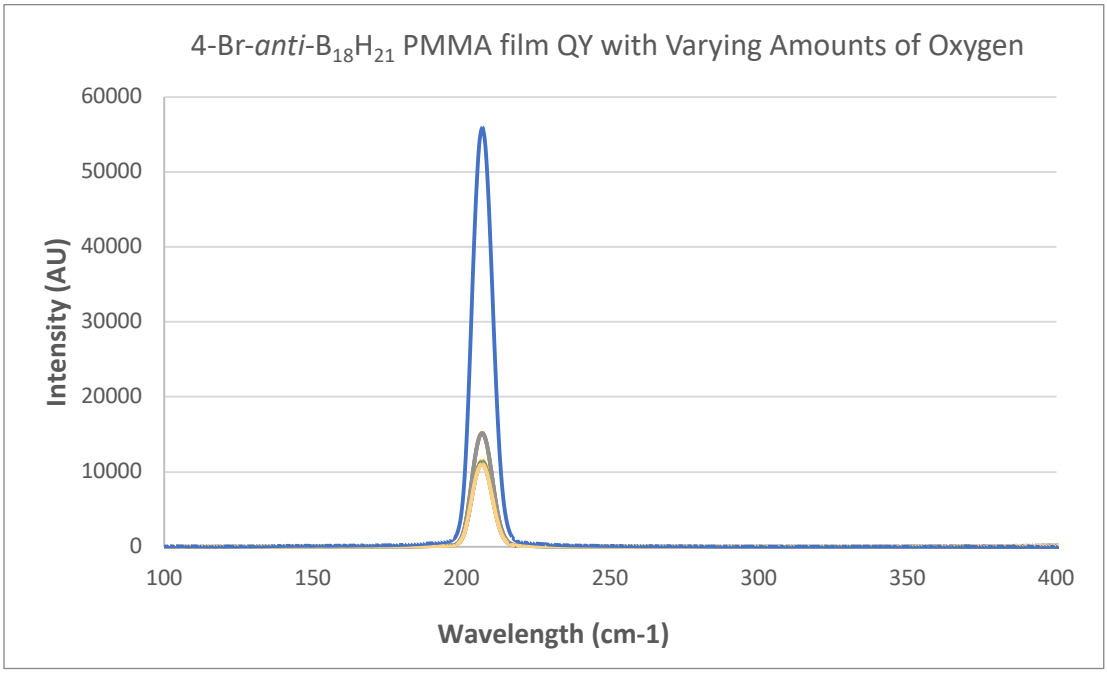
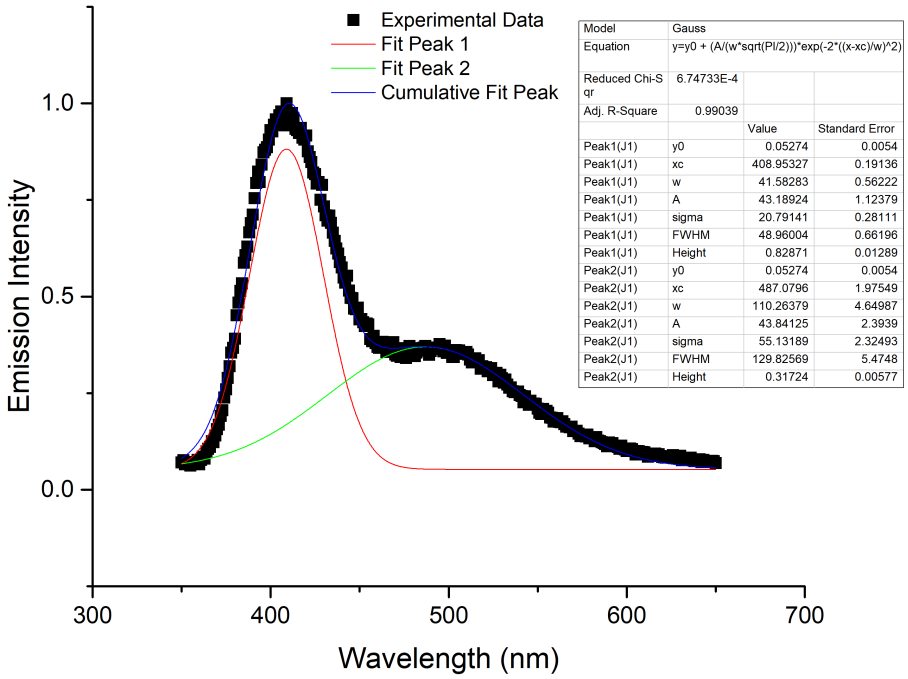
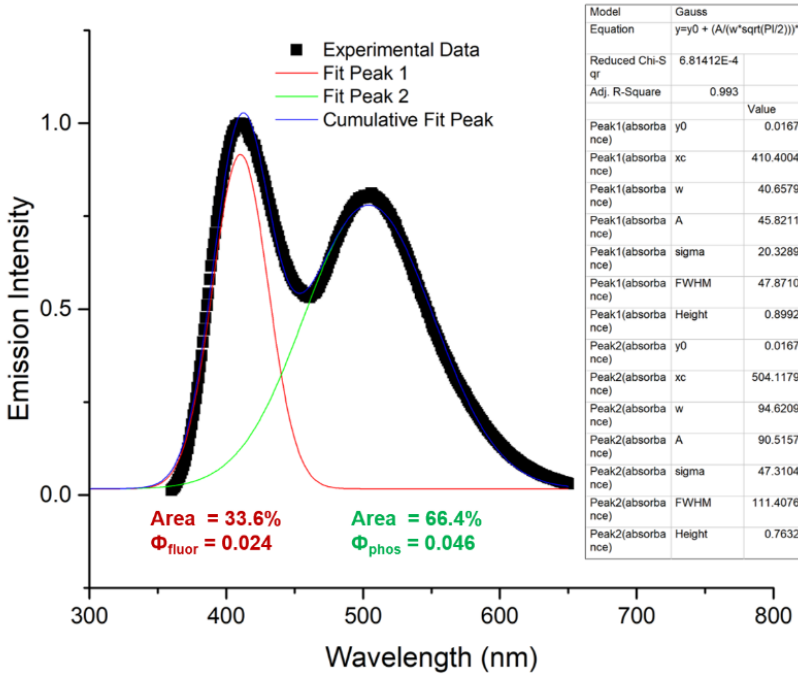


Figure S8: Quantum yield graph of a 4-Br-*anti*-$B_{18}H_{21}$ containing PMMA film taken over time under increasing amounts of oxygen. The baseline from a quartz plate was first measured (blue), then the sample was measured under ambient conditions (gray). The system was placed under the flow of oxygen and measurements were taken over 35 min until the system reached an equilibrium (yellow).



Model	Gauss		
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)		
Reduced Chi-Sqr	6.74733E-4		
Adj. R-Square	0.99039		
		Value	Standard Error
Peak1(J1)	y0	0.05274	0.0054
Peak1(J1)	xc	408.95327	0.19136
Peak1(J1)	w	41.58283	0.56222
Peak1(J1)	A	43.18924	1.12379
Peak1(J1)	sigma	20.79141	0.28111
Peak1(J1)	FWHM	48.96004	0.66196
Peak1(J1)	Height	0.82871	0.01289
Peak2(J1)	y0	0.05274	0.0054
Peak2(J1)	xc	487.0796	1.97549
Peak2(J1)	w	110.26379	4.64987
Peak2(J1)	A	43.84125	2.3939
Peak2(J1)	sigma	55.13189	2.32493
Peak2(J1)	FWHM	129.82569	5.4748
Peak2(J1)	Height	0.31724	0.00577

Figure S9: Deconvoluted emission spectrum of a cyclohexane solution of 4-Br-*anti*-$B_{18}H_{21}$ under ambient conditions. Peak percent as a function of area for each signal is listed, as well as the contribution to the overall quantum yield. QY contribution was calculated by multiplying peak percent by the quantum yield of the cyclohexane solution under ambient conditions (Φ=0.05). Fitting calculations were conducted with a nonlinear curve fit (Gauss) using Origin 9.1 Software.



Model	Gauss		
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)		
Reduced Chi-Sqr	6.81412E-4		
Adj. R-Square	0.993		
		Value	Standard Error
Peak1(absorbance)	y0	0.01671	0.00401
Peak1(absorbance)	xc	410.40043	0.18564
Peak1(absorbance)	w	40.65795	0.36764
Peak1(absorbance)	A	45.82113	0.52925
Peak1(absorbance)	sigma	20.32897	0.18382
Peak1(absorbance)	FWHM	47.87107	0.43287
Peak1(absorbance)	Height	0.89921	0.00656
Peak2(absorbance)	y0	0.01671	0.00401
Peak2(absorbance)	xc	504.11796	0.37735
Peak2(absorbance)	w	94.62098	1.00897
Peak2(absorbance)	A	90.51576	1.15693
Peak2(absorbance)	sigma	47.31049	0.50448
Peak2(absorbance)	FWHM	111.40769	1.18797
Peak2(absorbance)	Height	0.76327	0.00483

Figure S10: Deconvoluted emission spectrum of a cyclohexane solution of 4-Br-*anti*-$B_{18}H_{21}$ under oxygen-free conditions. Peak percent as a function of area for each signal is listed, as well as the contribution to the overall quantum yield. QY contribution was calculated by multiplying peak percent by

the quantum yield of the cyclohexane solution under oxygen-free conditions (Φ=0.07). Fitting calculations were conducted with a nonlinear curve fit (Gauss) using Origin 9.1 Software.

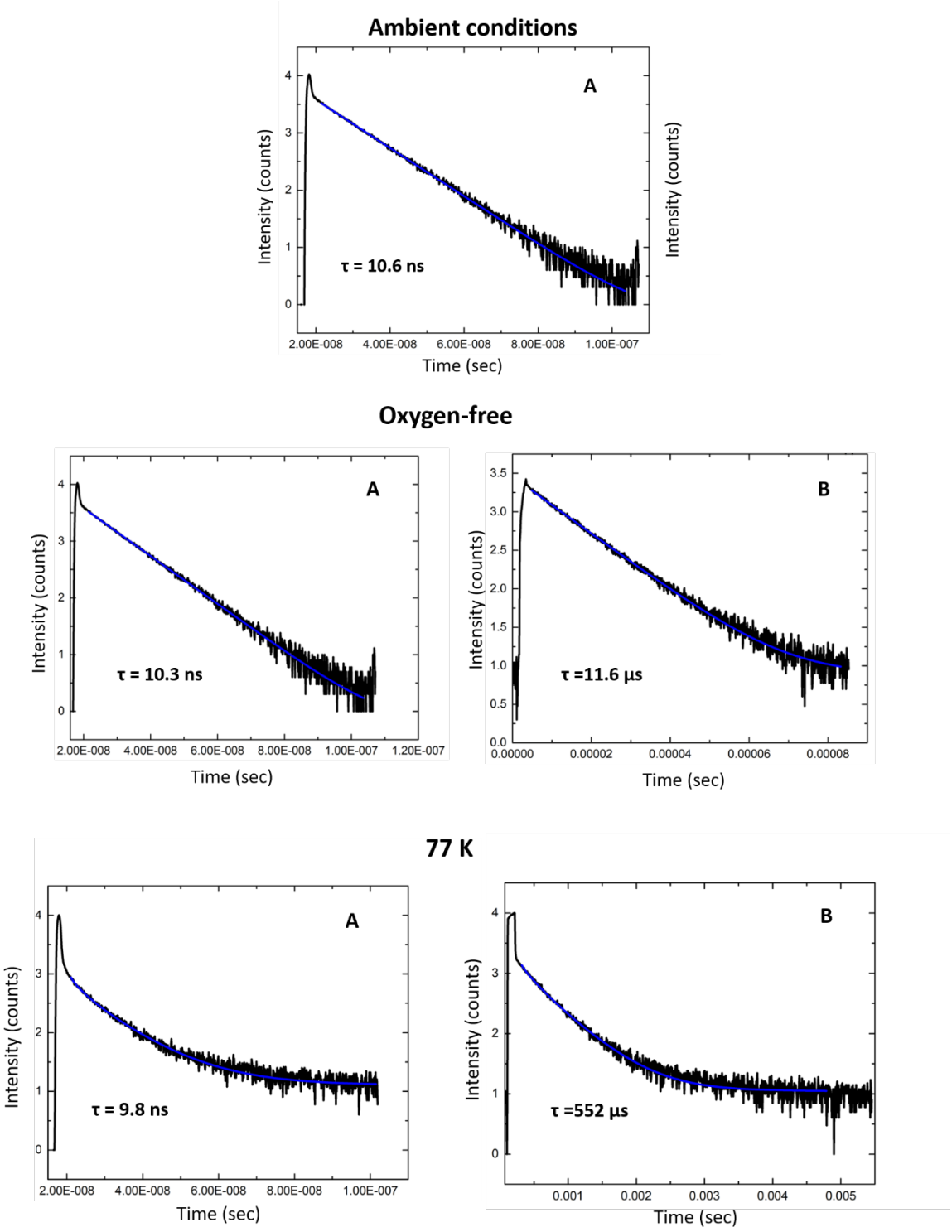


Figure S11: Luminescence decay curves (black) and fits (blue) for 4-Br-*anti*-$B_{18}H_{21}$ in cyclohexane at 298 K under ambient conditions (top) at 298 K under oxygen-free conditions (middle) at 77 K (bottom). A) Observed at 410 nm, excitation at 331 nm. B) Observed at 525 nm, excitation at 372 nm.

Oxygen sensing studies A nitrogen/oxygen gas mixture regulated with a calibrated mass-flow meter (GMR2-010123, G-METER 2-TUBE 150 mm ALUMINUM MFV, AALBORG Instruments) was bubbled through a cyclohexane solution of 4-Br-*anti*-$B_{18}H_{21}$ for 10 min, and then the emission spectra were measured under various oxygen concentrations.

Table S4: Flow rates of oxygen and nitrogen gas and the resulting percent of oxygen in solution.

N_2 scale reading	N_2 flow (mL/min)	O_2 scale reading	O_2 flow (mL/min)	Actual % O_2
100	102	0	0	0%
99	97	40	24	20%
71	61	60	41	40%
70	60	100	89	60%
40	29	120	119	80%
0	0	110	103	100%

Cyclic Voltammetry Cyclic voltammetry measurements of *anti*-$B_{18}H_{22}$ (5 mM) and 4-Br-*anti*-$B_{18}H_{21}$ (2 mM) were performed with a Gamry Instruments Interface 1010E potentiostat using a glassy carbon working electrode, platinum wire counter electrode and AgCl reference electrode (fill solution: saturated KCl in MeCN). Measurements were conducted at a scan rate of 100 mV/s with [TBA][PF_6] (0.15 M) supporting electrolyte under an inert atmosphere of N_2 in DCM, and referenced vs. an internal Fc/Fc^+ standard.

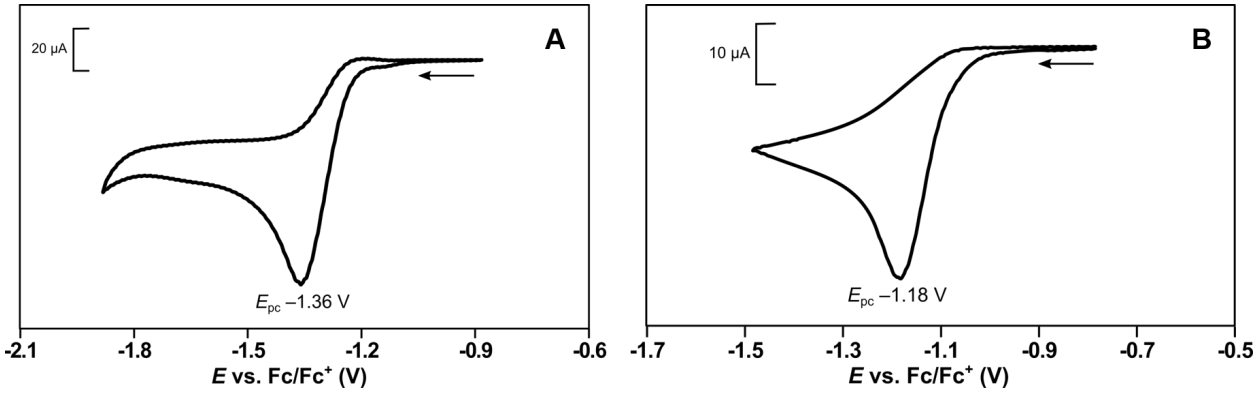


Figure S12 Cyclic voltammograms of A) *anti*-$B_{18}H_{22}$ and B) 4-Br-*anti*-$B_{18}H_{21}$.

Calculations

Calculations were performed using SCM ADF software with TD-DFT capabilities. Optimized geometries were calculated using the hybrid PBE0 functional and the DZP basis set with scalar relativistic effects considered. In all cases, frequency analyses were carried out to confirm the local minima.

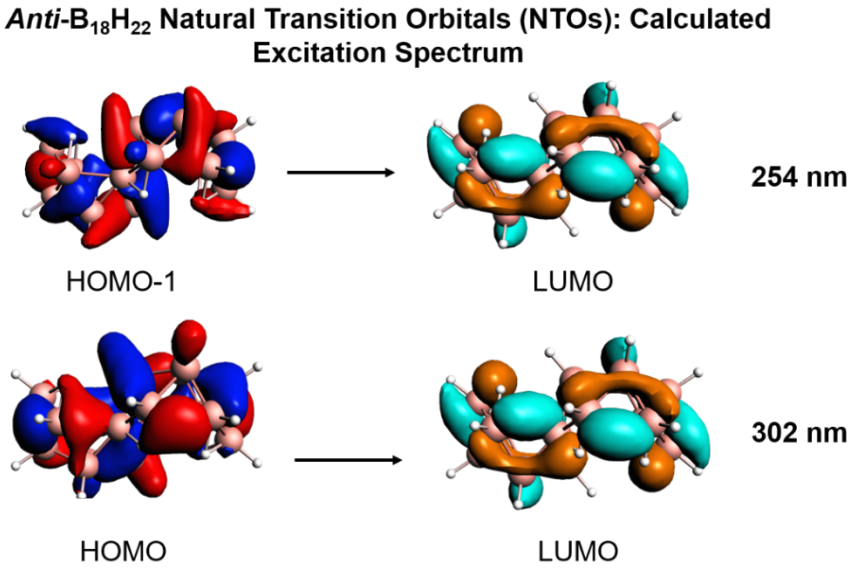


Figure S13 Natural Transition Orbitals of the excitation and emission spectra of *anti*-$B_{18}H_{22}$, calculated from the S_0 state optimized geometry Wavelengths at which these events are observed are listed on the right.

Table S5 Summary of the calculated absorption spectrum (Hybrid PBE0 DZP) for *anti*-$B_{18}H_{22}$, where λ_{VA} is the calculated vertical absorption wavelength and *f* is the oscillator strength. The excitation calculation was based on the S_0 optimized geometry. The energies of the HOMO and LUMO are listed on the right.

Anti-$B_{18}H_{22}$	State Transition	Composition	λ_{VA}	*f*
Excitation	$S_0 \rightarrow S_1$	HOMO → LUMO	302	0.1417
		HOMO-1 → LUMO	254	0.0553

Orbital	Energy
HOMO	-8.16 eV
HOMO-1	-9.19 eV
LUMO	-3.32 eV

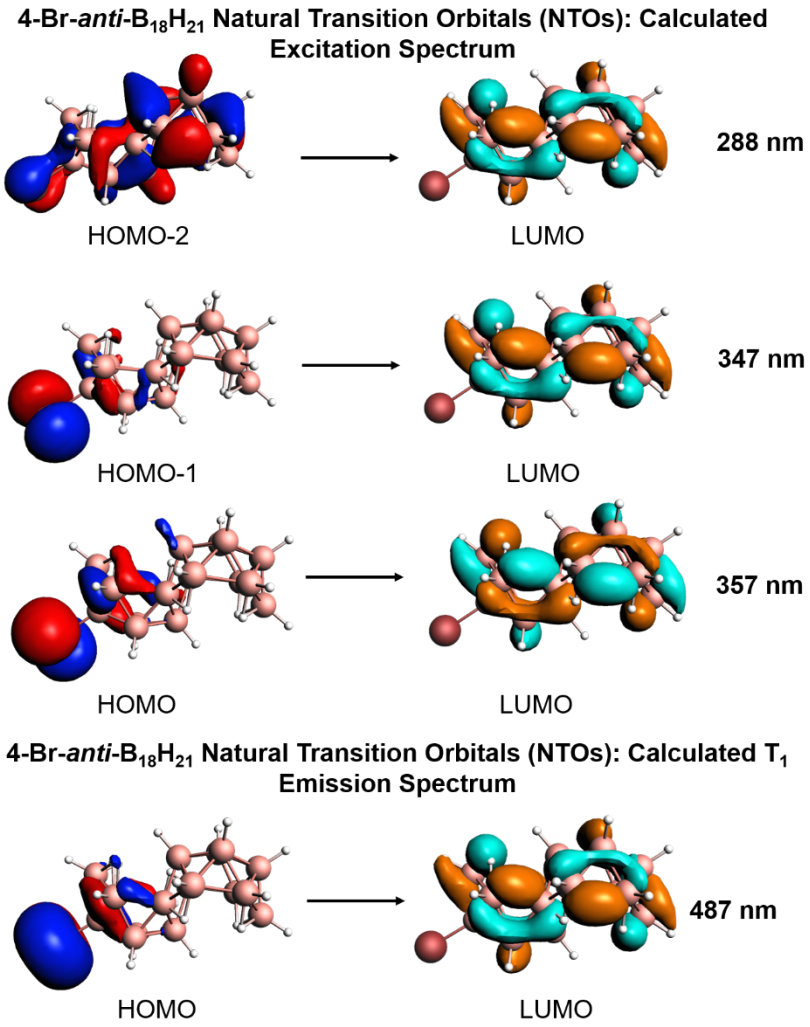


Figure S14 Natural Transition Orbitals of the excitation and emission spectra of 4-Br-*anti*-$B_{18}H_{21}$. The excitation spectrum was calculated from the S_0 state optimized geometry. The emission spectrum was calculated from the T_1 optimized geometry. Wavelengths at which these events are observed are listed on the right.

Table S6 The PBE0 DZP optimized geometry coordinates for the S_0 states of *anti*-$B_{18}H_{22}$

H	4.48287848	1.95785989	2.79187060
B	0.01627591	0.01074632	2.84364647
B	3.49709668	1.29945583	2.77240630
B	2.86037305	0.38170068	4.16864198
H	3.41877183	0.23679721	5.20433261
H	2.69948257	-0.82377351	3.66712297
B	2.08187407	1.85469417	3.67489933
B	2.05413514	1.87574577	1.89814074
H	2.13415808	2.82118037	1.18331513
B	2.87804696	0.44698862	1.35275234
H	3.36868498	0.36032607	0.27708424

H	2.73721806	-0.78956889	1.77640301
B	3.55651818	-0.40864508	2.73369330
H	4.47624933	-1.15386197	2.72961154
B	0.93456070	0.67013378	4.24621767
H	0.40351609	0.77198375	5.30061920
H	0.22808482	1.18606377	0.43532880
B	0.56152603	1.67685733	2.83207403
H	-0.20618408	2.58188473	2.84038899
B	0.93193824	0.62228141	1.43375130
H	-3.53537916	-1.32418171	1.48548743
H	2.20152279	2.78651155	4.40051874
B	-2.54951834	-0.66589381	1.50515227
B	-1.91224194	0.25230503	0.10917819
H	-2.47109111	0.39756452	-0.92622869
H	-1.75170321	1.45753109	0.61130038
B	-1.13449668	-1.22118413	0.60269541
B	-1.10639037	-1.24243328	2.37944088
H	-1.18638839	-2.18810923	3.09395651
B	-1.93072634	0.18599712	2.92510102
H	-2.42099563	0.27227476	4.00096371
H	-1.78972796	1.42279677	2.50203294
B	-2.60879734	1.04216495	1.54452867
H	-3.52856442	1.78733892	1.54860950
B	0.01254283	-0.03637460	0.03122354
H	0.54366258	-0.13861721	-1.02310894
H	0.71964100	-0.55266474	3.84242117
B	0.38592620	-1.04370902	1.44521721
H	1.15363226	-1.94874040	1.43631947
H	-1.25437052	-2.15275156	-0.12319757

Table S7 The PBE0 DZP frequency calculations for the S_0 state of *anti*-$B_{18}H_{22}$.

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm^{-1}	$1e^{-40}$ esu^2 cm^2	km/mole
---	---	---
105.937586	65.990902	1.752315
162.837355	103.884635	4.240172
204.808833	0.000125	0.000006
222.058488	36.999345	2.059394
254.025263	0.000192	0.000012
347.096464	6.412573	0.557905
371.651618	0.000310	0.000029
398.891872	45.968704	4.596164
413.639716	0.009461	0.000981
430.088061	108.727348	11.721259
469.217974	16.745509	1.969478
470.290238	0.143008	0.016858
481.065063	0.000400	0.000048

533.357191	0.000048	0.000006
559.517525	0.000114	0.000016
561.233244	1.742602	0.245143
579.536165	0.005607	0.000815
580.460440	16.926416	2.462724
594.456060	1.024292	0.152624
602.954237	0.000399	0.000060
616.883312	6.408804	0.990964
624.624001	0.000614	0.000096
630.401839	15.186489	2.399678
635.044888	0.000632	0.000101
639.842294	72.909325	11.693219
645.775284	0.000020	0.000003
663.773879	12.730244	2.118044
663.982937	0.135762	0.022595
685.204911	22.036816	3.784839
689.377677	0.000872	0.000151
703.577373	0.000733	0.000129
709.505430	87.431982	15.549059
716.969960	27.647452	4.968601
719.982903	0.006676	0.001205
725.913169	76.144527	13.854838
732.318259	0.001248	0.000229
742.612808	0.039349	0.007324
743.637115	32.332538	6.026691
746.196537	19.732053	3.690656
747.484693	0.005626	0.001054
750.642605	47.466918	8.931046
761.564497	0.000106	0.000020
766.830646	61.764431	11.871784
779.498010	0.000228	0.000045
791.444389	32.501974	6.447750
798.872968	0.000586	0.000117
802.730275	0.001276	0.000257
805.430094	47.203584	9.529737
808.264539	0.001874	0.000380
809.378500	5.318020	1.078896
824.992156	52.883261	10.935688
850.012684	0.000759	0.000162
859.018362	92.759704	19.972842
863.804728	0.005230	0.001132
867.008248	122.183347	26.552983
879.345242	0.000484	0.000107
892.417289	0.000190	0.000043
899.493297	18.837477	4.247161
914.693020	15.001529	3.439450
923.741808	0.000503	0.000116
925.983557	6.513150	1.511724
931.200979	0.006859	0.001601
934.103157	76.648194	17.946296
936.523437	0.007054	0.001656

942.107960	83.541178	19.727831
946.944027	0.252003	0.059815
947.024760	34.201972	8.118776
953.950896	0.000375	0.000090
961.124104	0.001066	0.000257
962.560923	80.613670	19.449793
965.647757	0.000718	0.000174
974.986017	85.494131	20.893575
980.652026	0.000955	0.000235
989.935504	21.839045	5.418993
999.273196	0.002195	0.000550
1003.922876	107.100198	26.950616
1014.648328	66.379298	16.882092
1018.688083	73.415830	18.746017
1022.194417	0.000724	0.000185
1036.151900	0.000146	0.000038
1041.504903	25.078618	6.547010
1049.267146	0.000018	0.000005
1056.146175	0.012278	0.003250
1056.738434	33.072867	8.760268
1103.977308	83.978593	23.238431
1106.011997	0.000474	0.000131
1578.704816	0.036538	0.014458
1584.896868	63.331557	25.159340
1675.257119	406.696764	170.777346
1677.535394	0.268898	0.113068
1721.680076	120.186232	51.866297
1721.932481	0.112251	0.048449
2043.596563	31.738088	16.257509
2044.097837	0.042906	0.021984
2080.948355	20.578382	10.733728
2081.179374	42.869456	22.363283
2105.449465	0.067726	0.035742
2107.784855	69.692436	36.820526
2678.148246	61.249527	41.116432
2678.378898	0.289557	0.194395
2683.280501	3.056964	2.056054
2683.340399	85.564956	57.550589
2690.874012	0.334616	0.225693
2691.008659	151.882939	102.447687
2700.364360	4.308051	2.915958
2700.448625	169.928286	115.021669
2707.451362	96.100797	65.217737
2707.721364	2.035259	1.381344
2710.706488	0.050721	0.034463
2711.660339	117.147544	79.624468
2714.893814	390.625259	265.822196
2715.758248	0.754010	0.513270
2729.615179	252.946907	173.064849
2730.227042	0.014564	0.009967

Table S8 The PBE0 DZP optimized geometry coordinates for the S_0, S_1, S_2 and T_1 states of 4-Br-*anti*-$B_{18}H_{21}$.

PBE0 DZP S_0

H	4.47687673	1.96167334	2.79306131
B	0.02303554	0.01355468	2.84030125
B	3.49513313	1.29684663	2.77253545
B	2.85511343	0.38183243	4.16813607
H	3.41016328	0.23496334	5.20485376
H	2.69417393	-0.82434133	3.66973798
B	2.08143287	1.85262351	3.67121385
B	2.05560133	1.87164043	1.89743960
H	2.12860927	2.81454244	1.17791795
B	2.88039307	0.44564708	1.35380595
H	3.36709768	0.35849853	0.27668440
H	2.73823303	-0.79073544	1.76970519
B	3.55445618	-0.40926220	2.73566485
H	4.46554458	-1.16571722	2.73248058
B	0.93357519	0.67326987	4.24171198
H	0.39771011	0.76900562	5.29352011
H	0.22207520	1.19016079	0.44274071
B	0.56393154	1.67474439	2.82883238
H	-0.20494979	2.57910167	2.83463105
B	0.93298804	0.62256790	1.43532653
Br	-4.17479155	-1.74950241	1.48692025
H	2.19161557	2.78242597	4.40135006
B	-2.54596070	-0.66481590	1.50741370
B	-1.90510961	0.25260463	0.10609751
H	-2.47596561	0.39115304	-0.92199114
H	-1.74998004	1.45736753	0.60688446
B	-1.12849197	-1.21580604	0.60565918
B	-1.09869876	-1.23624914	2.38023495
H	-1.18706961	-2.17860836	3.09666764
B	-1.92670353	0.18737129	2.92664837
H	-2.42190339	0.26960787	3.99898814
H	-1.78649302	1.42360549	2.50806042
B	-2.60469153	1.04300401	1.54493441
H	-3.52271502	1.78913061	1.55092168
B	0.01406894	-0.03252654	0.03431425
H	0.54378645	-0.13263275	-1.01996369
H	0.72698938	-0.55239482	3.83543198
B	0.38805379	-1.03968213	1.44448679
H	1.15227875	-1.94704426	1.43309389
H	-1.25703826	-2.14400410	-0.12169432

PBE0 DZP S_1

H	4.47101822	1.92718349	2.78660797
B	0.00320074	0.00579322	2.83550150
B	3.47327140	1.28520154	2.77236655
B	2.82864718	0.36771547	4.18596730
H	3.41196769	0.26430578	5.21366901
H	2.74221160	-0.87644759	3.68315015
B	2.05432808	1.86465881	3.67611623
B	2.06467700	1.89479572	1.91717171
H	2.11391448	2.85778531	1.22370987
B	2.79190188	0.40480426	1.35344913
H	3.29754552	0.31840774	0.28327906
H	2.78704860	-0.85811202	1.81918596
B	3.56041985	-0.42952855	2.76302714
H	4.56117945	-1.06319540	2.75146402
B	0.97072887	0.63746767	4.26241902
H	0.42296512	0.72163067	5.31052677
H	0.26191584	1.19852772	0.48547357
B	0.54807927	1.66151955	2.83414054
H	-0.21133096	2.57645606	2.76985989
B	0.95737980	0.61715874	1.43374007
Br	-4.17231802	-1.60760879	1.54272474
H	2.17901576	2.79477079	4.40592577
B	-2.49785610	-0.62846529	1.51220120
B	-1.87139059	0.27295277	0.08338714
H	-2.48969524	0.34752990	-0.92508751
H	-1.78506391	1.53794923	0.59025852
B	-1.08897475	-1.25767967	0.60417787
B	-1.10033734	-1.27792867	2.35870922
H	-1.19599720	-2.24469037	3.04095372
B	-1.80332646	0.22483843	2.94787419
H	-2.32637767	0.30461294	4.00824559
H	-1.86145664	1.51468857	2.45817213
B	-2.59740446	1.09753926	1.49866693
H	-3.64272007	1.65170308	1.50791748
B	-0.03976006	-0.00817495	0.00954853
H	0.47102680	-0.08144657	-1.05804953
H	0.72375070	-0.56716007	3.79627163
B	0.40877595	-1.04229096	1.43510171
H	1.15730759	-1.96367581	1.47306832
H	-1.27589332	-2.18997154	-0.10613360

PBE0 DZP S_2

H	4.49005281	1.95443804	2.81013068
B	0.00983533	0.01198064	2.87455964

B	3.48453479	1.32545229	2.76949609
B	2.80342010	0.41468952	4.14858823
H	3.30580276	0.20124998	5.20112618
H	2.62101795	-0.82624292	3.58013963
B	2.08219160	1.92176272	3.64484750
B	2.09484320	1.93439320	1.90968938
H	2.12147155	2.88188816	1.19293205
B	2.87150038	0.49825531	1.29432616
H	3.42641204	0.48282675	0.24682736
H	2.78263460	-0.76288777	1.68905257
B	3.50923787	-0.41693562	2.72860491
H	4.46066275	-1.12267940	2.74953347
B	0.91251710	0.70844873	4.22967223
H	0.42878192	0.79546108	5.30852321
H	0.42373270	1.14248792	0.36241955
B	0.56826668	1.65456855	2.75468337
H	-0.22771964	2.53188004	2.61657934
B	0.99246447	0.56435962	1.38952165
Br	-4.25253621	-1.56790552	1.48869204
H	2.17770560	2.87634438	4.34727872
B	-2.53164399	-0.66158984	1.50906748
B	-1.85217999	0.27073483	0.14338020
H	-2.37763296	0.51780431	-0.88845121
H	-1.61298725	1.47976018	0.75917403
B	-1.15367288	-1.26727808	0.60599712
B	-1.14895737	-1.32215138	2.34077008
H	-1.22083412	-2.28240077	3.03553445
B	-1.89817446	0.10314992	3.02302924
H	-2.45170297	0.06303487	4.06909251
H	-1.86413620	1.38132413	2.67365242
B	-2.53270992	1.08767819	1.58331387
H	-3.47654539	1.80044135	1.55902275
B	0.06325781	-0.08769084	0.03730703
H	0.49420663	-0.20261094	-1.06081046
H	0.59604320	-0.55655768	3.87906190
B	0.36624110	-1.08519964	1.48446910
H	1.13130072	-1.99267503	1.56989170
H	-1.31432769	-2.19598882	-0.11596666

PBE0 DZP T_1

H	4.47270767	1.92411517	2.78828724
B	0.00113709	0.01404912	2.83567166
B	3.47596262	1.28111985	2.77167808
B	2.83036777	0.36726471	4.18272703
H	3.40404302	0.25919990	5.21482324
H	2.74051700	-0.87939203	3.67903523
B	2.05685827	1.86638537	3.67353153
B	2.07140567	1.89625521	1.91852744
H	2.12233801	2.86020149	1.22724383

B	2.78677469	0.40227695	1.35020386
H	3.29249359	0.31566890	0.28048826
H	2.78881278	-0.86086630	1.81704479
B	3.55869737	-0.43292518	2.76136213
H	4.55604151	-1.07138880	2.75095536
B	0.96988215	0.63923425	4.26311116
H	0.43203156	0.71379133	5.31627876
H	0.26805378	1.20506706	0.49553759
B	0.55024952	1.67064336	2.83167431
H	-0.20859514	2.58301381	2.76104978
B	0.95732110	0.61994788	1.43450678
Br	-4.16719157	-1.63259463	1.53344038
H	2.18347409	2.79758679	4.40092916
B	-2.50378001	-0.63412854	1.51261533
B	-1.87444036	0.26816566	0.08406645
H	-2.48132232	0.34569427	-0.93046518
H	-1.79699770	1.54012531	0.59419846
B	-1.08693682	-1.25711053	0.60847970
B	-1.10635217	-1.27472148	2.35738098
H	-1.19407369	-2.24126584	3.03989096
B	-1.80180528	0.22972122	2.94990090
H	-2.32126119	0.30811489	4.01168089
H	-1.87075851	1.51261553	2.45799460
B	-2.60340434	1.09144477	1.49781277
H	-3.64569286	1.65031339	1.50748346
B	-0.04181112	-0.00254762	0.00690293
H	0.46375897	-0.06442501	-1.06310463
H	0.71773953	-0.56410744	3.78718364
B	0.41094041	-1.03991566	1.44128144
H	1.15935361	-1.95932119	1.49128433
H	-1.26416409	-2.19368548	-0.09793514

Table S9 The PBE0 DZP frequency calculations for the S_0, S_1, and T_1 states of 4-Br-*anti*-$B_{18}H_{21}$.

S_0 State

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm^{-1}	$1e^{-40}$ esu^2 cm^2	km/mole
----------	----------	----------
89.421380	27.521232	0.616861
103.215055	113.302579	2.931304
104.546349	9.734857	0.255104
183.073632	3.776321	0.173290
192.449049	4.688165	0.226150
230.135419	13.501517	0.778833

251.735232	1.113715	0.070274
300.646288	18.037203	1.359262
346.590838	16.219455	1.409066
388.407866	8.213674	0.799657
402.573080	42.210038	4.259303
413.509568	1.514116	0.156936
427.141867	80.605877	8.630122
468.862709	12.497112	1.468701
470.362778	4.746281	0.559583
483.041297	2.833757	0.343103
534.093757	0.374159	0.050090
558.973937	0.285904	0.040058
561.979573	6.443367	0.907635
579.404950	6.606215	0.959429
582.916953	18.038394	2.635619
598.457183	0.260763	0.039116
604.626176	15.048316	2.280620
618.653496	15.755736	2.443229
619.971338	19.964089	3.102410
627.875138	24.231521	3.813573
637.393493	32.503072	5.192902
645.216285	2.810909	0.454601
659.486099	10.010753	1.654819
662.889200	1.299263	0.215882
675.146678	60.994907	10.322141
685.051755	20.825630	3.576017
691.254177	36.533999	6.330136
706.435118	3.268695	0.578795
708.465996	123.370759	21.908332
715.920664	41.903365	7.519550
720.230313	89.241419	16.110757
728.101498	57.851774	10.558122
730.099188	1.936270	0.354345
741.364371	19.702113	3.661193
742.041678	4.213909	0.783775
745.222627	23.657871	4.419160
749.141291	0.530104	0.099541
759.792921	28.798571	5.484591
764.254403	3.941667	0.755085
768.465641	1.257911	0.242299
784.947593	21.934612	4.315675
793.554699	9.237095	1.837343
795.668402	21.299899	4.248032
799.204776	18.890430	3.784234
803.489557	22.600450	4.551718
812.003907	14.619582	2.975577
817.448865	96.578028	19.788688

823.980869	46.875795	9.681527
850.481003	19.663018	4.191726
857.461004	54.872219	11.793561
869.404330	18.868248	4.111795
873.583389	106.925626	23.413387
880.699701	40.223397	8.879421
889.688288	32.069268	7.151629
908.500489	458.545735	104.420530
920.160726	31.597367	7.287736
921.115890	36.417186	8.408117
926.374241	45.971596	10.674662
932.890986	50.456129	11.798394
934.884202	14.243770	3.337804
943.179257	20.292960	4.797530
944.946272	10.455983	2.476567
945.659453	27.604419	6.543219
952.706923	14.647536	3.497856
957.477738	4.373626	1.049659
962.929842	21.946107	5.297003
973.890696	50.147632	12.241615
978.794912	5.083322	1.247146
986.598271	10.739375	2.655813
995.031736	12.265705	3.059197
998.832949	93.912559	23.512272
1015.272507	68.033194	17.313368
1017.398466	55.501754	14.153891
1023.234430	50.434011	12.935306
1031.999561	11.477514	2.968967
1038.339433	25.699630	6.688740
1046.358059	12.195844	3.198676
1055.992299	48.856828	12.931952
1057.701484	13.205295	3.500977
1101.312317	10.335505	2.853121
1105.167699	41.002623	11.358419
1560.322613	12.405325	4.851775
1566.423077	75.341129	29.581437
1663.603114	311.332606	129.823228
1668.724954	72.347370	30.261160
1701.100190	105.244994	44.875511
1708.079441	82.680528	35.398868
2032.050191	4.785601	2.437525
2036.002736	2.729155	1.392787
2073.814479	44.965759	23.373831
2076.599127	25.368562	13.204641
2095.172355	8.216253	4.314909
2101.843572	20.330601	10.710967
2677.387212	29.177905	19.581383

2681.216730	55.116651	37.041862
2683.894053	41.325252	27.800906
2688.872462	78.854921	53.146795
2690.706238	26.898058	18.141169
2697.860698	73.941546	50.001856
2700.259109	76.343626	51.672121
2710.268367	47.876854	32.524900
2712.063289	48.352643	32.869879
2716.713571	35.502157	24.175567
2717.688738	85.274701	58.089547
2721.902092	123.488249	84.251221
2722.158641	46.696554	31.862242
2729.134257	119.132657	81.495532
2736.743315	53.751453	36.872480

S_1 State

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm^{-1}	$1e^{-40}$ esu^2 cm^2	km/mole
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76.923468	148.356706	2.860514
79.800678	195.415674	3.908805
95.238268	42.761272	1.020799
166.784404	327.070947	13.673367
178.666159	40.708256	1.823068
213.012852	22.498739	1.201274
233.833397	41.296513	2.420460
273.407219	70.845408	4.855118
333.999684	817.676722	68.455092
341.357276	95.492275	8.170629
356.641617	490.418621	43.840656
384.264989	0.230353	0.022187
394.794517	45.562972	4.508803
413.646292	8.516364	0.883001
452.676850	0.898052	0.101899
473.597020	78.828842	9.357766
510.950586	146.046438	18.704579
522.297352	9.442024	1.236121
542.862495	5.484229	0.746249
558.278578	0.974153	0.136319
564.204532	7.021846	0.993038
579.749231	3.878309	0.563587
589.472507	28.856953	4.263754
593.336745	36.470156	5.423966
609.509280	27.012849	4.126946
614.594041	136.404991	21.013417
621.579976	183.401321	28.574428

626.701300	71.073719	11.164717
634.375187	11.724166	1.864259
639.407350	9.342513	1.497336
655.406765	67.562943	11.099350
663.220310	59.127889	9.829428
670.827427	179.540340	30.189153
675.503800	27.613183	4.675438
686.722245	94.042198	16.187581
704.219799	141.802590	25.030554
706.268645	12.821786	2.269847
710.662165	25.926776	4.618381
717.798192	15.955759	2.870767
723.660333	202.502104	36.731814
731.170041	125.345029	22.972252
732.649401	50.660814	9.303502
737.195620	21.463303	3.966043
742.107046	9.022290	1.678268
750.764635	13.785170	2.594144
755.987557	28.927669	5.481585
769.299917	95.497628	18.414772
770.596161	52.349613	10.111565
780.600960	21.422845	4.191643
782.778698	59.561567	11.686466
790.529063	42.722928	8.465584
801.157248	73.932950	14.846835
803.922729	25.113531	5.060578
814.153348	320.622908	65.430288
826.518008	4.731959	0.980328
834.155434	36.995404	7.735223
838.154268	20.160051	4.235392
847.504611	44.057080	9.359138
851.278965	23.112292	4.931658
864.211046	76.065953	16.477381
877.715274	493.910967	108.662676
888.398397	30.673089	6.830356
895.731742	7.118590	1.598269
900.908121	101.459003	22.911270
905.273954	158.180698	35.893151
915.267049	19.843318	4.552398
918.313461	12.771914	2.939849
924.585851	76.131076	17.643603
925.101630	131.103094	30.400481
926.959882	4.580756	1.064330
933.387382	319.939829	74.852844
940.623749	4.338206	1.022832
947.111735	19.439700	4.614970
951.871618	5.710489	1.362479

955.464317	217.543405	52.100089
973.996021	2.939108	0.717548
976.426166	59.037417	14.449234
983.436137	28.357699	6.990290
985.805722	19.843191	4.903215
993.775829	18.352554	4.571545
996.390810	72.998344	18.231432
1005.040109	54.666828	13.771630
1010.109997	36.699988	9.292074
1047.304315	15.148895	3.976783
1059.777949	90.598795	24.066635
1077.040976	8.848205	2.388721
1090.530201	62.308442	17.031883
1440.194048	68.436996	24.705293
1461.092905	42.255147	15.475173
1534.569510	158.163867	60.837577
1574.837309	94.506061	37.305548
1622.495321	42.806475	17.408886
1642.753903	46.585974	19.182524
2028.598005	2.472627	1.257282
2035.736910	2.316116	1.181844
2070.358518	3.747325	1.944666
2074.517347	46.123123	23.983571
2078.095406	0.161219	0.083977
2097.570645	21.758937	11.440166
2664.468541	11.347489	7.578590
2675.919901	22.522647	15.106735
2677.344465	16.817750	11.286264
2680.659115	79.958524	53.725990
2685.885887	17.082309	11.500381
2691.539026	79.837124	53.862144
2699.317484	97.502262	65.970038
2705.685200	46.109321	31.271165
2708.982347	39.524339	26.837921
2711.259177	66.969656	45.512131
2712.363252	156.944266	106.701709
2717.668961	56.201058	38.284159
2719.561470	97.264227	66.302528
2724.354394	317.837738	217.043674
2730.533955	54.653316	37.406077

S_2 State

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm^{-1}	$1e^{-40}$ esu^2 cm^2	km/mole
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-642.049134	357.681338	-57.562894
-238.806262	21.424507	-1.282433
57.082440	124.193277	1.776964
82.170942	27.896820	0.574581
84.508460	20.742376	0.439376
167.055436	98.480089	4.123700
177.939538	53.062084	2.366654
208.347427	13.121863	0.685270
235.269248	289.728371	17.085758
279.744053	44.314021	3.107278
289.207028	61.085946	4.428210
365.881721	42.022737	3.853924
371.837044	394.314613	36.751375
378.753579	12.884118	1.223178
404.486903	102.529817	10.395197
437.293146	47.389420	5.194361
460.402378	35.811955	4.132793
471.940664	113.567979	13.434496
504.995050	142.126063	17.990321
525.704391	4.327012	0.570175
531.258784	23.430902	3.120134
547.449689	4.394338	0.602998
556.614584	107.532930	15.002863
569.864404	28.212008	4.029801
584.828814	8.248369	1.209135
602.820338	133.775385	20.213531
609.152702	95.522445	14.585109
613.856353	120.676587	18.568116
620.739924	19.311192	3.004670
626.750054	34.431375	5.409122
639.677233	12.176066	1.952297
647.143741	4.377900	0.710141
654.409353	138.915034	22.786458
659.481730	24.145070	3.991253
670.858117	0.979444	0.164698
682.626118	124.719436	21.340034
687.742928	24.491193	4.221960
697.192332	101.665022	17.766514
706.031422	12.887372	2.280691
710.914279	162.531805	28.962341
719.598765	150.058656	27.066340
723.612315	66.959135	12.144898
725.400552	67.800196	12.327838
732.725909	291.507838	53.538951
735.431717	71.080846	13.103069

741.507445	15.065111	2.800051
754.274485	14.934686	2.823603
764.104796	340.426277	65.200972
769.710033	1.582480	0.305312
771.648407	213.314344	41.258895
773.418362	125.947511	24.416429
781.969530	18.197696	3.566846
796.488151	292.722520	58.440446
808.308038	48.136914	9.752887
817.445299	37.001244	7.581464
823.827561	65.498701	13.525305
829.506316	29.071640	6.044596
836.153381	14.243259	2.985200
841.090979	77.713559	16.383921
848.988802	66.717803	14.197823
857.128546	488.652390	104.984227
872.088308	212.636714	46.481142
874.134297	8.883884	1.946521
891.788419	5.601079	1.252021
892.929960	69.205604	15.489476
895.634388	34.171346	7.671334
900.023606	5.385191	1.214879
911.299551	3.987974	0.910944
915.662752	86.417632	19.834259
920.918569	151.288712	34.922540
924.284113	20.734247	4.803655
929.769583	1.082796	0.252348
941.596122	35.001485	8.260935
948.073758	6.833573	1.623933
950.374676	13.345985	3.179242
955.882969	4.320233	1.035118
967.271060	4.318210	1.046960
974.810263	92.913154	22.702588
988.427814	13.441614	3.330232
993.511953	100.972816	25.145231
996.987188	89.072925	22.259395
1002.237538	328.112000	82.427257
1010.649799	8.145808	2.063540
1043.442895	8.156565	2.133310
1056.592961	23.458476	6.212774
1075.505347	30.356285	8.183503
1089.761142	8.947701	2.444111
1288.611459	50.200829	16.214776
1434.271500	15.485706	5.567247
1561.881284	225.279361	88.195717
1575.346959	27.183211	10.733838

1619.562254	127.724203	51.850019
1700.621610	1403.871948	598.429866
2003.758777	33.904555	17.028702
2021.875451	0.087013	0.044098
2036.304543	25.858889	13.198685
2044.097730	10.445889	5.352111
2065.636593	58.174947	30.120903
2088.380736	64.103656	33.556028
2662.801817	24.721391	16.500223
2674.328779	13.169367	8.827907
2675.612665	28.400631	19.047119
2679.699281	83.710123	56.226637
2689.075321	23.689948	15.967803
2694.447709	70.288138	47.471162
2696.048563	134.940297	91.190048
2708.070124	67.338566	45.709013
2708.901959	72.875801	49.482849
2714.982019	19.149114	13.031479
2716.269643	88.596591	60.320921
2719.754834	54.688317	37.282273
2721.884083	175.317875	119.611763
2725.530109	278.601192	190.332093
2735.233346	71.432337	48.974196

T_1 State

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm^{-1}	$1e^{-40}$ esu^2 cm^2	km/mole
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88.904879	183.349662	4.085863
93.690323	3.095207	0.072688
109.572250	71.506263	1.963915
180.438947	194.253246	8.785705
194.871221	12.856126	0.627966
224.245335	15.000661	0.843164
246.822269	36.648457	2.267348
296.853346	27.398763	2.038689
342.856064	25.228490	2.168109
373.012399	39.524977	3.695498
392.000427	356.430190	35.021851
437.108708	21.409370	2.345694
458.324991	52.868968	6.073687
462.389307	67.026245	7.768385
488.104833	27.297727	3.339779
496.001013	280.034772	34.815497

513.733386	4.264995	0.549205
516.318608	21.561006	2.790390
536.351619	223.516253	30.049467
541.464577	51.542286	6.995388
549.655649	66.725489	9.193069
557.893576	10.520737	1.471213
575.258305	30.912482	4.457331
578.529653	82.593006	11.976970
590.722174	82.540176	12.221562
598.950865	47.176782	7.082679
609.129185	109.059751	16.651447
619.822493	65.783612	10.220288
623.743298	38.320723	5.991253
638.249887	9.867440	1.578604
647.998422	17.881761	2.904439
661.303880	28.251370	4.682941
674.133981	90.317778	15.261511
678.428324	38.921788	6.618732
680.870443	12.068412	2.059647
694.105350	104.058825	18.104327
704.282830	19.741928	3.485096
705.663460	14.692526	2.598796
707.000780	7.526671	1.333831
714.514765	55.743220	9.983466
719.505613	87.725285	15.821114
728.619166	3.264207	0.596151
731.242023	56.358367	10.329936
738.046603	74.500111	13.782207
746.080198	37.630203	7.037204
755.378078	11.738906	2.222645
761.669480	19.338386	3.692027
770.207008	51.968292	10.032842
773.208550	76.862016	14.896577
778.948586	54.457651	10.632754
783.329251	96.266176	18.901494
785.590645	21.658226	4.264786
789.627288	56.254012	11.134064
794.808511	27.188758	5.416640
820.188636	143.709175	29.544477
825.396472	12.534978	2.593369
834.957923	93.545122	19.577796
846.857948	46.205443	9.808030
849.228592	56.225313	11.968358
860.599297	182.507865	39.369567
873.792509	122.204068	26.765296
882.948273	200.393281	44.350292
893.166797	12.252223	2.742998

895.373553	107.729171	24.177737
898.412888	19.752819	4.448188
901.357835	48.139832	10.876268
908.001123	6.060286	1.379296
910.650639	272.088470	62.106922
918.670678	38.825163	8.940282
921.506587	34.134996	7.884540
929.838482	27.657871	6.446208
943.509466	71.880185	16.999397
949.071345	87.796280	20.885893
949.697489	31.488461	7.495745
953.531825	45.890065	10.968114
962.200837	61.203684	14.761190
969.437710	116.475255	28.302946
977.793679	23.556483	5.773454
987.708610	62.446789	15.460268
994.134506	8.682691	2.163603
999.760657	67.943441	17.026354
1009.758869	39.992859	10.122277
1015.150693	55.457450	14.111347
1033.320271	9.019183	2.336040
1051.018842	54.993101	14.487611
1070.943656	2.415126	0.648313
1090.172146	15.662708	4.279963
1363.348381	38.430398	13.132875
1509.331208	11.809630	4.467853
1541.127279	136.966651	52.909227
1571.172803	128.917306	50.770711
1599.173628	146.397475	58.682320
1651.646360	67.740683	28.044307
2028.948839	1.934735	0.983944
2037.085532	16.168512	8.255766
2058.308434	6.786795	3.501493
2095.341973	8.554160	4.492730
2106.921521	10.058453	5.311995
2131.174827	18.845685	10.067209
2657.992690	20.164388	13.434357
2675.234741	28.673440	19.227365
2679.577909	23.108808	15.521082
2688.843661	43.721948	29.467488
2691.067405	18.000600	12.141983
2695.114308	73.095667	49.379524
2698.182354	53.404940	36.118591
2701.377791	86.228471	58.386720
2702.346569	113.530449	76.900909
2706.274061	47.351177	32.120376
2710.378998	124.845979	84.816950

2714.370120	94.109079	64.029286
2717.004475	82.226188	55.998782
2719.864850	230.777899	157.332922
2727.131351	54.334828	37.141755

DFT Screening Data

To determine which method works best for this system, we first screened a variety of basis sets and functionals. UV/Vis spectra were calculated and compared to experimental data to find the most suitable method (PBE0 DZP). The optimized geometries of the S_0 state for each method tested are shown below in Table S10. Scalar relativistic effects were used in all calculations.

Table S10

B3LYP-D3 DZP

H	4.49417643	1.97113952	2.79401503
B	0.02294936	0.00995206	2.84744990
B	3.52222828	1.29549852	2.77756692
B	2.88468652	0.38125075	4.18784602
H	3.44072027	0.24599567	5.22237937
H	2.73379483	-0.82677299	3.69127726
B	2.09619679	1.85101206	3.68467482
B	2.06845780	1.86942390	1.89789953
H	2.14521269	2.81680316	1.18845791
B	2.90373168	0.43943245	1.35269372
H	3.39357848	0.35444344	0.28012416
H	2.77490294	-0.79605603	1.77599136
B	3.58636147	-0.41772173	2.74543403
H	4.50507929	-1.16130191	2.74181505
B	0.94197138	0.66751131	4.25841869
H	0.40914430	0.77085527	5.30745395
H	0.22213250	1.19390494	0.43067471
B	0.57034066	1.67351298	2.83895192
H	-0.19389934	2.57727078	2.84752939
B	0.93275692	0.63011132	1.42801414
Br	-4.21881825	-1.77862810	1.48870000
H	2.20679232	2.78613728	4.40401734
B	-2.57958610	-0.66745687	1.50226867
B	-1.93517497	0.25090009	0.08579435
H	-2.50113100	0.38141211	-0.94247328
H	-1.78867949	1.45578462	0.58608405
B	-1.14295834	-1.21374351	0.59302091
B	-1.11161254	-1.23263637	2.38016726
H	-1.19511425	-2.17841346	3.08825325
B	-1.95119232	0.19292549	2.92687891
H	-2.44460479	0.27854685	3.99623763
H	-1.82184451	1.42619761	2.49766190
B	-2.63781780	1.04878600	1.53374163
H	-3.55819232	1.78805917	1.53986026

B	0.00565520	-0.02411845	0.01881986
H	0.53317529	-0.13104943	-1.03246729
H	0.72752579	-0.55284423	3.84668204
B	0.38149524	-1.03501717	1.43572260
H	1.14241357	-1.94063252	1.42212464
H	-1.26247936	-2.14685411	-0.12500311

B3LYP DZP Cyclohexane

H	4.49120459	1.97481642	2.79354884
B	0.02527724	0.00830170	2.84800289
B	3.52088262	1.29609893	2.77753959
B	2.88740345	0.37967492	4.18789255
H	3.44387357	0.25030425	5.22295694
H	2.74011653	-0.82831393	3.69636152
B	2.09573826	1.84925453	3.68354668
B	2.06804261	1.86591781	1.89619261
H	2.14395872	2.81363739	1.18751332
B	2.90844029	0.43694130	1.35430006
H	3.39823066	0.35306638	0.28177915
H	2.77805511	-0.79726709	1.77693873
B	3.58946321	-0.41727197	2.74791483
H	4.50967229	-1.15837709	2.74435009
B	0.94381662	0.66394400	4.25742904
H	0.41110261	0.76458686	5.30691900
H	0.21805108	1.19560921	0.43331990
B	0.57114381	1.67208277	2.83874597
H	-0.19336643	2.57534035	2.84704752
B	0.93045506	0.62916995	1.42817309
Br	-4.21577987	-1.78151509	1.48787340
H	2.20619715	2.78534634	4.40204394
B	-2.57423916	-0.66375035	1.50182447
B	-1.93590738	0.25446960	0.08587082
H	-2.50363958	0.37894312	-0.94215919
H	-1.79343325	1.45985802	0.58148475
B	-1.14335068	-1.21252264	0.59381012
B	-1.11228338	-1.22985294	2.38178085
H	-1.19822858	-2.17627819	3.08836571
B	-1.95481712	0.19645663	2.92559897
H	-2.44950370	0.27936371	3.99444584
H	-1.82465195	1.42955302	2.49829602
B	-2.63882370	1.05096796	1.53156869
H	-3.56191279	1.78616539	1.53729124
B	0.00405332	-0.02208055	0.01963864
H	0.53156444	-0.12755335	-1.03183814
H	0.73207356	-0.55677736	3.84396429
B	0.37970748	-1.03619155	1.43557570

H	1.13965616	-1.94231645	1.42218890
H	-1.26586824	-2.14618157	-0.12333787

B3LYP-D3 TZP Cyclohexane

H	4.49679514	1.97671927	2.79363286
B	0.02673945	0.00521994	2.84964227
B	3.52598604	1.29995137	2.77693532
B	2.88718805	0.37920379	4.19221204
H	3.43960987	0.24839994	5.22847834
H	2.73732632	-0.83252428	3.69873708
B	2.09488082	1.85531763	3.68604502
B	2.06706712	1.87179257	1.89527170
H	2.13972276	2.81807349	1.18558998
B	2.90612147	0.43764778	1.34949182
H	3.38708077	0.35396210	0.27379913
H	2.77655395	-0.80000524	1.77064661
B	3.58722324	-0.42082714	2.74610935
H	4.50631313	-1.16322553	2.74163216
B	0.93976174	0.66567296	4.26164950
H	0.40674743	0.76578530	5.30998987
H	0.22443900	1.19537180	0.42835674
B	0.56711507	1.67496830	2.83879424
H	-0.20189125	2.57304605	2.84200623
B	0.93001634	0.63060978	1.42653563
Br	-4.22375757	-1.78251339	1.48847705
H	2.20462527	2.79058981	4.40483472
B	-2.57664835	-0.66508859	1.50237212
B	-1.93394264	0.25678300	0.08190637
H	-2.50048903	0.38057761	-0.94607472
H	-1.78969124	1.46610322	0.57905481
B	-1.14209468	-1.21775972	0.59108905
B	-1.11087626	-1.23545193	2.38218017
H	-1.19903873	-2.18120657	3.08806768
B	-1.95060179	0.19667709	2.93041808
H	-2.43840667	0.27681295	4.00178265
H	-1.82258947	1.43378331	2.50579262
B	-2.63440789	1.05596579	1.53380640
H	-3.55912166	1.78904700	1.54046371
B	0.00886969	-0.02451225	0.01492410
H	0.53664958	-0.12988837	-1.03544193
H	0.72707442	-0.55777530	3.84870323
B	0.38395108	-1.04066025	1.43513507
H	1.14795458	-1.94203637	1.42648676
H	-1.26988049	-2.15098643	-0.12477431

wB97 TZP

H	4.51407391	1.96418289	2.79855857
B	0.01596923	0.00875021	2.84505619
B	3.52439388	1.31070442	2.77877350
B	2.87871684	0.38470399	4.18481236
H	3.43659587	0.24545641	5.22347782
H	2.72503179	-0.83388545	3.68269007
B	2.09709713	1.86670734	3.68244005
B	2.07051475	1.88411001	1.89854054
H	2.14859085	2.82579232	1.17785315
B	2.90403493	0.44806775	1.34991792
H	3.39992606	0.36776440	0.27412924
H	2.76977172	-0.79927040	1.77150412
B	3.58869693	-0.41080039	2.74157208
H	4.51788106	-1.14712881	2.73911853
B	0.94301998	0.67232273	4.25510085
H	0.40595740	0.77448863	5.30854647
H	0.23060781	1.18914496	0.42764645
B	0.56584179	1.68436088	2.83264857
H	-0.20363958	2.58928895	2.83716399
B	0.94026744	0.62016126	1.43166509
Br	-4.21128010	-1.72747114	1.47458130
H	2.21241794	2.79419312	4.41484187
B	-2.56609834	-0.66726435	1.49946308
B	-1.92378388	0.25562485	0.09115989
H	-2.50129503	0.38431572	-0.93716580
H	-1.77500188	1.47364298	0.59729219
B	-1.14582967	-1.22998327	0.59308546
B	-1.11596911	-1.25150620	2.37768658
H	-1.21966395	-2.19468321	3.09188655
B	-1.94756787	0.18513592	2.93159897
H	-2.45836293	0.25243236	4.00024916
H	-1.81610822	1.43484567	2.51173185
B	-2.63224349	1.05091865	1.54148036
H	-3.57510158	1.76806394	1.54657875
B	0.00623052	-0.03727595	0.02055745
H	0.53655467	-0.14623227	-1.03533389
H	0.72055595	-0.55876303	3.84966579
B	0.38429759	-1.05620971	1.44029613
H	1.14705700	-1.96605589	1.43019826
H	-1.28978283	-2.15502981	-0.13631005

BP86-D3 TZP Cyclohexane

H	4.51181513	1.97063191	2.79535203
B	0.02090436	0.00205106	2.85083200

B	3.52287127	1.30594513	2.77801060
B	2.88327966	0.38507776	4.19316472
H	3.43723531	0.25121829	5.23896587
H	2.73432574	-0.83789792	3.69716352
B	2.09335448	1.86627165	3.68783170
B	2.06692128	1.88319583	1.89429936
H	2.14459225	2.83592474	1.17987231
B	2.89836136	0.44342114	1.34665891
H	3.38250359	0.35487233	0.26238691
H	2.76742529	-0.80681576	1.77415405
B	3.58738433	-0.41702221	2.74377215
H	4.51782862	-1.15887894	2.73882924
B	0.93989867	0.67039591	4.26622946
H	0.40439897	0.76756123	5.32452286
H	0.22955678	1.19247192	0.41969107
B	0.56196236	1.68220936	2.83739437
H	-0.21741373	2.58338873	2.83890241
B	0.93643624	0.62559229	1.42502091
Br	-4.22732903	-1.74256949	1.47903089
H	2.21030024	2.80715062	4.41225222
B	-2.56469814	-0.66268042	1.50014860
B	-1.92594555	0.25764486	0.08272687
H	-2.50021402	0.38297746	-0.95191208
H	-1.78360844	1.47861179	0.58425438
B	-1.14186046	-1.22885781	0.58637787
B	-1.11097895	-1.25126195	2.38106145
H	-1.21419324	-2.20499991	3.08887782
B	-1.94015994	0.18860856	2.93532029
H	-2.43722739	0.26443937	4.01340815
H	-1.81280982	1.44155780	2.51127466
B	-2.62994596	1.05718861	1.54078747
H	-3.57183893	1.78255137	1.54969332
B	0.00897944	-0.03411022	0.00847729
H	0.53811693	-0.13851812	-1.05203649
H	0.72193017	-0.56157161	3.85802650
B	0.38802498	-1.05497229	1.43389671
H	1.16065183	-1.96098214	1.42569823
H	-1.28846109	-2.16620047	-0.13565909

PBE-D3BJ TZP Cyclohexane

H	4.48792406	1.96002543	2.79362244
B	0.02498310	0.00617218	2.84703554
B	3.51120878	1.29663851	2.77633453
B	2.87955013	0.38315835	4.18495352
H	3.43521721	0.25727590	5.21795972
H	2.73645526	-0.82510939	3.69160928

B	2.08957586	1.84958521	3.68077038
B	2.06281026	1.86669849	1.89763563
H	2.14422235	2.81247429	1.19341655
B	2.89644619	0.44153014	1.35334977
H	3.38537657	0.36267501	0.28299436
H	2.77048414	-0.79273435	1.77807507
B	3.57790421	-0.41609870	2.74312652
H	4.50406649	-1.14533619	2.73787953
B	0.93911304	0.66529265	4.25613797
H	0.40887014	0.76551755	5.30398077
H	0.23045240	1.18233482	0.43561929
B	0.56518526	1.67176890	2.83583431
H	-0.19921251	2.56968387	2.83863591
B	0.93139112	0.62530327	1.42929621
Br	-4.20748710	-1.74384269	1.48314938
H	2.20910400	2.78278046	4.39574285
B	-2.55286935	-0.65417733	1.50240818
B	-1.92496288	0.25586958	0.08979877
H	-2.49719194	0.37353686	-0.93361800
H	-1.78734863	1.46226256	0.58790756
B	-1.13797367	-1.21293343	0.59508711
B	-1.10753529	-1.23314113	2.37927925
H	-1.20876195	-2.17878658	3.07860642
B	-1.93990290	0.19210921	2.92795987
H	-2.43931385	0.26313463	3.99249927
H	-1.81620120	1.42707847	2.50166261
B	-2.62362100	1.05435755	1.53878162
H	-3.55885216	1.76971708	1.54718903
B	0.00982320	-0.02814812	0.01997148
H	0.53382704	-0.13473761	-1.03017366
H	0.72146940	-0.54946297	3.84135709
B	0.38471546	-1.04171194	1.43738414
H	1.14312519	-1.94396219	1.42899442
H	-1.27969180	-2.14317790	-0.11749519

PBE0-dDsC TZP

H	4.47937444	1.95430686	2.78980612
B	0.02388488	0.00682286	2.84225330
B	3.49204136	1.30172634	2.77115938
B	2.85229463	0.38482986	4.16981716
H	3.40633779	0.24367003	5.20695702
H	2.69384478	-0.82626083	3.67387788
B	2.07671151	1.85943914	3.67225694
B	2.04978191	1.87731204	1.89744010
H	2.12750989	2.81957308	1.18157066
B	2.86760256	0.44449266	1.35355478

H	3.35220004	0.35554734	0.27679387
H	2.72536557	-0.79317819	1.77790319
B	3.54590147	-0.40915270	2.73491787
H	4.46680623	-1.15235254	2.72944478
B	0.93451829	0.66846963	4.24368912
H	0.40182896	0.76658126	5.29584509
H	0.22856420	1.18891091	0.44041529
B	0.55662075	1.67461968	2.82923151
H	-0.21703858	2.57156739	2.83465096
B	0.93148158	0.62271929	1.43365783
Br	-4.18648939	-1.72121516	1.48606904
H	2.19291751	2.78826787	4.39928226
B	-2.54117782	-0.66409648	1.50717266
B	-1.89909457	0.25386497	0.10599928
H	-2.46793195	0.38976475	-0.92270436
H	-1.74325621	1.46258792	0.60703371
B	-1.12675598	-1.22342453	0.60302695
B	-1.09591375	-1.24551489	2.37842498
H	-1.19227342	-2.18794942	3.09008093
B	-1.91257031	0.18688211	2.92743942
H	-2.40548735	0.26861856	3.99988533
H	-1.76991190	1.42541338	2.50339161
B	-2.59131480	1.04639900	1.54795779
H	-3.51963229	1.77861404	1.55704548
B	0.01336124	-0.03193738	0.03211651
H	0.54061169	-0.13554941	-1.02211625
H	0.72248405	-0.55647407	3.83734152
B	0.39285055	-1.04535205	1.44325153
H	1.16118212	-1.94601644	1.43179198
H	-1.26485506	-2.14890645	-0.12297374

PBE0 TZ2P Cyclohexane

H	4.48842791	1.96309533	2.79155012
B	0.02182932	0.00637094	2.84611034
B	3.50454608	1.30352237	2.77460928
B	2.86775036	0.38312708	4.17726205
H	3.42291258	0.24997198	5.21583749
H	2.71931856	-0.83187019	3.68672577
B	2.08511900	1.85886018	3.67763198
B	2.05853934	1.87673890	1.89757358
H	2.13755695	2.82033052	1.18190680
B	2.88496503	0.44128903	1.35482744
H	3.37480326	0.35633644	0.27920590
H	2.75281374	-0.80065325	1.77675011
B	3.56759819	-0.41142615	2.74137001
H	4.49280468	-1.14981000	2.73660721

B	0.94040105	0.66593337	4.25090080
H	0.41132627	0.76538940	5.30591417
H	0.22957521	1.19192982	0.43202758
B	0.56080875	1.67696603	2.83372855
H	-0.21095045	2.57657899	2.84068681
B	0.93350454	0.62292569	1.43013001
Br	-4.19347934	-1.73435470	1.48412560
H	2.20121322	2.79019709	4.40365683
B	-2.55273345	-0.66410374	1.50374618
B	-1.91415395	0.25619303	0.09812755
H	-2.48388896	0.38398780	-0.93211388
H	-1.76909780	1.46892752	0.59387784
B	-1.13529629	-1.22286938	0.59769711
B	-1.10496755	-1.24474754	2.37857511
H	-1.20322402	-2.18861593	3.08990231
B	-1.92943494	0.19111681	2.92648172
H	-2.42758370	0.26911870	3.99771043
H	-1.79763429	1.43395390	2.50432413
B	-2.61279186	1.04988344	1.54132460
H	-3.54529550	1.77740963	1.54959965
B	0.00753090	-0.03005238	0.02501999
H	0.53031217	-0.13578145	-1.03229087
H	0.72127648	-0.56032422	3.84548955
B	0.38808680	-1.04835049	1.43899589
H	1.15352661	-1.95249446	1.42619938
H	-1.27364030	-2.15107961	-0.12704561

PBE0 TZP Cyclohexane

H	4.49165581	1.96307928	2.79235646
B	0.02136498	0.00755016	2.84586493
B	3.50598290	1.30348756	2.77509154
B	2.86916665	0.38399875	4.17818155
H	3.42513731	0.24969522	5.21672924
H	2.71933817	-0.83124858	3.68687146
B	2.08671693	1.85883135	3.67799737
B	2.05997410	1.87677653	1.89809738
H	2.13982300	2.82140719	1.18280482
B	2.88619427	0.44222586	1.35460150
H	3.37731282	0.35800647	0.27897249
H	2.75242197	-0.79993450	1.77698238
B	3.56878271	-0.41061629	2.74174724
H	4.49338695	-1.15016873	2.73719520
B	0.94179032	0.66694294	4.25119748
H	0.41248204	0.76626257	5.30642621
H	0.22778919	1.19220753	0.43350436
B	0.56261647	1.67718271	2.83397255

H	-0.20865818	2.57803915	2.84128314
B	0.93415156	0.62272928	1.43060715
Br	-4.20267461	-1.73772141	1.48220607
H	2.20303665	2.79075538	4.40458750
B	-2.55442614	-0.66490889	1.50321361
B	-1.91587114	0.25460050	0.09693208
H	-2.48579397	0.38347387	-0.93352535
H	-1.76962475	1.46746534	0.59329666
B	-1.13606230	-1.22268446	0.59766774
B	-1.10581775	-1.24428355	2.37839636
H	-1.20378678	-2.18908257	3.08955488
B	-1.93107481	0.19017143	2.92659320
H	-2.43012676	0.26813074	3.99783741
H	-1.79740012	1.43278063	2.50338514
B	-2.61447584	1.04843334	1.54053433
H	-3.54594792	1.77754175	1.54846215
B	0.00642360	-0.03036370	0.02509196
H	0.52967795	-0.13540186	-1.03232400
H	0.72314353	-0.55971465	3.84453640
B	0.38694360	-1.04761699	1.43924190
H	1.15211288	-1.95276268	1.42619458
H	-1.27331070	-2.15164617	-0.12760758

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