

Supporting Information for the paper entitled,

A Super-Oxidized Radical Cationic Icosahedral Boron Cluster

Julia M. Stauber,¹ Josef Schwan,² Xinglong Zhang,² Jonathan C. Axtell,^{1,3} Dahee Jung,¹
Brendon J. McNicholas,² Paul H. Oyala,² Andrew J. Martinolich,² Jay R. Winkler,²
Kimberly A. See,² Thomas F. Miller III,^{2*} Harry B. Gray,^{2*} Alexander M. Spokoyny^{1,4*}

¹*Department of Chemistry and Biochemistry, University of California, Los Angeles, 607 Charles E. Young Dr E., Los Angeles, California, 90095, United States*

²*Division of Chemistry and Chemical Engineering, California Institute of Technology, 1200 East California Boulevard, Pasadena, California, 91125, United States*

³*The Dow Chemical Company, 633 Washington St., Midland, Michigan, 48674, United States*

⁴*California NanoSystems Institute, University of California, Los Angeles, 570 Westwood Plaza, Los Angeles, California, 90095, United States*

*Correspondence to: spokoyny@chem.ucla.edu (A. M. S.), hbgray@caltech.edu (H. B. G.), tfm@caltech.edu (T. F. M.)

S9. Computational details

S9.1. Methods

Density functional theory (DFT) calculations were performed with *Gaussian 16* rev. C.01.⁶ To find the best functional for the system, geometry optimizations were carried out separately using B3LYP,^{7–10} B3LYP with Grimme's dispersion with Becke-Johnson damping¹¹ (Gaussian keyword "empiricaldispersion=GD3BJ"), denoted herein B3LYP-D3 and CAM-B3LYP¹² functionals with a Pople split-valence double- ζ basis set¹³ 6-31G(d) for all atoms. Geometry minima on the potential energy surface (PES) were confirmed as such by harmonic frequency analysis, showing zero imaginary frequency, at the same level of theory. Gibbs energies were evaluated at 298.15K, using a quasi-rigid rotor harmonic oscillator (quasi-RRHO) treatment of vibrational entropies^{14,15} at a cut-off of 100 cm⁻¹. Briefly, a free-rotor approximation was used for all vibrational frequencies less than 100 cm⁻¹ and a damping function was used to interpolate between the RRHO and the free-rotor vibrational entropy to avoid a discontinuity. The values were further corrected at 1 mol L⁻¹ when going from gas-phase to the solution phase.

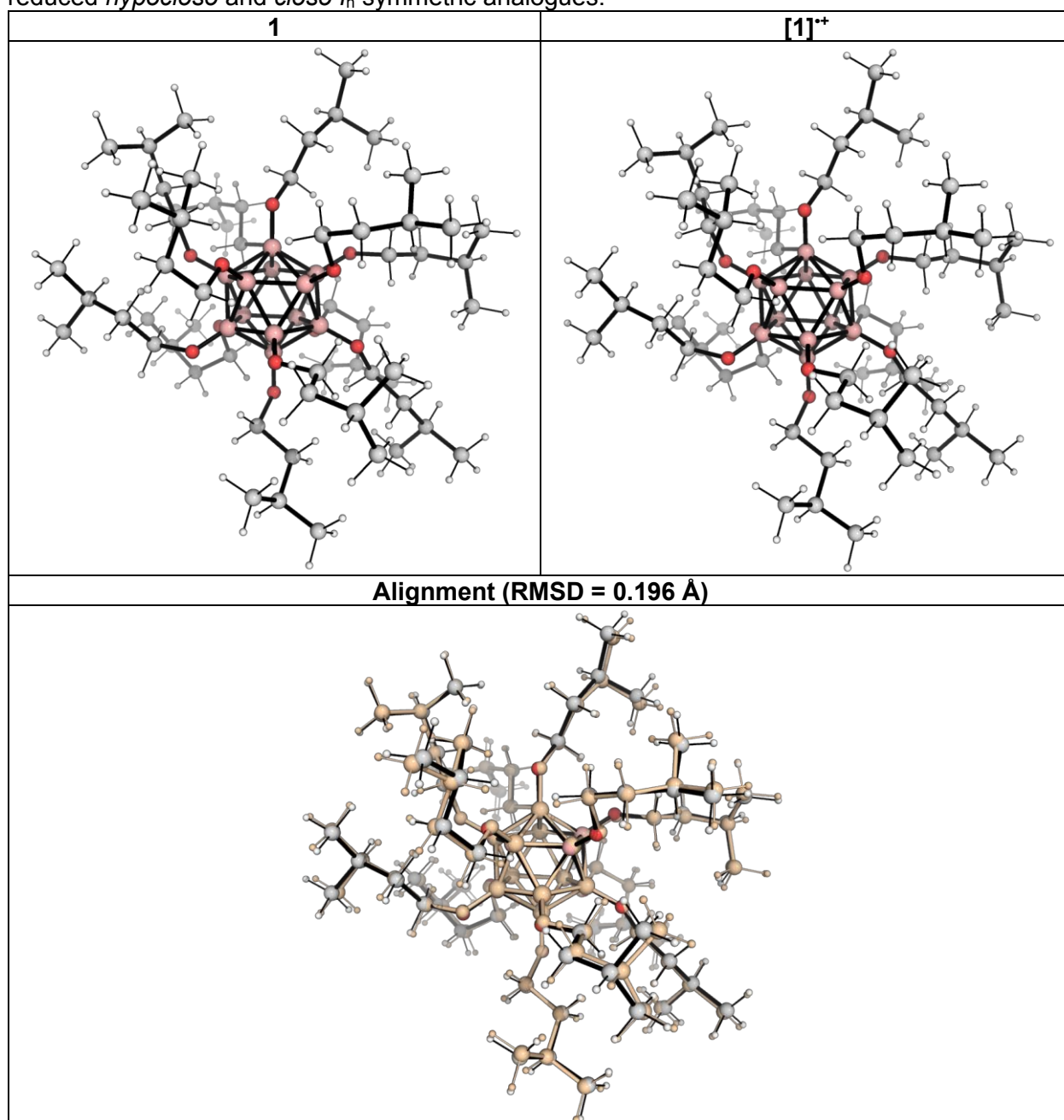
For time-dependent DFT (TD-DFT) calculations, CAM-B3LYP functional was adopted due to its robust performance for the study of excited states.^{16,17} In this case, 6-31+G(d,p) basis set¹³ for all atoms was used. The SMD continuum solvation model¹⁸ was used to account for the implicit solvent effect of dichloromethane (DCM), which was the solvent used for UV-vis measurements. For UV-vis spectra, Gaussian function, with a standard deviation of wavenumber (σ) of 0.4 eV, was used to broaden the peaks, as described on the *Gaussian 16* webpage.¹⁹

For electrochemical potential estimation, the solvation energies were calculated at B3LYP-D3/def2-SVP^{20–22} level of theory using SMD model for DCM, at geometries optimized at B3LYP-D3/6-31G(d) level of theory (we denote this model chemistry as SMD(DCM)-B3LYP-D3/def2-SVP//B3LYP-D3/6-31G(d)). For ¹¹B NMR calculations, using the B3LYP-D3 optimized geometries, the chemical shielding tensors were calculated at B3LYP/def2-SVP level of theory with SMD solvation model to account for the effect of chloroform solvent. The Gauge-Including Atomic Orbitals (GIAOs)²³ method with the Gaussian keyword "nmr = (GIAO,Mixed)" was used. This level of theory (B3LYP/def2-SVP) has been shown to be computationally efficient and to give good agreement with experimental measurements for a variety of boron-containing compounds.^{24,25}

Molecular orbitals were visualized using an isosurface value of 0.05 a.u. throughout. All molecular structures and molecular orbitals were visualized using *PyMOL* software.²⁶ Coordinates of the optimized geometries have been deposited within this Supporting Information (**Section S9.8**).

S9.2. Geometry optimization and structural comparison of **1** and **[1]⁺**

Geometry optimizations were carried out on the **1** and **[1]⁺** clusters at the B3LYP^{7,9,10,27}-D3BJ/6²⁸-31G(d)¹³ level of theory and the optimized structures are given in **Figure S25**. These calculations show that the geometry of **1** is not significantly altered upon single-electron oxidation as indicated by the small RMSD when the two structures are aligned (RMSD = 0.196 Å). The B–O bond lengths of **[1]⁺** are shortened on average by ca. 0.02 Å when compared with those of **1**, suggesting that the B–O bonds are strengthened upon cluster oxidation. The B–B bond lengths show greater variability, suggesting some degree of geometrical distortion upon oxidation. This deviation from idealized icosahedral symmetry is consistent with Jahn-Teller distortion observed crystallographically for the oxidized, D_{3d} symmetric *hypercloso* species when compared with their reduced *hypocloso* and *closo* I_h symmetric analogues.^{1,3,29}



Bond	Bond length (Å)	
	1	[1] ⁺
B–B (type 1)	1.73	1.75; 1.76
B–B (type 2)	1.84; 1.85	1.80; 1.81; 1.82; 1.86; 1.87; 1.89
B–O	1.39	1.37

Figure S25. B3LYP-D3 optimized geometry of **1** and [1]⁺ and key bond lengths in Å. Their structural alignment is given, with [1]⁺ displayed in black/gray superimposed on **1**, which is displayed in pale pink. The naming of B–B bond lengths as “type 1” vs “type 2” is arbitrary.

S9.3. Calculated UV-vis spectra of **1** and [1]⁺

For all UV-vis spectra calculations, we used TD-DFT SMD(DCM)-CAM-B3LYP/6-31+G(d,p)//B3LYP-D3/6-31G(d) with 50 excited states for simulation.

S9.3.1. 1

The main transitions giving rise to the peaks shown in **Figure S26** are given in **Table S1**. All transitions arise from exciting the electrons from the lower occupied orbitals to the LUMO of the molecule (MO # 325). The peak at ~450 nm arises from the transitions from HOMO-5 (MO # 319), HOMO-4 (MO # 320) and HOMO-3 (MO # 321) to the LUMO, as shown in **Table S1**. The selected MOs are given in **Figure S27**. The electron distributions are centered around the B₁₂ cluster and the O-atoms of the cluster and are rarely on the alkyl side chains.

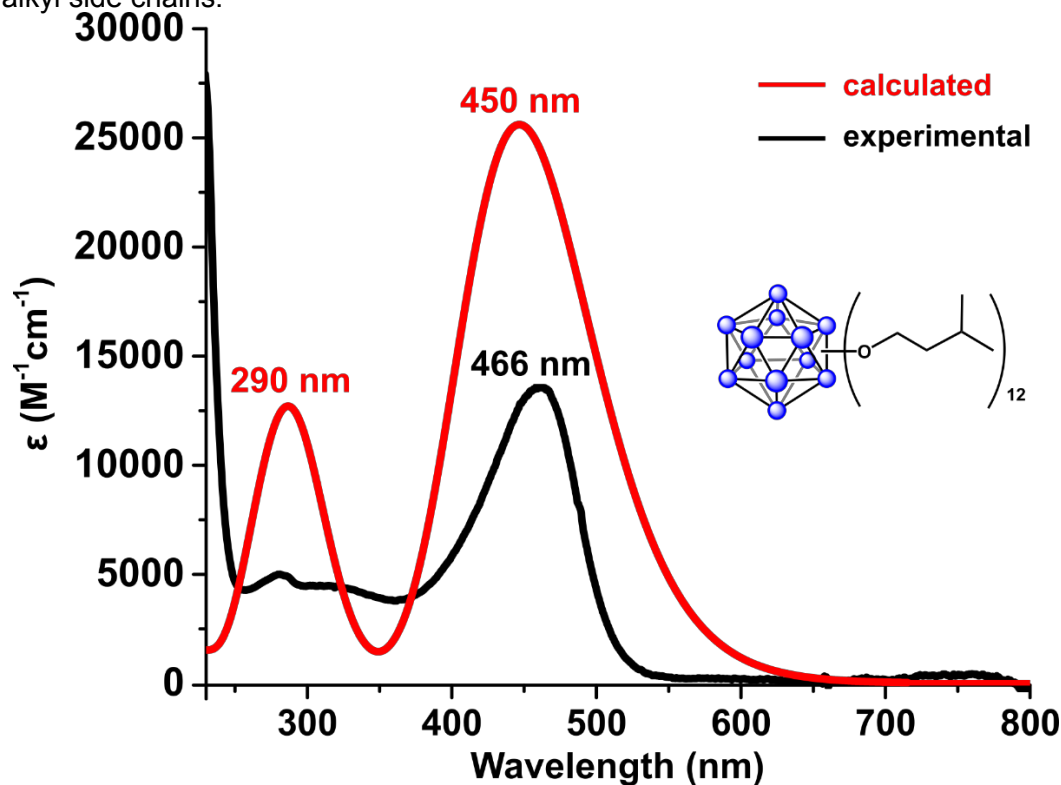


Figure S26. Calculated and experimental (DCM, 80 μM) UV-vis spectra of **1**.

Excited State No.	Excitation Energy / eV	Absorption Wavelength / nm	Oscillator Strength	MO transitions	Contribution
4	2.7313	453.95	0.2002	321 → 325	0.975
5	2.7598	449.24	0.2309	320 → 325	0.974
6	2.8363	437.14	0.2087	319 → 325	0.974
8	4.028	307.8	0.0142	272 → 325 311 → 325 312 → 325 313 → 325 314 → 325 316 → 325 318 → 325	0.043 0.042 0.096 0.043 0.272 0.031 0.336
9	4.155	298.4	0.059	311 → 325 314 → 325 316 → 325 317 → 325 318 → 325	0.022 0.090 0.094 0.380 0.308
11	4.2043	294.9	0.0735	312 → 325 314 → 325 315 → 325 316 → 325 317 → 325	0.027 0.023 0.357 0.476 0.043
12	4.2816	289.58	0.0536	308 → 325 311 → 325 312 → 325 314 → 325 315 → 325 316 → 325 317 → 325	0.031 0.044 0.408 0.274 0.053 0.033 0.036
13	4.3216	286.89	0.0298	310 → 325 312 → 325 313 → 325 314 → 325 315 → 325	0.035 0.029 0.725 0.061 0.020
15	4.4551	278.3	0.034	302 → 325 309 → 325 310 → 325 311 → 325 313 → 325	0.047 0.097 0.543 0.041 0.051
16	4.5389	273.16	0.0128	303 → 325 304 → 325 306 → 325 307 → 325 308 → 325 311 → 325 312 → 325	0.046 0.044 0.424 0.103 0.087 0.032 0.022
18	4.6087	269.02	0.0332	277 → 325 285 → 325 304 → 325	0.039 0.032 0.104

				305 → 325	0.024
				306 → 325	0.081
				307 → 325	0.399
				309 → 325	0.047
				310 → 325	0.060
				311 → 325	0.022
19	4.6673	265.65	0.031	270 → 325	0.026
				271 → 325	0.029
				298 → 325	0.043
				303 → 325	0.050
				304 → 325	0.033
				305 → 325	0.040
				306 → 325	0.081
				307 → 325	0.021
				308 → 325	0.270
				309 → 325	0.158
				311 → 325	0.053
20	4.7035	263.6	0.0198	268 → 325	0.022
				298 → 325	0.042
				300 → 325	0.036
				302 → 325	0.023
				303 → 325	0.026
				304 → 325	0.106
				305 → 325	0.182
				306 → 325	0.022
				307 → 325	0.046
				308 → 325	0.224
				309 → 325	0.022

Table S1. Computed electronic transitions for **1**. Oscillator strengths greater than 0.01 are included. For **1**, MO #325 is the HOMO and MO #324 is the LUMO.

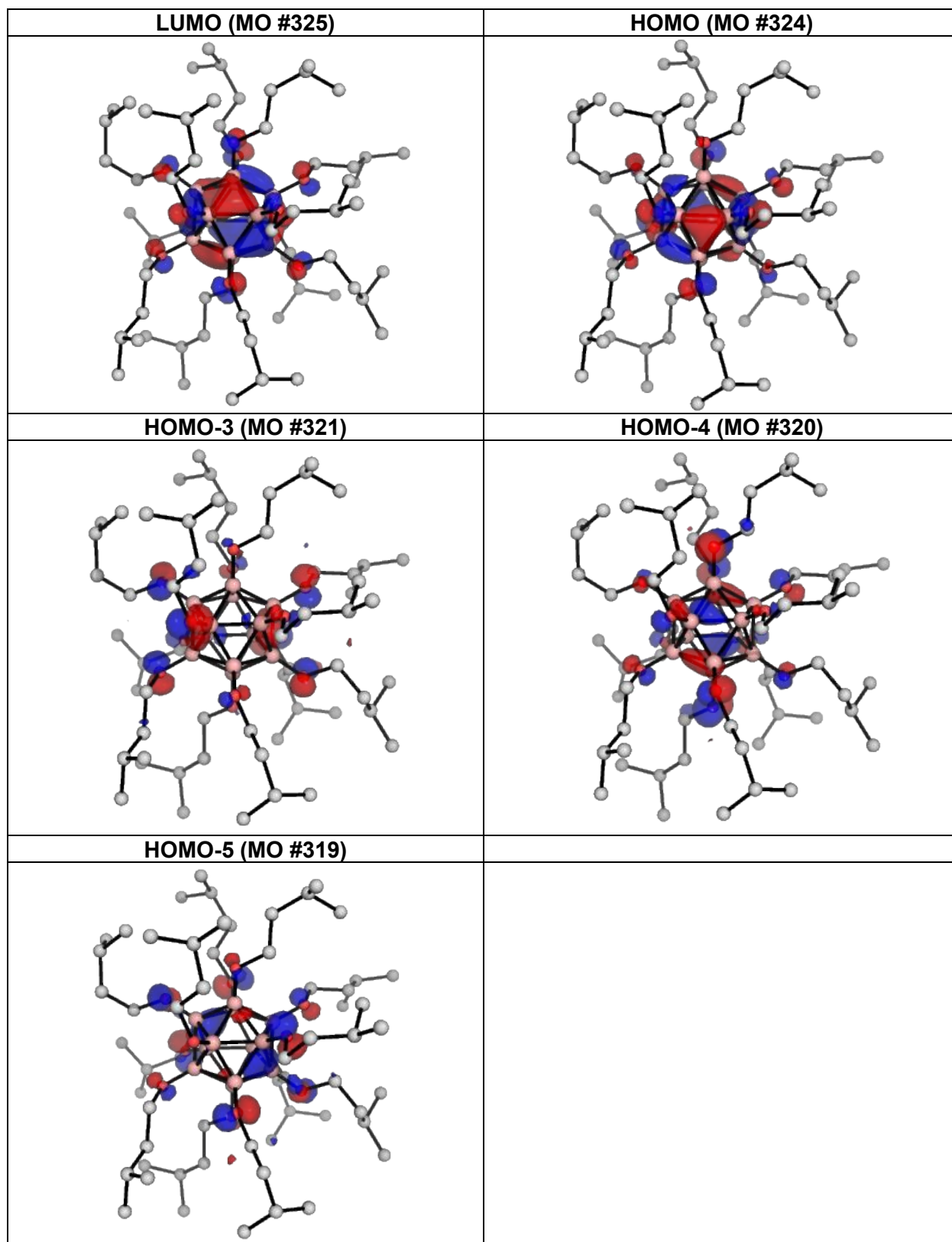


Figure S27. Selected MOs for 1. H-atoms are hidden for clarity.

S9.3.2. [1]⁺

The peaks arise from transitions from the lower occupied MOs to the LUMO (MO #325A) of the α -spin orbitals and the LUMO (MO #324B) and LUMO+1 (MO #325B) of the β -spin orbitals (**Table S2**). The computed transition around 820 nm, which likely corresponds to the experimentally observed peak at 720 nm, arises from the excitations from the ground state to excited states 7, 9 and 10, which result from the excitation of β -electron from MOs #319B, 320B, 321B to β -spin LUMO #324B (**Table S2**). These MOs are shown in **Figure S29**. These suggest that the long-wavelength transition in the [1]⁺ system (inset, **Figure S28**) arise from charge transfer from the periphery (O-atoms) to the B₁₂-core. The peak at around 464 nm arises from the transition from the ground state to the excited states 14, 15 and 16, where both α - and β -electronic transitions occur (the dominant contributions are given in bold in **Table S2**).

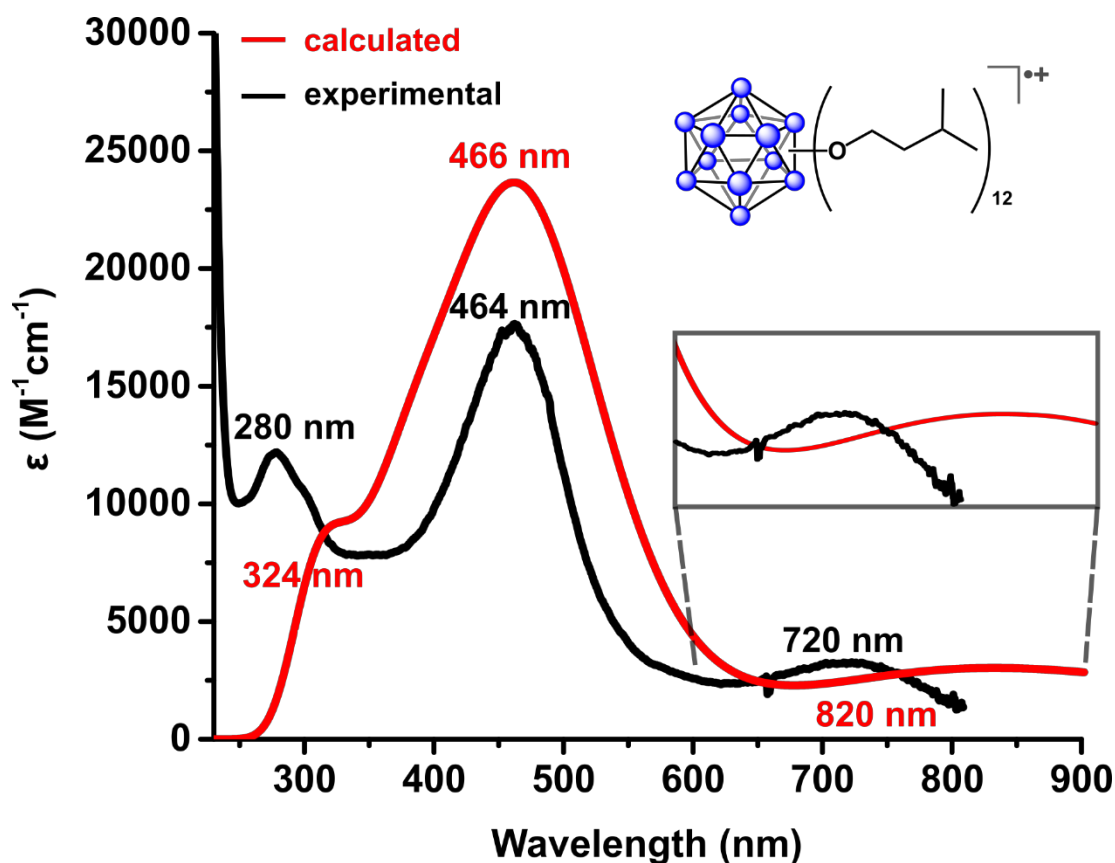


Figure S28. Calculated and experimental (DCM, 70 μM) UV-vis spectra of [1]⁺.

Excited State No.	Excitation Energy / eV	Absorption Wavelength / nm	Oscillator Strength	MO transitions	Contribution
7	1.3921	890.65	0.0337	319A → 325A 321A → 325A 323A → 325A 320B → 325B 321B → 324B 323B → 325B	0.013 0.066 0.017 0.022 0.838 0.015
9	1.4777	839.03	0.0264	320A → 325A 321A → 325A 319B → 324B 320B → 324B	0.055 0.020 0.015 0.864
10	1.6413	755.39	0.0149	320A → 325A 321A → 325A 319B → 324B 320B → 324B 321B → 325B	0.027 0.030 0.765 0.040 0.091
14	2.5497	486.26	0.171	320A → 325A 316B → 324B 320B → 324B 320B → 325B 321B → 325B	0.590 0.010 0.021 0.032 0.279
15	2.5782	480.89	0.2123	319A → 325A 321A → 325A 318B → 324B 319B → 324B 320B → 325B 321B → 325B	0.011 0.501 0.016 0.020 0.365 0.018
16	2.7239	455.18	0.1454	319A → 325A 321A → 325A 316B → 324B 318B → 324B 319B → 325B 321B → 324B	0.459 0.019 0.012 0.060 0.348 0.017
17	3.0231	410.12	0.0802	319A → 325A 276B → 324B 277B → 324B 311B → 324B 312B → 324B 314B → 324B 315B → 324B 317B → 324B 318B → 324B 319B → 325B	0.048 0.019 0.014 0.012 0.027 0.014 0.013 0.229 0.452 0.017
18	3.0785	402.75	0.082	319A → 325A 282B → 324B 307B → 324B 309B → 324B 312B → 324B	0.026 0.022 0.011 0.011 0.011

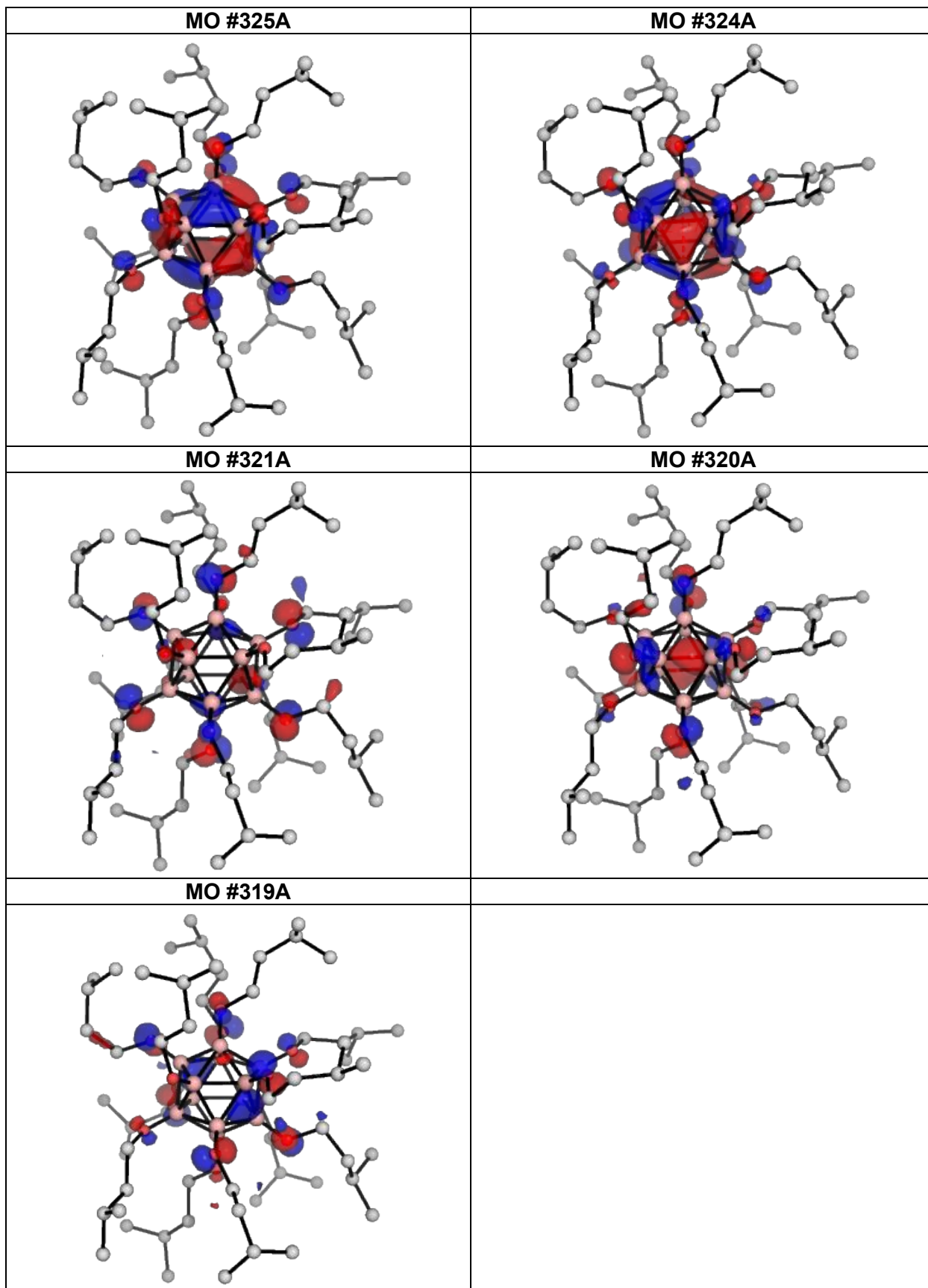
				313B → 324B 315B → 324B 316B → 324B 317B → 324B 318B → 324B 319B → 325B	0.020 0.017 0.089 0.495 0.137 0.011
20	3.2306	383.78	0.0625	320A → 325A 273B → 324B 274B → 324B 278B → 324B 281B → 324B 300B → 324B 302B → 324B 305B → 324B 309B → 324B 312B → 324B 314B → 324B 315B → 324B 316B → 324B 317B → 324B	0.013 0.017 0.014 0.022 0.015 0.015 0.020 0.010 0.011 0.173 0.017 0.244 0.244 0.039
21	3.2598	380.35	0.0261	276B → 324B 278B → 324B 282B → 324B 307B → 324B 309B → 324B 310B → 324B 311B → 324B 313B → 324B 314B → 324B 315B → 324B 318B → 324B	0.016 0.024 0.022 0.017 0.024 0.044 0.047 0.313 0.219 0.036 0.040
22	3.3367	371.58	0.0262	274B → 324B 279B → 324B 281B → 324B 307B → 324B 310B → 324B 312B → 324B 313B → 324B 314B → 324B 315B → 324B 318B → 325B	0.079 0.026 0.038 0.011 0.025 0.053 0.127 0.383 0.053 0.019
23	3.3628	368.69	0.0283	317A → 325A 273B → 324B 276B → 324B 277B → 324B 297B → 324B 299B → 324B 307B → 324B 308B → 324B 309B → 324B	0.012 0.034 0.020 0.041 0.023 0.022 0.046 0.053 0.014

				311B → 324B 312B → 324B 313B → 324B 315B → 324B 316B → 324B 317B → 324B 318B → 324B	0.096 0.108 0.095 0.022 0.155 0.019 0.010
26	3.5227	351.96	0.015	313A → 325A 316A → 325A 317A → 325A 318A → 325A 270B → 324B 305B → 324B 307B → 324B 308B → 324B 312B → 324B 313B → 324B 313B → 325B 314B → 324B 316B → 325B 318B → 325B	0.024 0.034 0.054 0.061 0.016 0.030 0.045 0.034 0.020 0.013 0.021 0.027 0.076 0.191
33	3.7438	331.17	0.0159	312A → 325A 313A → 325A 314A → 325A 315A → 325A 316A → 325A 318A → 325A 274B → 325B 276B → 325B 299B → 324B 304B → 324B 305B → 325B 307B → 325B 309B → 324B 310B → 324B 310B → 325B 313B → 325B 314B → 324B 314B → 325B 315B → 325B 317B → 325B 318B → 325B	0.014 0.035 0.022 0.024 0.061 0.115 0.015 0.019 0.019 0.015 0.011 0.012 0.020 0.028 0.012 0.063 0.011 0.073 0.022 0.030 0.089
36	3.8123	325.22	0.0108	272A → 325A 273A → 325A 277A → 325A 307A → 325A 308A → 325A 311A → 325A 312A → 325A 313A → 325A 314A → 325A	0.011 0.019 0.015 0.036 0.016 0.117 0.031 0.041 0.016

				316A → 325A 317A → 325A 272B → 324B 301B → 324B 304B → 324B 305B → 324B 306B → 324B 310B → 325B 315B → 325B 316B → 325B 317B → 325B	0.011 0.058 0.027 0.040 0.011 0.012 0.019 0.020 0.028 0.151 0.024
42	3.9195	316.33	0.0107	310A → 325A 311A → 325A 312A → 325A 316A → 325A 317A → 325A 272B → 324B 290B → 324B 295B → 324B 296B → 324B 298B → 324B 299B → 324B 300B → 324B 307B → 325B 309B → 324B 312B → 325B 314B → 325B 317B → 325B 318B → 325B	0.014 0.020 0.026 0.188 0.026 0.045 0.020 0.033 0.040 0.038 0.012 0.015 0.011 0.010 0.049 0.013 0.059 0.026
44	3.9597	313.12	0.0323	307A → 325A 312A → 325A 313A → 325A 315A → 325A 316A → 325A 318A → 325A 270B → 324B 273B → 324B 274B → 324B 275B → 324B 299B → 324B 300B → 324B 301B → 324B 302B → 324B 303B → 324B 305B → 324B 308B → 324B 313B → 325B 315B → 325B 316B → 325B 318B → 325B	0.023 0.021 0.021 0.053 0.024 0.024 0.021 0.012 0.011 0.011 0.011 0.011 0.030 0.013 0.040 0.043 0.073 0.067 0.133 0.041 0.027
45	3.9679	312.47	0.0169	278A → 325A	0.012

				279A → 325A	0.017
				307A → 325A	0.032
				309A → 325A	0.011
				312A → 325A	0.010
				313A → 325A	0.070
				314A → 325A	0.068
				315A → 325A	0.054
				316A → 325A	0.037
				317A → 325A	0.050
				318A → 325A	0.028
				293B → 324B	0.011
				299B → 324B	0.029
				303B → 324B	0.012
				305B → 325B	0.010
				307B → 325B	0.041
				309B → 325B	0.013
				312B → 325B	0.012
				313B → 325B	0.013
				314B → 325B	0.030
				315B → 325B	0.042
				316B → 325B	0.056
				317B → 325B	0.062
				318B → 325B	0.011
47	4.0086	309.29	0.0598	308A → 325A	0.019
				312A → 325A	0.019
				313A → 325A	0.026
				314A → 325A	0.088
				315A → 325A	0.027
				318A → 325A	0.057
				275B → 324B	0.015
				293B → 324B	0.011
				301B → 324B	0.015
				305B → 324B	0.118
				307B → 325B	0.019
				308B → 324B	0.010
				313B → 325B	0.121
				314B → 325B	0.055
				315B → 325B	0.033
318B → 325B	0.039				

Table S2. Computed electronic transitions for [1]²⁺. Oscillator strengths greater than 0.01 are included. A denotes α -MO; B denotes β -MO, a β -electron is removed from MO #324 of **1**, such that MO #324A is the SOMO of [1]²⁺.



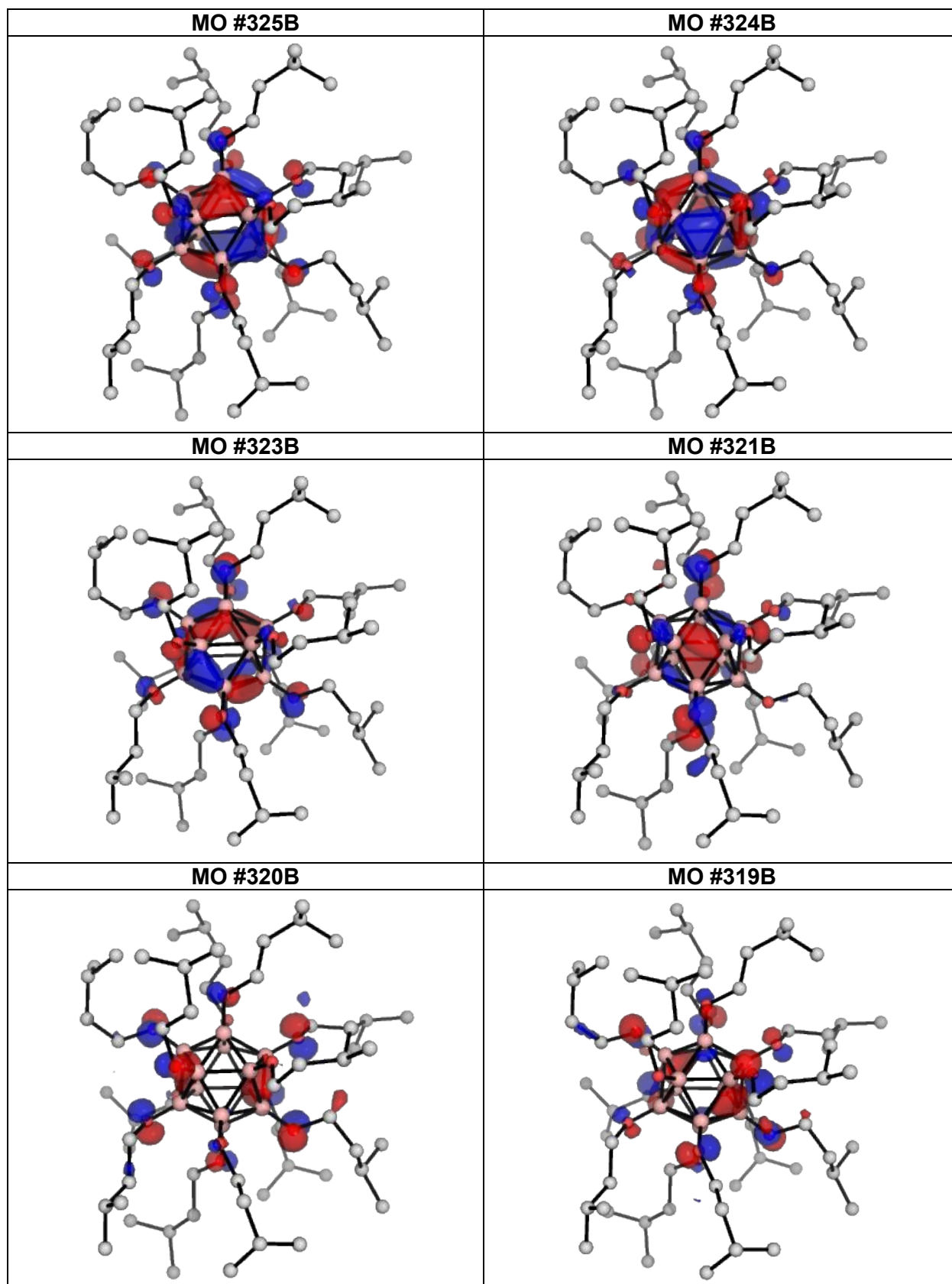


Figure S29. Selected MOs for $[1]^{*+}$. H-atoms are hidden for clarity.

S9.4. Electrostatic potential (ESP) of **1** and spin density plot of $[1]^{+\bullet}$

The electrostatic potential (ESP) of **1** and the spin density of the $[1]^{+\bullet}$ are displayed in **Figure S30**. In *hypercloso-1*, the B₁₂-core is positively charged, with the negative charge is localized on the O-atoms. This is perhaps unsurprising given that the oxygen atom is more electronegative than the boron atom. For $[1]^{+\bullet}$, the unpaired electron/radical is mostly delocalized over the electronegative O atoms and the B₁₂-cluster core, as shown by the spin density plot.

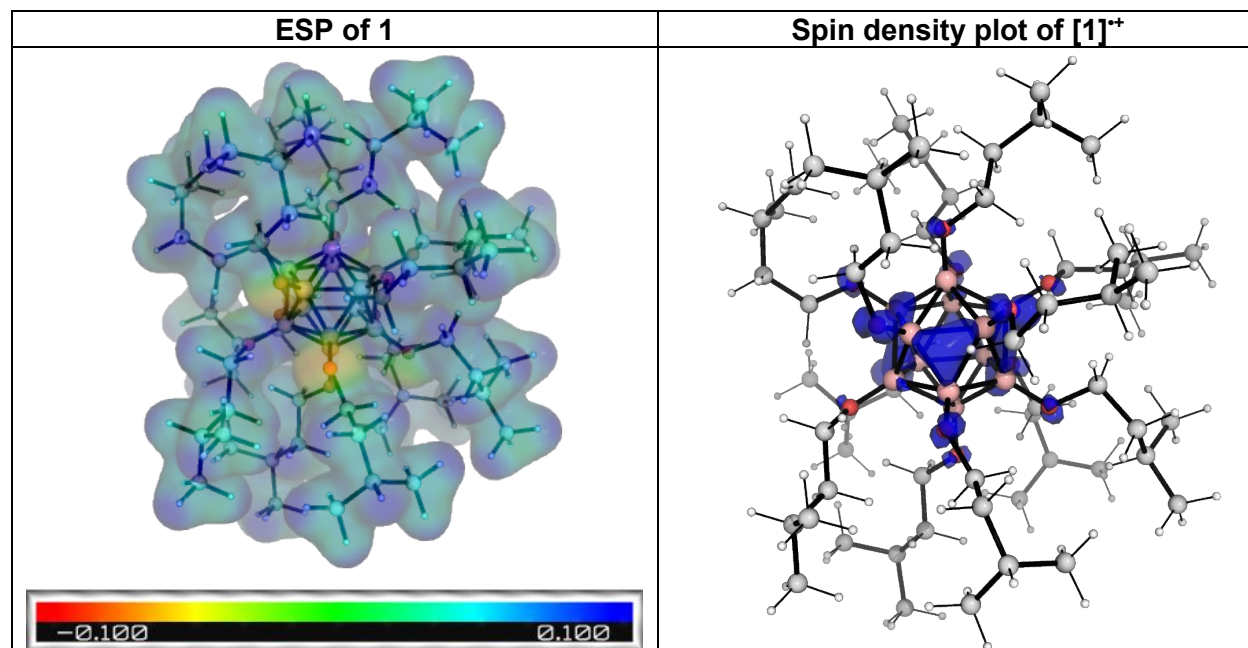
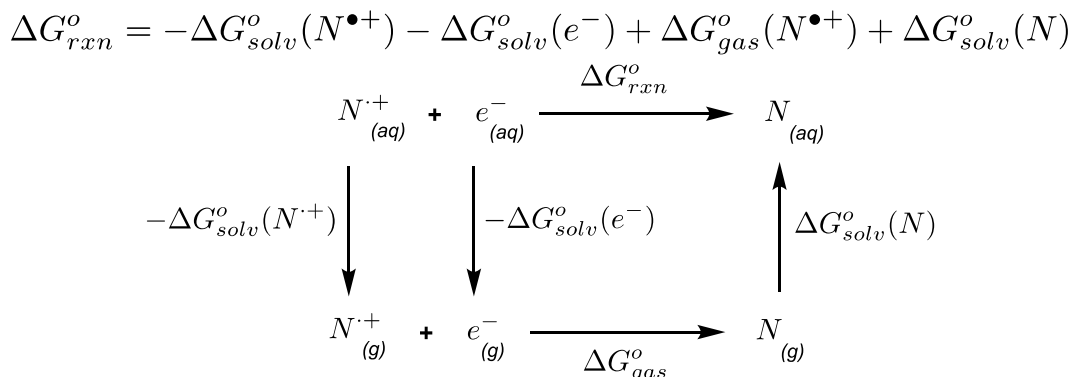


Figure S30. Electrostatic potential (ESP; isovalue of 0.02) of **1** and spin density plot (isovalue of 0.005) of $[1]^{+\bullet}$.

S9.5. [1]^{0/+} redox potential calculation

We estimated the adiabatic reduction potential of [1]⁺ by constructing a thermodynamic cycle (**Scheme S1**) and using separate gas phase geometry optimizations with single point solvation energy of each *optimized* species (thus the name adiabatic). The overall Gibbs energy of reaction ΔG_{rxn}^o is expressed in terms of the free energy of reaction in the gas phase, ΔG_{gas}^o , and the free energies of solvation, ΔG_{solv}^o , of the reacting species:^{30,31}



Scheme S1. Computation of the potential for the reduction of [1]⁺ to **1**.

The reduction potential of the reaction is then given by:

$$E_{cell} = -\frac{\Delta G_{rxn}^o}{nF} - E_{SHE}$$

where E_{SHE} is the reference potential of the standard hydrogen electrode. We need not consider the free energy of solvation of the electron as their contribution cancels out when we consider the full reaction against experimentally measured values.³¹ Using this thermodynamic cycle, we found that the absolute redox potential of the [1]^{0/+} couple to be 5.25 V. Together with the absolute redox potential of the ferrocene/ferrocenium (Fc/Fc⁺) redox couple of 4.8 ± 0.1 V in dichloromethane,³² we estimate that the redox potential of the [1]^{0/+} couple to be 0.45 ± 0.1 V in dichloromethane (*cf.* experimental value of 0.62 V, **Figure S10**).

S9.6. ¹¹B NMR chemical shift calculation of **1**

The ¹¹B NMR chemical shift of **1** was calculated. We adopted SMD(chloroform)-B3LYP/def2-SVP//B3LYP-D3/6-31G(d) level of theory as this gives good agreement with experimental measurements for a variety of boron-containing compounds.^{24,25} The computed ¹¹B NMR isotropic shielding tensor value of 113.8 ppm for the reference compound BF₃·OEt₂ was used as a reference. Averaging the peaks for all boron atoms in **1** gives a final ¹¹B NMR chemical shift of 34.8 ppm (*cf.* experimental value of 41.4 ppm, **Figure S2**). The difference of 6.6 ppm is considered a good agreement due to the wide chemical shift range of >200 ppm for ¹¹B NMR.

S9.7. Absolute energies from the optimized structures

Absolute values (in Hartrees) for SCF energy, zero-point vibrational energy (ZPE), enthalpy and quasi-harmonic Gibbs free energy (at 298K) for optimized structures are given below. Single point (SP) corrections in SMD dichloromethane using B3LYP-D3 functional are also included.

Structure	E/au	ZPE/au	H/au	G/au	qh-G/au	SP
1	-3567.927079	1.950308	-3565.8692	-3566.1275	-3566.0986	-3565.3931
[1] ⁺⁺	-3567.695672	1.9482	-3565.6388	-3565.9023	-3565.8718	-3565.1956

S9.8. Coordinates of the optimized structures

S9.8.1. 1

	x	y	z
B	0.78966	0.29457	1.56052
O	1.52345	0.73771	2.65876
B	-0.65409	-0.63701	1.77972
O	-1.04347	-1.00634	3.05892
B	0.65572	1.32397	0.03899
O	1.29784	2.55215	-0.07690
C	0.61316	3.79824	0.07167
H	0.03242	3.79455	0.99936
H	-0.10358	3.91446	-0.74786
C	1.64893	4.91151	0.09080
H	2.28828	4.76743	0.97099
H	1.12466	5.86790	0.23271
B	1.58340	-0.13589	-0.04365
O	2.96689	-0.07365	-0.19213
C	3.73462	-1.23397	-0.51703
H	3.66491	-1.41151	-1.59877
H	3.31602	-2.10776	-0.01411
C	5.18000	-0.99000	-0.11465
H	5.48507	-0.01266	-0.50844
H	5.24353	-0.92211	0.98056
B	-0.92645	-1.73942	0.30798
B	-1.04323	1.03255	-0.60624
O	-1.56610	-2.96459	0.43135
O	-1.74857	2.05105	-1.23854
C	-2.00740	2.00801	-2.64610
H	-2.97835	1.52154	-2.80836
H	-1.25094	1.39955	-3.14134
C	-2.02117	3.42848	-3.19041
H	-2.88989	3.96115	-2.78292
H	-1.13173	3.95311	-2.81841
B	-1.85001	-0.28339	0.40227
B	-0.81808	1.07139	1.10903
O	-3.23082	-0.33542	0.56569
O	-1.42627	2.07870	1.84744
B	0.78445	-1.45249	0.96125
B	-1.04559	-0.70583	-1.20947
O	1.50426	-2.47327	1.56649
O	-1.77443	-1.08230	-2.33194
C	1.83618	-2.48112	2.95806
C	-2.89195	-1.96853	-2.26324
H	1.44688	-3.41859	3.37773
H	-3.41242	-1.84595	-1.31127
H	1.35088	-1.65055	3.47107
H	-2.52045	-3.00022	-2.30945
C	3.35264	-2.42805	3.10038
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H	2.81593	-0.22909	-4.09253
H	1.95838	-3.55504	-4.54513
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C	-3.32434	-0.62736	3.80749
H	-3.08491	-0.33619	4.83995
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H	-5.82008	-0.24729	0.07635
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C	-1.64764	-5.27238	1.14014
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H	-1.67494	-4.96565	2.19434
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C	4.53715	2.77848	3.74176
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C	4.73512	3.78910	2.60210
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H	8.30037	-2.43559	-0.66665
H	7.85934	-0.71745	-0.69705
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H	2.87361	-4.22278	-1.70976
C	4.09476	-4.90800	-3.33551
H	4.53330	-5.75035	-2.78796
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S9.8.2. [1]⁺

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C	3.45884	-2.12031	3.19046
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C	2.23046	-3.51031	-3.33326
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H	2.92418	-2.67292	-3.48890
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C	4.02393	-2.28719	4.60997
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H	5.82570	-1.11903	4.24203
C	3.39699	-1.30648	5.60925
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H	2.89510	1.68737	4.60053
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H	-5.15469	-3.63364	-1.47331
H	-6.09866	-2.26412	-2.08259

S10. References

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