

**Supporting Information:** Tris(carbene)borates; New alternatives to cyclopentadienyls in organolanthanide chemistry

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Open Data are available for this manuscript as a Mendeley Data set doi: [10.17632/3ymr2wv4p3.1](https://doi.org/10.17632/3ymr2wv4p3.1)

## General information

All moisture and air sensitive materials were manipulated using standard high-vacuum Schlenk-line techniques and MBraun gloveboxes and stored under an atmosphere of dried and deoxygenated argon. All glassware items, cannulae and Fisherbrand 1.2  $\mu\text{m}$  retention glass microfibre filters were dried in a 160  $^{\circ}\text{C}$  oven overnight before use. Hexanes, tetrahydrofuran (THF), diethyl ether ( $\text{Et}_2\text{O}$ ) and toluene for use with moisture and air sensitive compounds were dried using an MBRAUN SPS 800 Manual solvent purification system and stored over activated 3  $\text{\AA}$  molecular sieves. Benzene- $d_6$  was purchased from Cambridge Isotope Laboratories and were refluxed over potassium metal for 24 hours, freeze-pump-thaw degassed and purified by trap-to-trap distillation prior to use. THF- $d_8$  was purchased from Cambridge Isotope Laboratories and dried over sodium/benzophenone before being freeze-pump-thaw degassed and purified by trap-to-trap distillation prior to use. Methylene dichloride- $d_2$  was purchased from Cambridge Isotope Laboratories and dried over calcium hydride and purified by trap-to-trap distillation before use. All solvents were purchased from Sigma-Aldrich or Fisher Scientific and stored over 3  $\text{\AA}$  molecular sieves for 4 hours before being used.  $\text{CeI}_3(\text{thf})_4$ ,  $\text{YbI}_3(\text{thf})_{1.5}$ , lithium diisopropyl amide,  $\text{KC}_8$  and phenylborontrimethylimidazolium ditriflate ( $[\text{C}_3\text{H}_3]_2[\text{OTf}]$ ) were prepared according to literature methods.<sup>1-4</sup> All other chemicals were purchased from commercial suppliers and degassed and/or dried under vacuum or over 3  $\text{\AA}$  molecular sieves for 12 hours before use. NMR spectra were recorded on Bruker Avance 400 or 500 MHz spectrometers and are referenced to residual protio solvent (3.58 and 1.72 ppm for THF- $d_8$ , 7.16 ppm for benzene- $d_6$ , 5.32 for dichloromethane- $d_2$ ) for  $^1\text{H}$  NMR spectroscopy. Chemical shifts are quoted in ppm. NMR spectra were measured at 25 $^{\circ}\text{C}$  unless otherwise noted. Elemental analyses were carried out by the microanalytic services in the College of Chemistry at the University of California, Berkeley. 10 mm pathlength quartz cells with Teflon lined screw caps were used for collecting photophysical data of all air sensitive compounds: the samples were prepared under an argon atmosphere for electronic absorption spectra (UV-Vis). UV-Vis measurements were collected on an Agilent Varian Cary 50 UV-Vis spectrophotometer. Single crystal X-ray diffraction data of all other compounds were collected using a Rigaku Xtalab Synergy-S diffractometer fitted with a HyPix-6000HE photon counting detector using  $\text{MoK}\alpha$  ( $\lambda = 0.71073 \text{ \AA}$ ) or  $\text{CuK}\alpha$  ( $\lambda = 0.15418 \text{ \AA}$ ) radiation. All structures were solved using SHELXT in Olex2 and refined using SHELXL in Olex2.<sup>13, 5, 6</sup> Absorption corrections were completed using CrysAlis PRO (Rigaku Oxford Diffraction) software. Analytical numeric absorption corrections used a multifaceted crystal model based on expressions derived by Clark and Reid.<sup>7</sup> Numerical absorption correction was based on a Gaussian integration over a multifaceted crystal model.

## Synthetic Methods and Characterisation

### Li[C3]

Prepared via a minor modification of a previously reported method.<sup>8</sup> To a stirred suspension of phenylborontrimethylimidazolium ditriflate ( $[\text{C}_3\text{H}_3]_2[\text{OTf}]$ ) (1.0 g, 1.75 mMol) in diethyl ether, 10 mL, was added 3.3 equivalents of lithium diisopropyl amide (0.62 g, 5.8 mMol) with stirring. The suspension was stirred for 2 hours until the supernatant liquors were yellow/brown and a fine powdery pale tan precipitate formed. The mixture was left to stand at -35 $^{\circ}\text{C}$  overnight, then the supernatant was removed by decantation. The remaining pale tan precipitate was washed once with diethyl ether (5 mL) and twice with hexane (5 mL); each time after allowing the precipitate to settle by storage at -35 $^{\circ}\text{C}$  for at least one

hour. The precipitate was dried under vacuum to yield **Li[C3]** as a white to tan powder (0.52 g, 0.15 mmol, 88 % yield). This crude product was used in preparing the metal complexes.

$^1\text{H}$  NMR (400 MHz, THF)  $\delta$  7.44-7.23 (m, 5H, Ar-CH), 6.68 (s, 6H, Im-CH), 3.09 (s, 9H, Im-Me).

$^{11}\text{B}$  NMR (400 MHz, THF)  $\delta$  0.6 (s, br).

### **Ce(C3)<sub>2</sub>I**

$\text{CeI}_3(\text{thf})_{2.2}$  (100 mg, 0.15 mmol) and **Li[C3]** (100 mg, 0.15 mmol) were suspended in thf (5 mL) with stirring. After approximately 5 minutes all solid material had dissolved and a yellow-orange solution formed. Diethyl ether (6 mL) was added dropwise until a grey precipitate formed. The reaction mixture was filtered through a glass microfiber filter pipette. The solution was concentrated to 2 mL and a few drops of diethyl ether were added. This mixture was allowed to stand until orange crystals of **Ce(C3)<sub>2</sub>I** formed; these were isolated from the solution by filtration and dried under vacuum (94 mg, 0.10 mmol, 69 % yield).

### **NMR:**

$^1\text{H}$  NMR (500 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  16.39 (4H, Ar-CH), 16.21 (6H, Im-CH), 10.93 (2H, Ar-CH), 10.22 (4H, Ar-CH), 6.91 (6H, Im-CH), 3.59 (2H, thf  $\text{CH}_2$ ), 1.43 (2H, thf  $\text{CH}_2$ ), -13.66 (18H, Im-Me).

$^{11}\text{B}$  NMR (160 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  44.35 (s, br).

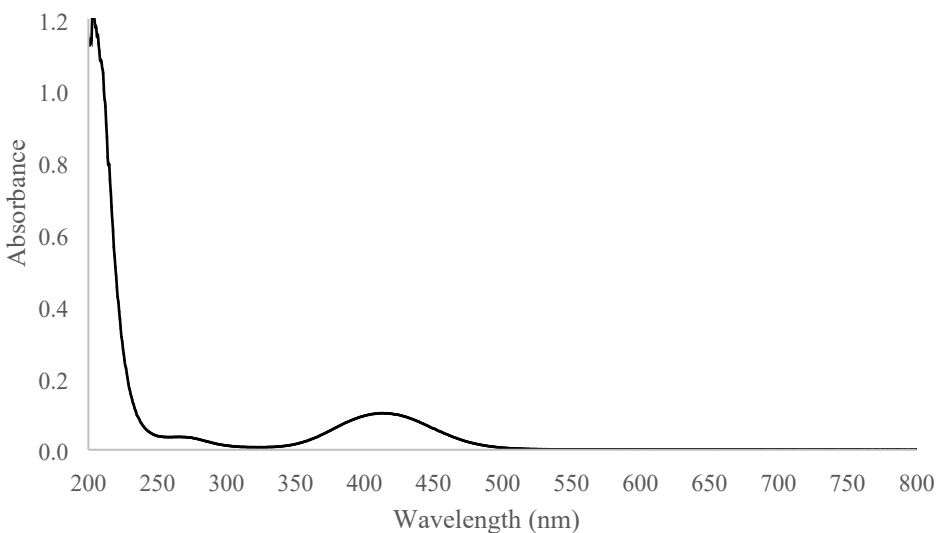
### **Elemental analysis (CHN):**

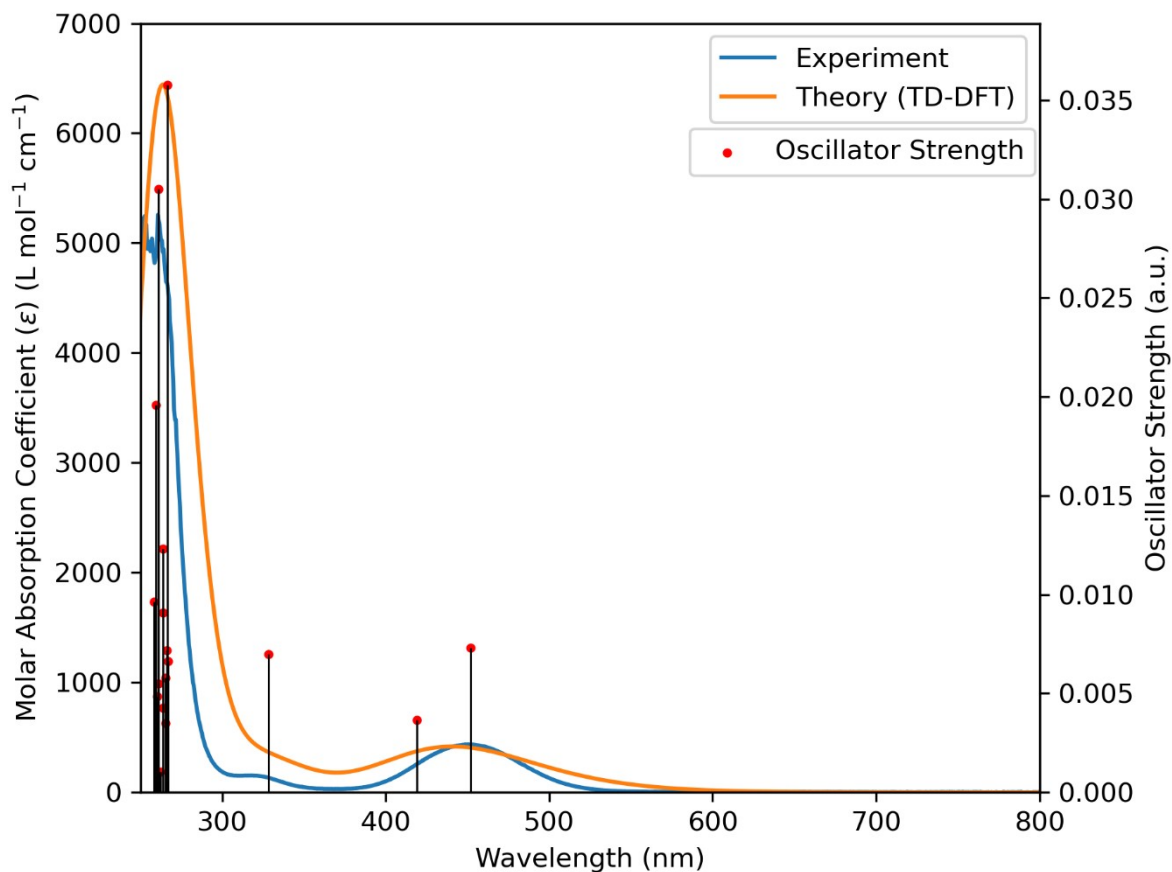
Expected: C 46.52 %; H 4.34 %; N 18.08 %,

Found: C 46.76 %; H 4.61 %; N 17.83 %.

### **UV-Vis:**

$\lambda_{\text{max}}$ : 452nm,  $\epsilon = 440 \text{ molL}^{-1}\text{cm}^{-1}$

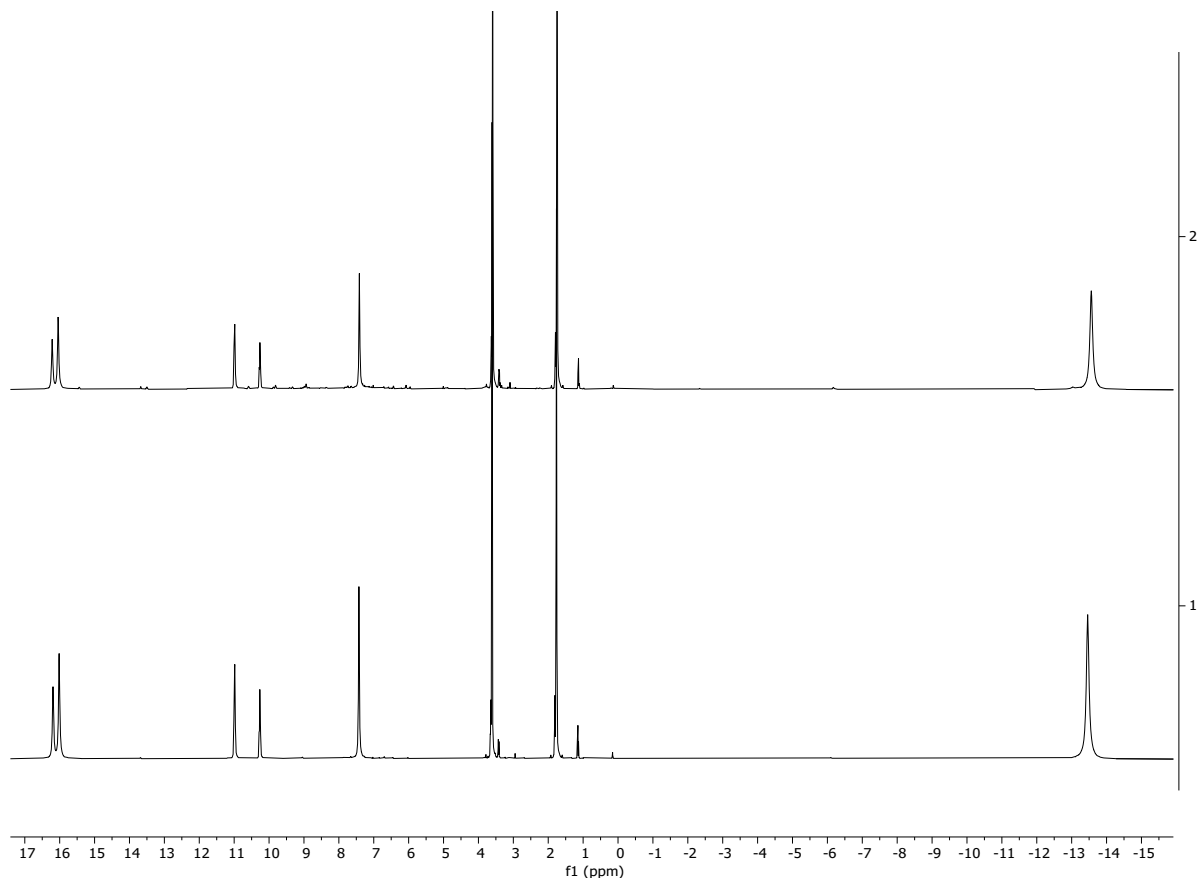




**Figure S1:** Comparison of calculated (orange) and experimental (blue) UV-Vis absorption spectra for  $\text{Ce}(\text{C3})_2\text{I}$

**Thermal stability study of  $\text{Ce}(\text{C3})_2\text{I}$  complex:**

$\text{Ce}(\text{C3})_2\text{I}$  (10mg, 0.011 mmol) was dissolved in  $\text{thf-d}_8$  (0.4 mL) in a Young's tap sealed NMR tube to give an orange-yellow solution. The resulting solution was heated to  $66^\circ\text{C}$  for 8 hours after which time a  $^1\text{H-NMR}$  spectrum was collected; no degradation was evident in the spectrum at this point (Spectrum 1, Figure 2). The sample was heated for a further 72 hours. Very minor degradation was observed to have occurred after this time (Spectrum 2, Figure 2).



**Figure S2:**  $^1\text{H}$ -NMR spectra (400 MHz, 300K) of a sample of  $\text{Ce}(\text{C}_3)_2\text{I}$  in  $\text{thf-d}_8$  after heating for 8 hours at  $66^\circ\text{C}$  (spectrum 1) and after 80 hours at  $66^\circ\text{C}$  (spectrum 2).

### **$[\text{Li}(\text{thf})_4][\text{CeC}_3\text{I}_3]$**

$\text{CeI}_3(\text{thf})_{2.2}$  (100 mg, 0.15 mmol) and  $\text{Li}[\text{C}_3]$  (50 mg, 0.15 mmol) were suspended in thf (5 mL) with stirring. After two hours the resulting yellow solution was concentrated to approx. 1 mL in volume and toluene (1 mL) was added. The solution was filtered and stored at  $-35^\circ\text{C}$  overnight, resulting in crystallization of yellow needles suitable for single crystal X-ray diffraction. This solid was isolated via filtration and dried under vacuum, yielding  $[\text{Li}(\text{thf})_4][\text{CeC}_3\text{I}_3]$  (111 mg, 0.10 mMol, 66% yield).

#### **NMR:**

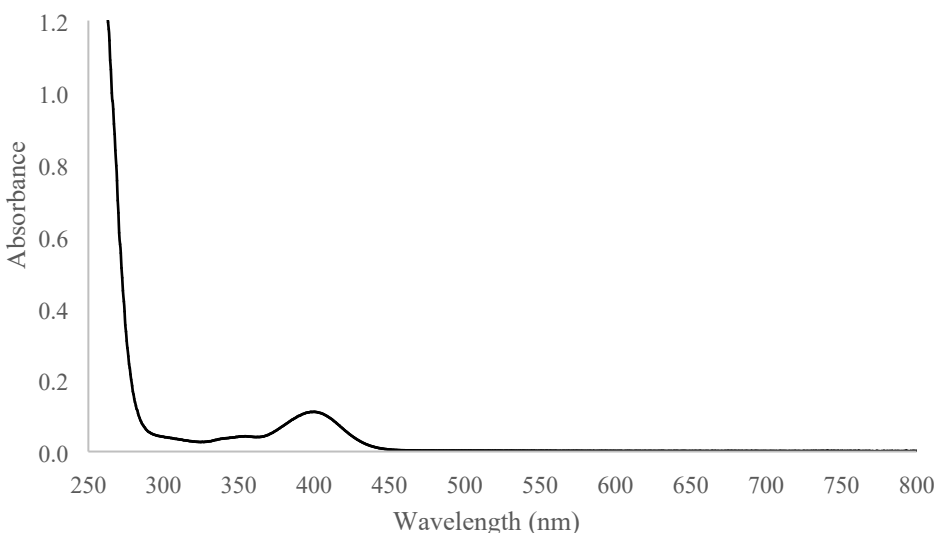
$^1\text{H}$  NMR (500 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  15.49 (2H, Ar- $\text{CH}$ ), 13.96 (3H, Im- $\text{CH}$ ), 10.56 (2H, Ar- $\text{CH}$ ), 9.85 (1H, Ar- $\text{CH}$ ), 5.92 (16H, thf  $\text{CH}_2$ ), 5.75 (Im- $\text{CH}$ ), 2.57 (16H, thf  $\text{CH}_2$ ), -11.36 (9H, Im-Me).

$^{11}\text{B}$  NMR (160 MHz,  $\text{C}_6\text{D}_6$ )  $\delta$  -37.8 (s, br).

#### **Elemental analysis (CHN):**

Expected ( $[\text{Li}(\text{thf})_4][\text{CeC}_3\text{I}_3] \cdot 0.5(\text{C}_7\text{H}_8)$ ): C 38.60 %; H 4.82 %; N 6.93 %,

Found: C 38.30 %; H 4.74 %; N 6.44 %. Low in N, potentially due to boron nitride formation.

**UV-Vis:** $\lambda_{\text{max}}$ : 400 nm,  $\epsilon = 1050 \text{ molL}^{-1}\text{cm}^{-1}$ **Ce(C3)<sub>2</sub>bipy**

**Ce(C3)<sub>2</sub>I** (100mg, 0.11 mMol) was dissolved in thf (5 mL), to which K[bipy] (21 mg, 0.13 mMol) was added: the solution was observed to change color from orange to a deep red. The mixture was stirred for 2 hours, and then allowed to stand for 72 hours, during which time a white precipitate formed. The mixture was filtered, then concentrated to approximately 1 mL in volume, followed by addition of toluene (3 mL). After standing overnight, the reaction was again filtered and concentrated *in vacuo* to incipient crystallization. Upon standing at room temperature overnight a crop of an extremely air and moisture sensitive deep red microcrystalline solid was observed to have formed (48mg, 0.05 mMol, 46% yield). Crystals suitable for X-ray diffraction were grown from thf/toluene solutions of **Ce(C3)<sub>2</sub>bipy**.

**NMR:**

<sup>1</sup>H-NMR (400MHz, thf-d<sub>8</sub>): 15.11 (9H Im-Me), 13.53 (3H Im-CH), 11.83 (9H, Im-Me), 10.76 (3H Im-CH), 8.21 (3H Im-CH), 8.19 (3H Im-CH), 8.10 (2H, bipy-CH), 8.01 (2H, bipy-CH), 7.70 (10H, overlapping Ar-CH), 5.19 (2H, bipy-CH), -0.19 (2H, bipy-CH).

<sup>11</sup>B-NMR (128MHz, thf-d<sub>8</sub>):  $\delta$  1.7 (s, br).

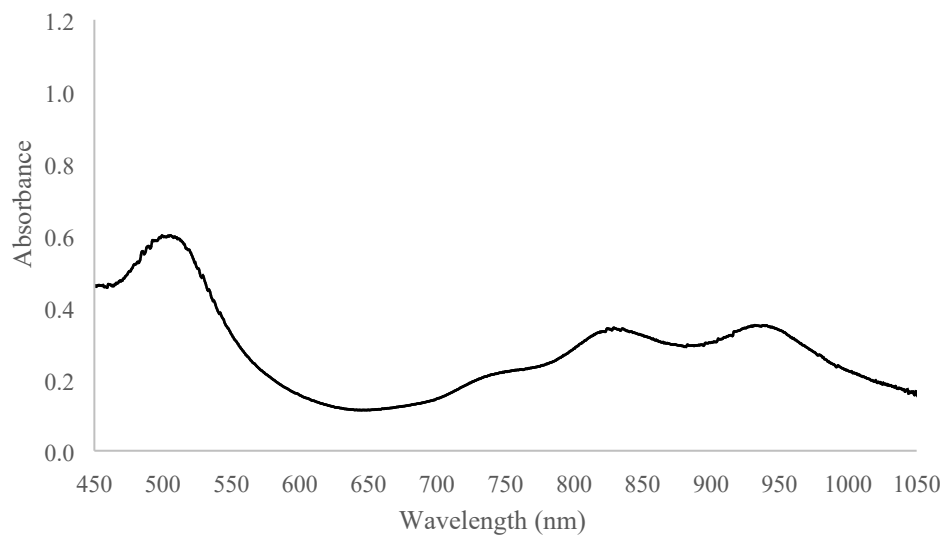
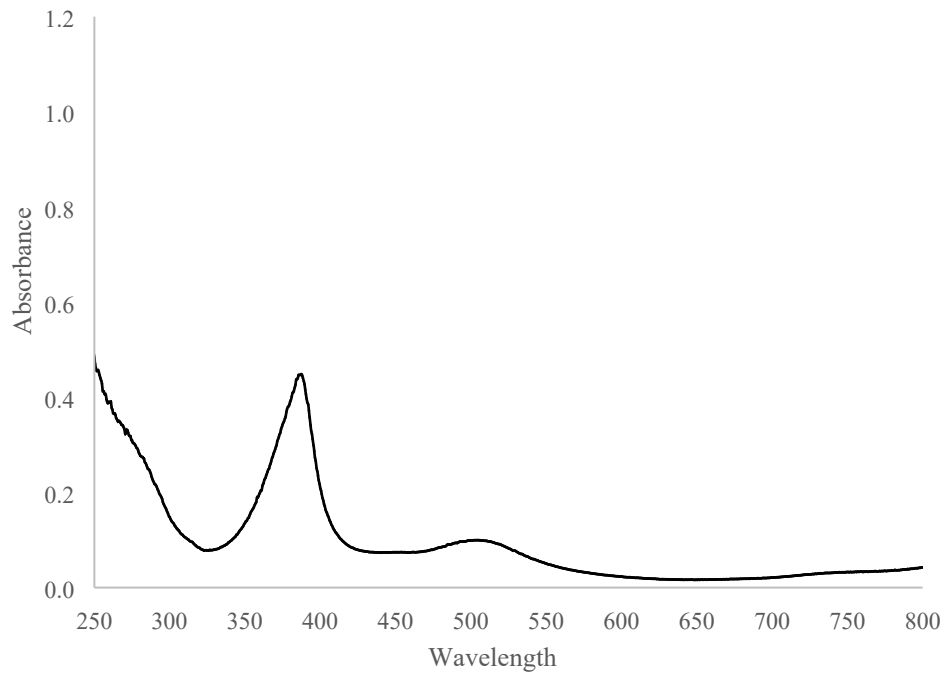
**Elemental Analysis (CHN, Ce(C3)<sub>2</sub>bipy.thf):**

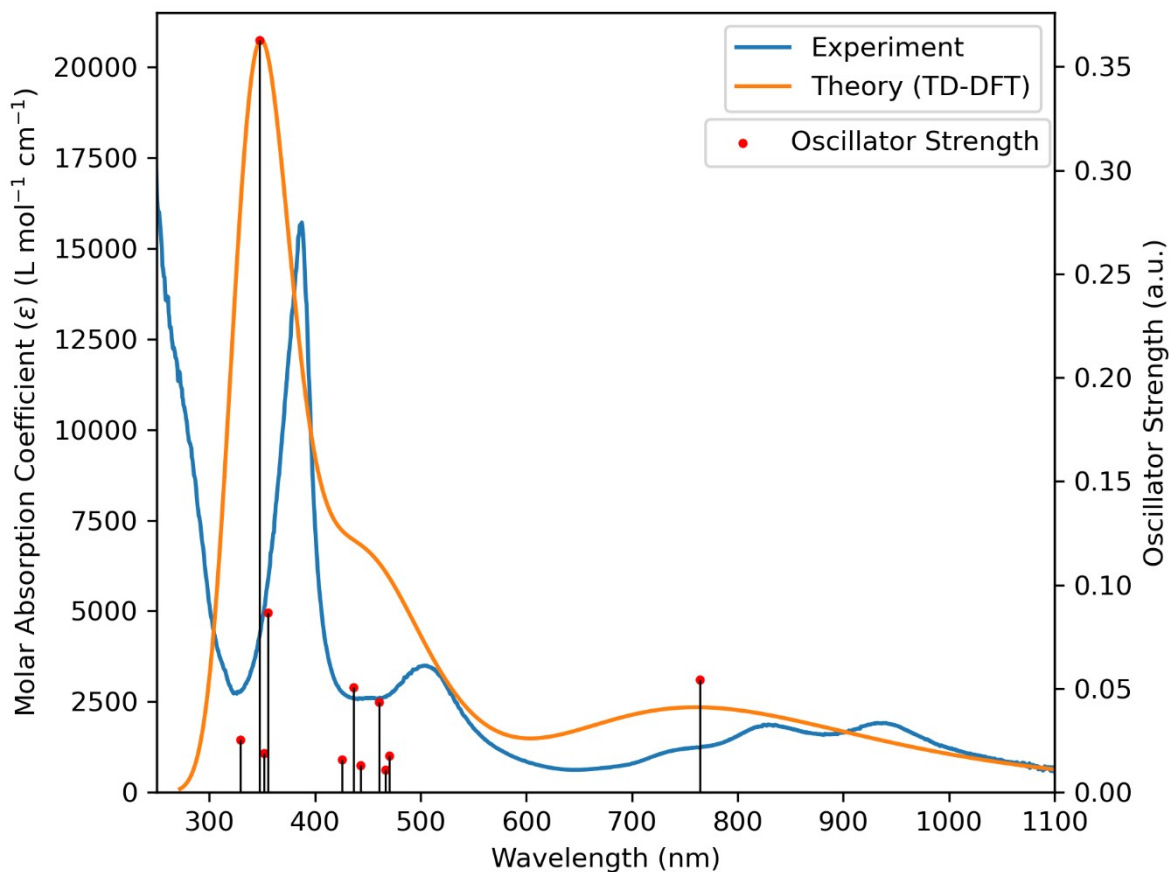
Expected: C, 58.26%; H, 5.48%; N, 19.02%.

Found: C, 58.01%; H, 5.08%; N, 18.64%.

**UV-Vis:**

Absorptions were observed at 937, 835, 758, 506 and 387nm with respective  $\epsilon$  values of: 1910, 1860, 1170, 3490 and 15700 mol<sup>-1</sup>Lcm<sup>-1</sup>.





**Figure S3:** Comparison of calculated (orange) and experimental (blue) UV-Vis absorption spectra for  $\text{Ce}(\text{C}3)_2\text{bipy}$

#### Testing the lability of the Ce – bound [C3] ligand:

The addition of two equivalents of  $\text{Li}[\text{C}3]$  (5.2 mg, 0.16 mmol) to  $\text{CeI}_3\text{thf}_{2.2}$  (5 mg, 0.0078 mmol) in thf (0.4 mL) led to the formation of a pale-orange/yellow solution almost immediately. A range of  $^1\text{H-NMR}$  resonances are observed for this solution between 16.2–13.6 ppm by no-D  $^1\text{H-NMR}$  corresponding to  $\text{Ce}(\text{C}3)_2\text{I}$ . The addition of a further equivalent of  $\text{CeI}_3\text{thf}_{2.2}$  (5 mg, 0.0078 mmol) rapidly results in the formation of the pale yellow solution associated with  $[\text{Li}(\text{thf})_4][\text{Ce}(\text{C}3)_3\text{I}_3]$ ; corresponding resonances between 14.8 and -10.4 ppm in the  $^1\text{H-NMR}$  spectrum were observed. This can be reversed through the addition of a further equivalent of  $\text{Li}[\text{C}3]$  (5.2 mg, 0.16 mmol) again over a period of minutes, giving  $\text{Ce}(\text{C}3)_2\text{I}$  ( $^1\text{H-NMR}$  signals again observed between 16.2-13.6 ppm).

#### $\text{Yb}(\text{C}3)_2\text{I}$

$\text{Li}[\text{C}3]$  (0.24 g, 0.71 mmol) was added to  $\text{YbI}_3(\text{thf})_{2.5}$  (0.25 g, 0.35 mmol) in thf (7 mL); the resulting suspension was stirred at room temperature for 30 minutes, then left to stand for one hour, after which time dme (5 mL) was added, giving an off-white solid. The reaction was filtered, retaining the solid. The solid was extracted into dcm (4 mL) to remove salts and swiftly filtered (slow degradation of the desired



product occurs in dcm), followed by removal of the solvent *in vacuo*. The resulting solid (0.11 g, 0.11 mmol, 33% yield) was determined to be  $[\text{Yb}(\text{C3})_2]\text{I}$ . Colorless single crystals suitable for X-ray diffraction could be grown directly from small scale reactions of  $\text{Li}[\text{C3}]$  (9 mg, 0.026 mmol) and  $\text{YbI}_3(\text{thf})_{2.5}$  (10 mg, 0.014 mmol) in thf (0.4 mL) that were allowed to stand overnight.

#### NMR:

$^1\text{H}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  31.15 (18H, Im-Me), 9.39 (6H, Im-CH), 2.30 (2H, Ar-CH), 1.03 (4H, Ar-CH), -5.64 (Im-CH), -7.57(4H, Ar-CH).

$^{11}\text{B}$  NMR (128 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  -74.88 (s, br).

#### Elemental Analysis (CHN):

Expected: C, 44.93%; H, 4.19%; N, 17.47%.

Found: C, 44.72%; H, 4.14%; N, 17.21%.

#### Reaction to target $\text{Yb}(\text{C3})_2$

To  $\text{YbI}_2(\text{thf})_4$  (10 mg, 0.014 mmol) and  $\text{Li}[\text{C3}]$  (10 mg, 0.028 mmol) was added thf (2 mL), with stirring. The resulting solution (a dark purple red) was stirred for 10 minutes until all material had dissolved. The solution was left to stand overnight: the solution was observed to have changed color over this time to colorless, and colorless crystals had formed, alongside a grey powder. The crystals were found to be  $\text{Yb}(\text{C3})_2\text{I}$  by checking the unit cell.

### SAMBVCA 2.1 steric profile analysis of $\text{Tp}^*$ vs C3 in $[\text{YbL}_2]\text{X}$ complexes

The SAMBVCA applet 2.1 was used to estimate the volume that one  $[\text{C3}]^-$  or  $\text{Tp}^*$  ligand occupies around a Yb(III) ion within a sphere of 3.5 Å radius, centered on the metal centre (%V\_Bur).<sup>9</sup> Coordinates for the ligands were taken from complexes of the structure  $[\text{YbL}_2]\text{X}$  where X is an outersphere anion ( $\text{I}^-$ ,  $\text{OTf}^-$ ) and L =  $\text{Tp}^*$  or C3). The coordinates used for the  $\text{Tp}^*$  ligand for Yb were taken from CCDC structure 1234400<sup>10</sup> and are given below while the coordinates for the  $[\text{C3}]^-$  ligand were taken from the structure reported here for  $\text{Yb}[\text{C3}]_2\text{I}$ . All default parameters in the SAMBVCA applet were used as found, unless otherwise stated.

#### Method:

- 1) The coordinate file was loaded into the applet.
- 2) Yb was set as the centre of the sphere
- 3) The z-axis was defined by clicking on Yb (0) and B(10) for the  $\text{Tp}^*$  ligand, and Yb(0) and B(24) for the C3 ligand.
- 4) The xz-plane was defined by clicking on Yb(0), N(1), N(4) and B(10) for the  $\text{Tp}^*$  ligand, and Yb(0), C(16), N(4) and B(24) for the C3 ligand.
- 5) The Yb(0) atom was deleted.
- 5) The Bondi van der Waals radii were scaled by 1.17 (applet default).

6) The sphere radius was set to 3.5 Å (applet default).

7) The distance of the coordination point from the centre of the sphere was set to 0.

8) The mesh spacing for numerical integration was set to 0.10 (applet default) and the job was then submitted to the applet

**Coordinates for Tp\* ligand coordinated to a Yb center:**

Yb	0.00000	0.00000	0.00000
N	-1.12302	-1.47920	1.36293
N	-1.12302	1.47920	1.36293
N	-2.02999	-0.00000	-1.17934
N	-2.45884	-1.26183	1.59460
C	-0.85579	-2.70412	1.87523
N	-2.45884	1.26183	1.59460
C	-0.85579	2.70412	1.87523
N	-3.18095	-0.00000	-0.45548
C	-2.40137	-0.00000	-2.44960
B	-3.16448	0.00000	1.09454
C	-2.96951	-2.31587	2.21094
C	-1.97754	-3.22772	2.39278
C	0.53073	-3.24139	1.78344
C	-2.96951	2.31587	2.21094
C	-1.97754	3.22772	2.39278
C	0.53073	3.24139	1.78344
C	-4.22540	-0.00000	-1.28862
C	-3.76094	-0.00000	-2.54314
C	-1.39184	-0.00000	-3.56075
C	-4.40848	-2.41840	2.56675
C	-4.40848	2.41840	2.56675
C	-5.63128	-0.00000	-0.81478

**Coordinates for C3 ligand on Yb center:**

Yb	7.06785	9.57488	24.83233
N	4.20741	8.39311	23.15215
N	5.05289	12.19330	24.94739
N	8.35993	11.55311	22.18477
N	4.36213	10.54054	23.13130
N	6.31861	12.05851	22.69632
N	5.63085	11.96712	27.01124
C	3.38689	8.81831	22.13786
C	3.88599	13.14976	22.87994
C	3.49470	10.16708	22.11421
C	2.50349	12.95426	23.00862
C	4.30025	13.08905	25.70590
C	4.30224	14.43585	22.49387
C	6.63703	12.70572	21.51646
C	9.67655	10.93220	22.17074
C	5.87940	11.48210	25.76564
C	4.83428	9.43067	23.76192
C	7.38668	11.30369	23.11767
C	4.38509	6.98144	23.51617
C	7.91173	12.40130	21.20777
C	4.65860	12.94834	26.99520
C	1.58315	13.95697	22.71597
C	3.38190	15.43154	22.17475
C	2.03034	15.19528	22.28139
B	4.90316	12.00153	23.39269
C	6.32060	11.51958	28.21435

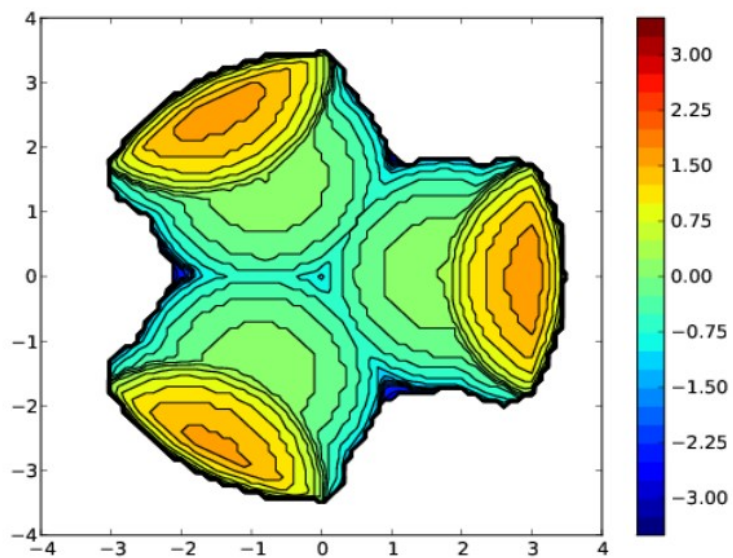
Results of the SAMBVCA 2.1 analysis:

For  $Yb^{III}(Tp^*)$ :

%V Free	%V Buried	% V Tot/V Ex
52.1	47.9	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	21.1	23.8	44.9	47.0	53.0
NW	20.6	24.2	44.9	46.0	54.0
NE	25.7	19.1	44.9	57.4	42.6
SE	26.1	18.8	44.9	58.1	41.9

Steric Map

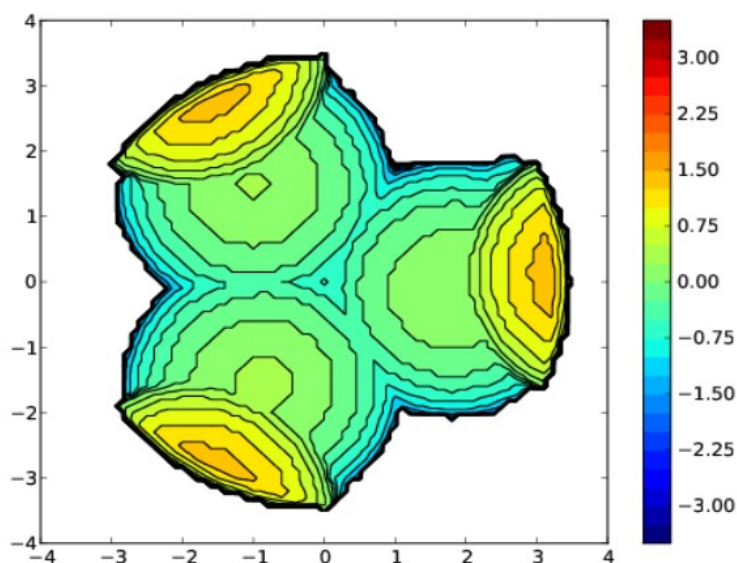


### For Yb[C3]<sub>2</sub>I:

%V Free	%V Buried	% V Tot/V Ex
53.5	46.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	21.9	22.9	44.9	48.9	51.1
NW	21.5	23.4	44.9	47.9	52.1
NE	26.9	18.0	44.9	59.9	40.1
SE	25.8	19.1	44.9	57.4	42.6

**Steric Map**



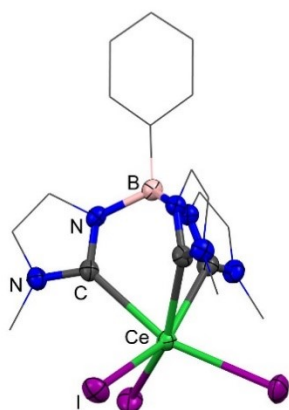
The percent buried volume (%VBur) of the Tp\* ligand around the Yb(III) center is calculated to be 47.9 %VBur, while that for C3 around a Yb(III) center is 46.5 %VBur, showing the similar steric bulk of the two ligand sets. The maps showing the distribution of steric bulk around the metal center are also similar for Tp\* and C3, with the distribution of steric bulk being similar in each of the 4 quadrants around the metal center within a sphere of 3.5 Å radius.

## Crystallography

Cifs are deposited with the CCDC with codes 2235950-2235953.

### Additional information for the structure of $[\text{Li}(\text{thf})_4][\text{Ce}(\text{C3})\text{I}_3]$ .

$[\text{Li}(\text{thf})_4][\text{Ce}(\text{C3})\text{I}_3]$  crystallizes as an ion pair in the  $P2_1/c$  space group with  $Z=4$  (Figure 2). The Ce-C distances range between 2.591(3) to 2.662(3) Å, which are comparable to the distances observed for the Ce-C bonds in  $\text{Ce}(\text{C3})_2\text{I}$  (range 2.631(2)-2.781(2) Å). The Ce-I distances range from 3.1324(3) to 3.1428(3) Å for  $[\text{Li}(\text{thf})_4][\text{Ce}(\text{C3})\text{I}_3]$ , which are slightly shorter than that seen in  $\text{Ce}(\text{C3})_2\text{I}$  (3.2951(2) Å), presumably due to reduced steric hindrance about Ce.



**Figure S4:** Solid-state structure of  $[\text{Li}(\text{thf})_4][\text{Ce}(\text{C3})\text{I}_3]$ ; thf-coordinated lithium counterion and disordered co-crystallized toluene omitted for clarity. Phenyl and backbone carbons set respectively to wireframe and capped sticks; hydrogens are omitted for clarity. C= grey, Ce= green, N=blue B=pink, I=purple.

### Crystallographic data tables

Compound	$\text{Ce}(\text{C3})_2\text{I}$
Empirical formula	$\text{C}_{36}\text{H}_{40}\text{B}_2\text{N}_{12}\text{ICe}$
Formula weight	929.44
Temperature/K	100.00(11)
Crystal system	monoclinic
Space group	$P2_1/n$
$a/\text{Å}$	8.61860(10)
$b/\text{Å}$	21.6975(3)
$c/\text{Å}$	20.3758(3)
$\alpha/^\circ$	90
$\beta/^\circ$	92.7150(10)
$\gamma/^\circ$	90
Volume/ $\text{Å}^3$	3806.04(9)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.622
$\mu/\text{mm}^{-1}$	2.051
$F(000)$	1844.0
Crystal size/ $\text{mm}^3$	$0.3 \times 0.16 \times 0.06$
Radiation	Mo $K\alpha$ ( $\lambda = 0.71073$ )
$2\theta$ range for data collection/ $^\circ$	4.002 to 52.74

<i>Index ranges</i>	-10 ≤ h ≤ 10, -27 ≤ k ≤ 27, -25 ≤ l ≤ 25
<i>Reflections collected</i>	79661
<i>Independent reflections</i>	7779 [R <sub>int</sub> = 0.0425, R <sub>sigma</sub> = 0.0191]
<i>Data/restraints/parameters</i>	7779/0/475
<i>Goodness-of-fit on F<sup>2</sup></i>	1.051
<i>Final R indexes [I ≥ 2σ (I)]</i>	R <sub>1</sub> = 0.0217, wR <sub>2</sub> = 0.0481
<i>Final R indexes [all data]</i>	R <sub>1</sub> = 0.0265, wR <sub>2</sub> = 0.0498
<i>Largest diff. peak/hole / e Å<sup>-3</sup></i>	0.87/-0.53

<b>Compound</b>	<b>[Yb(C3)<sub>2</sub>]I</b>
<i>Empirical formula</i>	C <sub>36</sub> H <sub>40</sub> B <sub>2</sub> IN <sub>12</sub> Yb
<i>Formula weight</i>	962.36
<i>Temperature/K</i>	100.00(13)
<i>Crystal system</i>	orthorhombic
<i>Space group</i>	Pbcm
<i>a/Å</i>	9.98200(10)
<i>b/Å</i>	21.9170(2)
<i>c/Å</i>	40.0903(3)
<i>α/°</i>	90
<i>β/°</i>	90
<i>γ/°</i>	90
<i>Volume/Å<sup>3</sup></i>	8770.78(14)
<i>Z</i>	8
<i>ρ<sub>calc</sub>/cm<sup>3</sup></i>	1.458
<i>μ/mm<sup>-1</sup></i>	9.771
<i>F(000)</i>	3784.0
<i>Crystal size/mm<sup>3</sup></i>	0.16 × 0.115 × 0.052
<i>Radiation</i>	Cu Kα (λ = 1.54184)
<i>2θ range for data collection/°</i>	8.068 to 148.996
<i>Index ranges</i>	-12 ≤ h ≤ 12, -27 ≤ k ≤ 17, -50 ≤ l ≤ 48
<i>Reflections collected</i>	160321
<i>Independent reflections</i>	9095 [R <sub>int</sub> = 0.0580, R <sub>sigma</sub> = 0.0211]
<i>Data/restraints/parameters</i>	9095/0/477
<i>Goodness-of-fit on F<sup>2</sup></i>	1.044
<i>Final R indexes [I ≥ 2σ (I)]</i>	R <sub>1</sub> = 0.0408, wR <sub>2</sub> = 0.0951
<i>Final R indexes [all data]</i>	R <sub>1</sub> = 0.0425, wR <sub>2</sub> = 0.0962
<i>Largest diff. peak/hole / e Å<sup>-3</sup></i>	1.29/-0.91

<b>Compound</b>	<b>[Li(thf)<sub>4</sub>][Ce(C3)I<sub>3</sub>]</b>
<i>Empirical formula</i>	C <sub>41</sub> H <sub>60</sub> BCeI <sub>3</sub> LiN <sub>6</sub> O <sub>4</sub>
<i>Formula weight</i>	1239.52
<i>Temperature/K</i>	100.00(10)
<i>Crystal system</i>	monoclinic
<i>Space group</i>	P2 <sub>1</sub> /c
<i>a/Å</i>	11.0280(2)

<i>b/Å</i>	13.4919(2)
<i>c/Å</i>	33.1783(6)
<i>α/°</i>	90
<i>β/°</i>	98.164(2)
<i>γ/°</i>	90
<i>Volume/Å<sup>3</sup></i>	4886.53(15)
<i>Z</i>	4
<i>ρ<sub>calc</sub>/g/cm<sup>3</sup></i>	1.685
<i>μ/mm<sup>-1</sup></i>	2.870
<i>F(000)</i>	2420.0
<i>Crystal size/mm<sup>3</sup></i>	0.32 × 0.225 × 0.077
<i>Radiation</i>	Mo Kα (λ = 0.71073)
<i>2θ range for data collection/°</i>	3.264 to 52.738
<i>Index ranges</i>	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -41 ≤ l ≤ 41
<i>Reflections collected</i>	102572
<i>Independent reflections</i>	10000 [R <sub>int</sub> = 0.0482, R <sub>sigma</sub> = 0.0222]
<i>Data/restraints/parameters</i>	10000/1204/767
<i>Goodness-of-fit on F<sup>2</sup></i>	1.030
<i>Final R indexes [I &gt; 2σ (I)]</i>	R <sub>1</sub> = 0.0295, wR <sub>2</sub> = 0.0676
<i>Final R indexes [all data]</i>	R <sub>1</sub> = 0.0378, wR <sub>2</sub> = 0.0720
<i>Largest diff. peak/hole / e Å<sup>-3</sup></i>	1.98/-1.44

<b>Complex</b>	<b>Ce(C3)<sub>2</sub>bipy</b>
<i>Empirical formula</i>	C <sub>53</sub> H <sub>56</sub> B <sub>2</sub> CeN <sub>14</sub>
<i>Formula weight</i>	1050.85
<i>Temperature/K</i>	100.00(10)
<i>Crystal system</i>	monoclinic
<i>Space group</i>	P2 <sub>1</sub> /c
<i>a/Å</i>	27.31031(17)
<i>b/Å</i>	8.65621(4)
<i>c/Å</i>	22.48352(12)
<i>α/°</i>	90
<i>β/°</i>	109.4313(7)
<i>γ/°</i>	90
<i>Volume/Å<sup>3</sup></i>	5012.44(5)
<i>Z</i>	4
<i>ρ<sub>calc</sub>/g/cm<sup>3</sup></i>	1.393
<i>μ/mm<sup>-1</sup></i>	7.422
<i>F(000)</i>	2160.0
<i>Crystal size/mm<sup>3</sup></i>	0.422 × 0.085 × 0.064
<i>Radiation</i>	Cu Kα (λ = 1.54184)
<i>2θ range for data collection/°</i>	6.864 to 149.008
<i>Index ranges</i>	-33 ≤ h ≤ 33, -10 ≤ k ≤ 10, -28 ≤ l ≤ 28
<i>Reflections collected</i>	187985

<i>Independent reflections</i>	10234 [ $R_{\text{int}} = 0.0665$ , $R_{\text{sigma}} = 0.0202$ ]
<i>Data/restraints/parameters</i>	10234/385/703
<i>Goodness-of-fit on <math>F^2</math></i>	1.053
<i>Final R indexes [<math>I &gt; 2\sigma(I)</math>]</i>	$R_1 = 0.0236$ , $wR_2 = 0.0633$
<i>Final R indexes [all data]</i>	$R_1 = 0.0245$ , $wR_2 = 0.0639$
<i>Largest diff. peak/hole / <math>e \text{ \AA}^{-3}</math></i>	0.77/-0.78

## Computational Methods and Additional Information

All quantum chemistry computations were performed using the unrestricted B3LYP<sup>11-13</sup> hybrid density functional augmented with Grimme's D4<sup>14, 15</sup> dispersion scheme using the Orca 5.0.3<sup>16</sup> program package. The tetrahydrofuran (THF) solvent environment was modeled using the SMD<sup>17</sup> implicit solvent scheme. The metal complex geometries were optimized using the double zeta Karlsruhe basis set, def2-SVP<sup>18, 19</sup> on the ligand atoms and the corresponding triple zeta basis (def2-TZVP<sup>18, 19</sup>) on the metal center, which automatically assigns def2-ECP<sup>20</sup> pseudopotential for the core electrons of the heavier elements (viz., Yb, Ce, and I in the present work). To obtain accurate electronic energies (and hence, binding energies), single-point energy calculations were performed on the optimized structures with the triple zeta basis set, def2-TZVP, on all the atoms. The metal-ligand bonding character was analyzed using various QTAIM<sup>21</sup> metrics, which were computed using the Multiwfn<sup>22</sup> software. Furthermore, accurate partial atomic charges were computed using the natural population analysis (NPA) scheme implemented within the NBO 7.0<sup>23</sup> framework. The theoretical UV-Vis spectra for DFT-optimized Ce complexes were simulated using the time-dependent density functional theory (TD-DFT) method incorporating 50 excited states utilizing the B3LYP-D4/def2-TZVP level of theory and the implicit THF solvation scheme. The TD-DFT computed UV-Vis spectra were analyzed using the Multiwfn package.

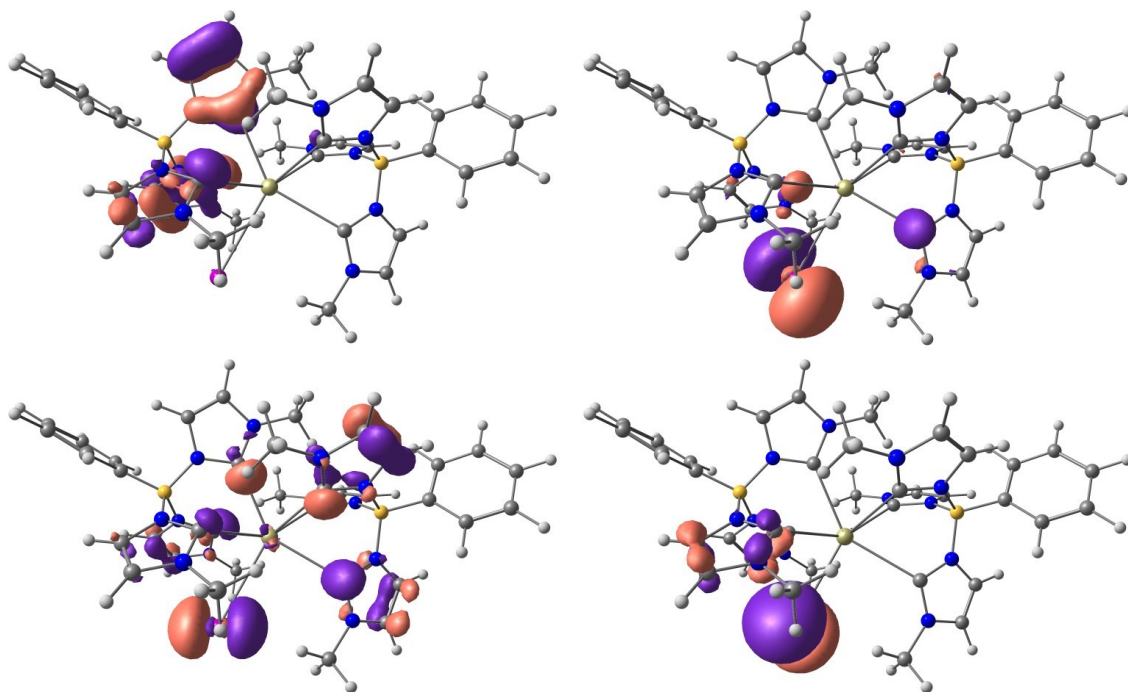
**Table S1.** QTAIM and NPA charges for the metal atoms in the optimized lanthanide borate systems

Complex	Metal atom	QTAIM Charges	NPA Charges (From NBO)
Ce(C3) <sub>2</sub> I	Ce	2.01	1.34
Ce(C3) <sub>2</sub> (bipy)	Ce	2.04	1.32
Ce(Tp*) <sub>2</sub> (bipy)	Ce	2.19	1.73
[Yb(C3) <sub>2</sub> ]I	Yb	2.10	1.63
[Yb(Tp*) <sub>2</sub> ]I	Yb	2.24	1.96

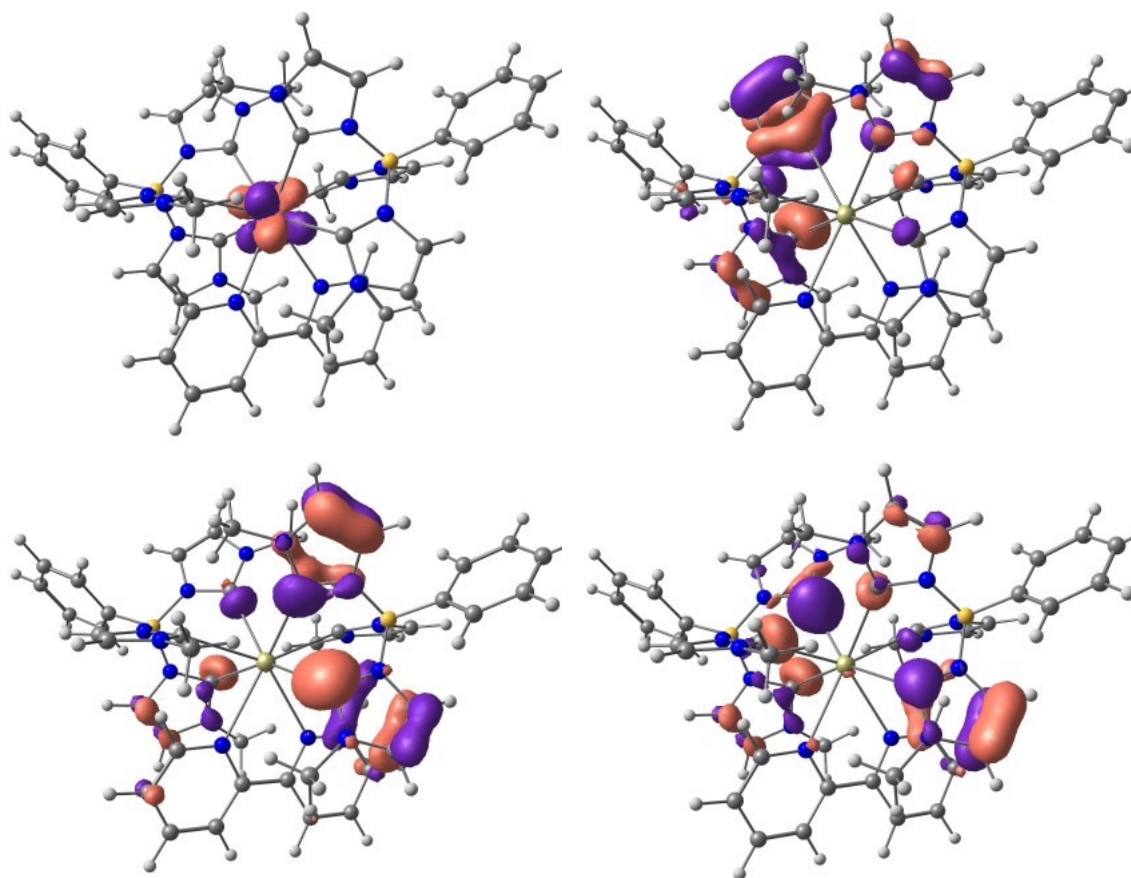


## (HOMO-1) Alpha to (HOMO-4) Alpha Molecular Orbitals for Lanthanide Borate Complexes

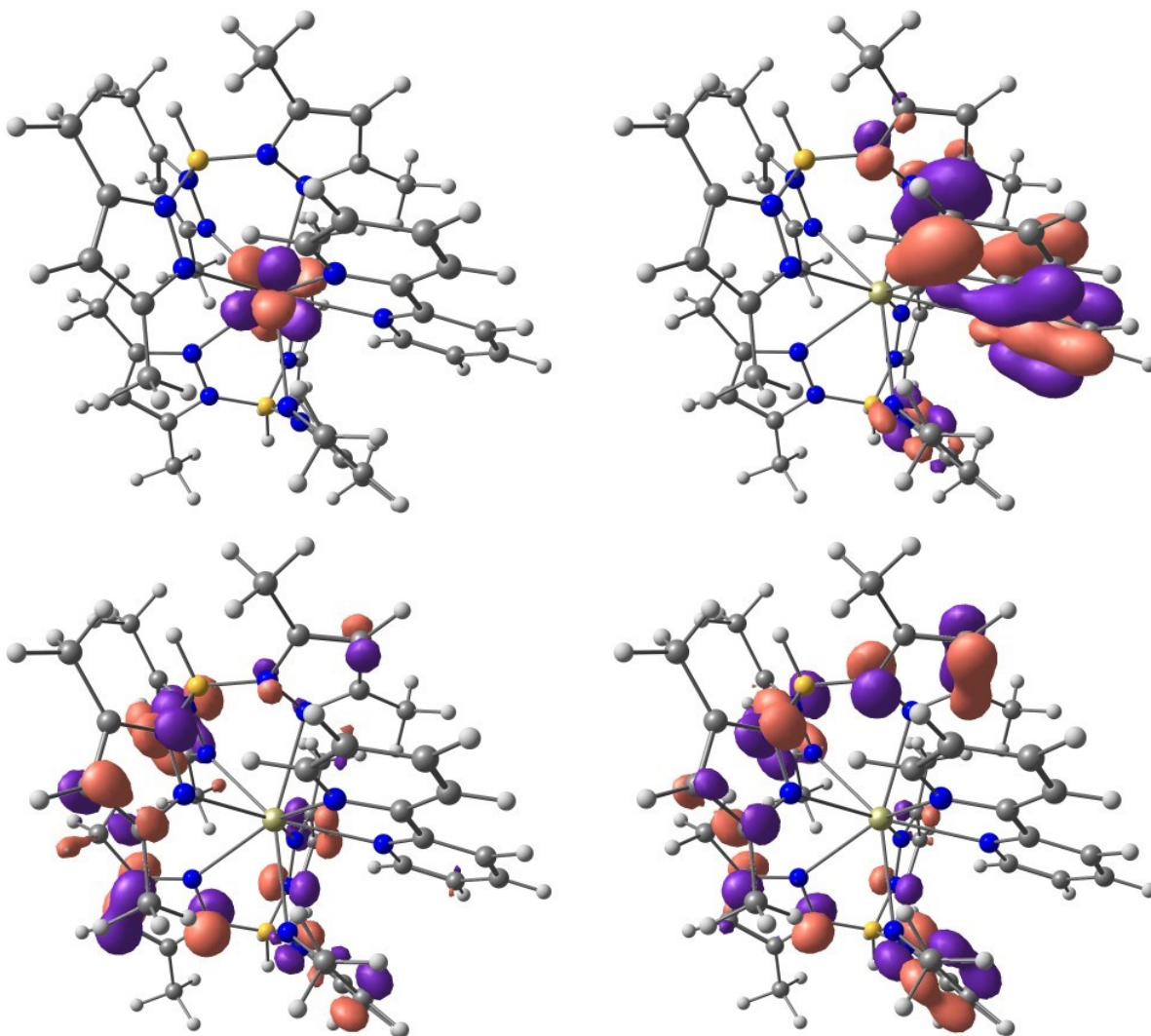
### 1) Ce(C3)<sub>2</sub>I



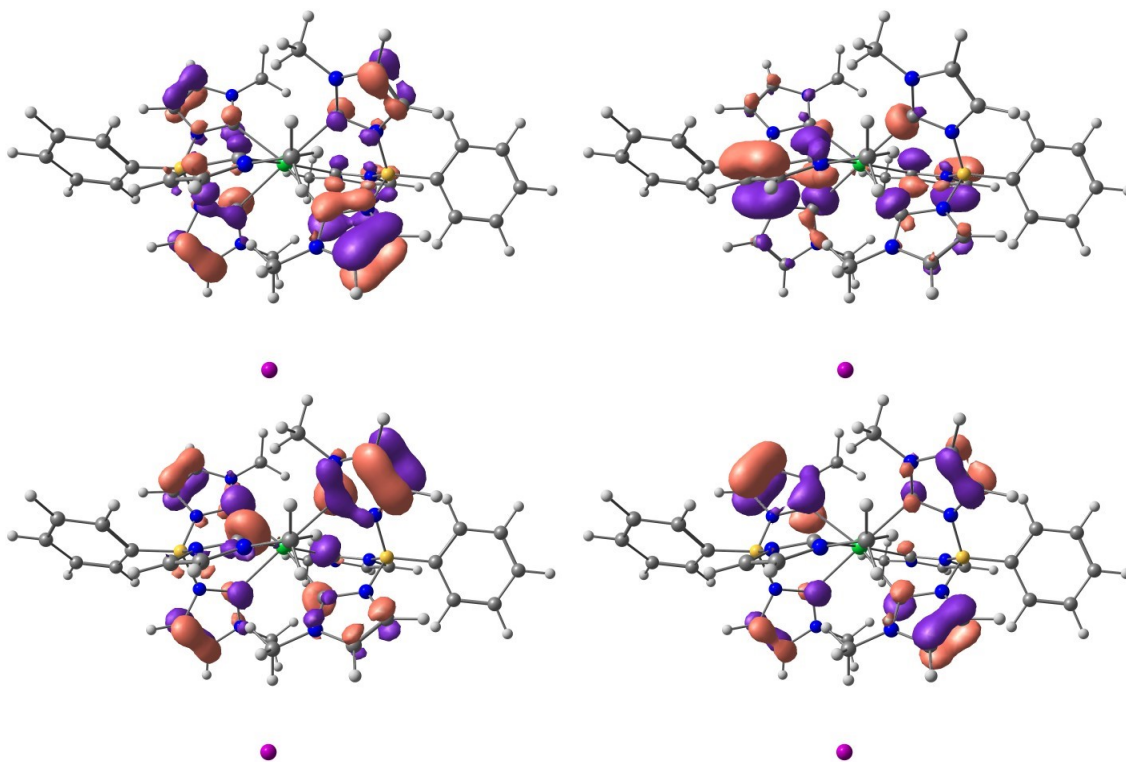
## 2) $\text{Ce}(\text{C3})_2\text{bipy}$



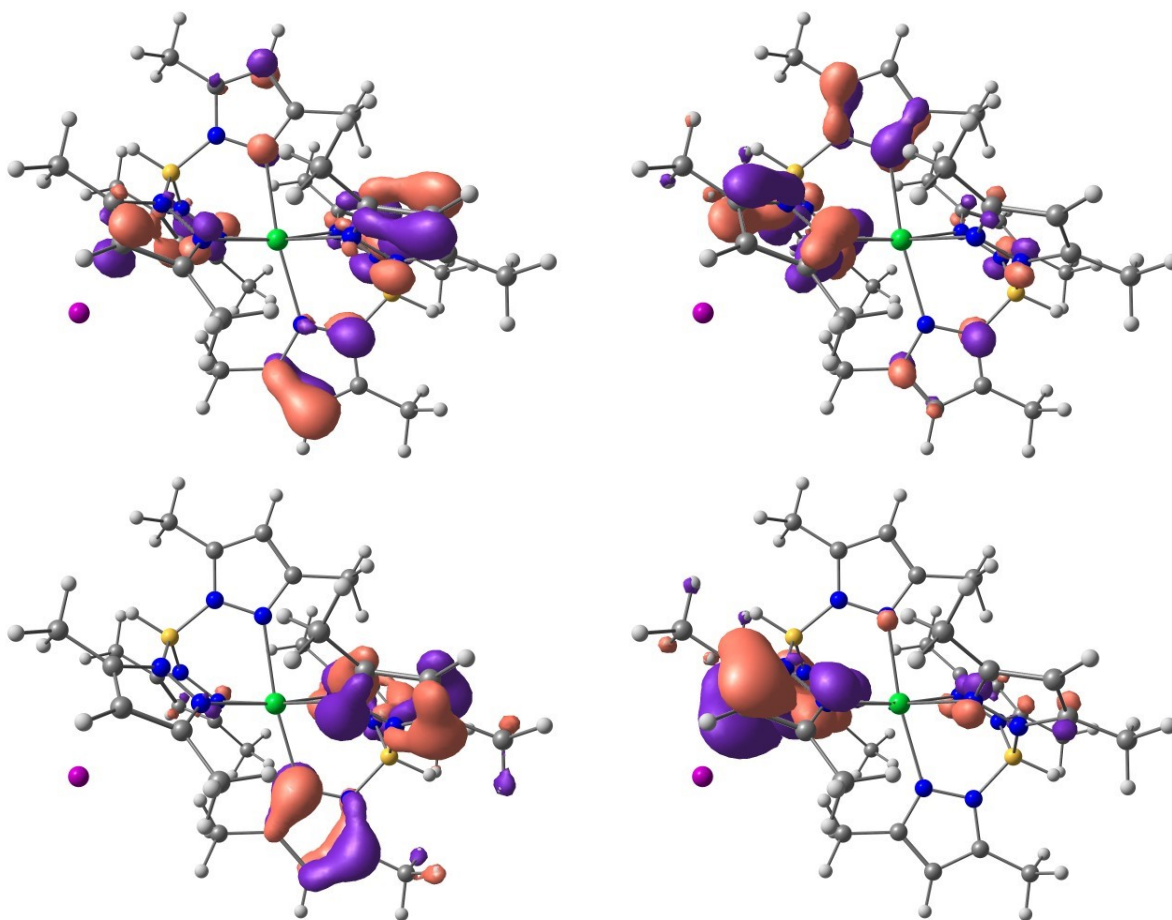
### 3) $\text{Ce}(\text{Tp}^*)_2\text{bipy}$

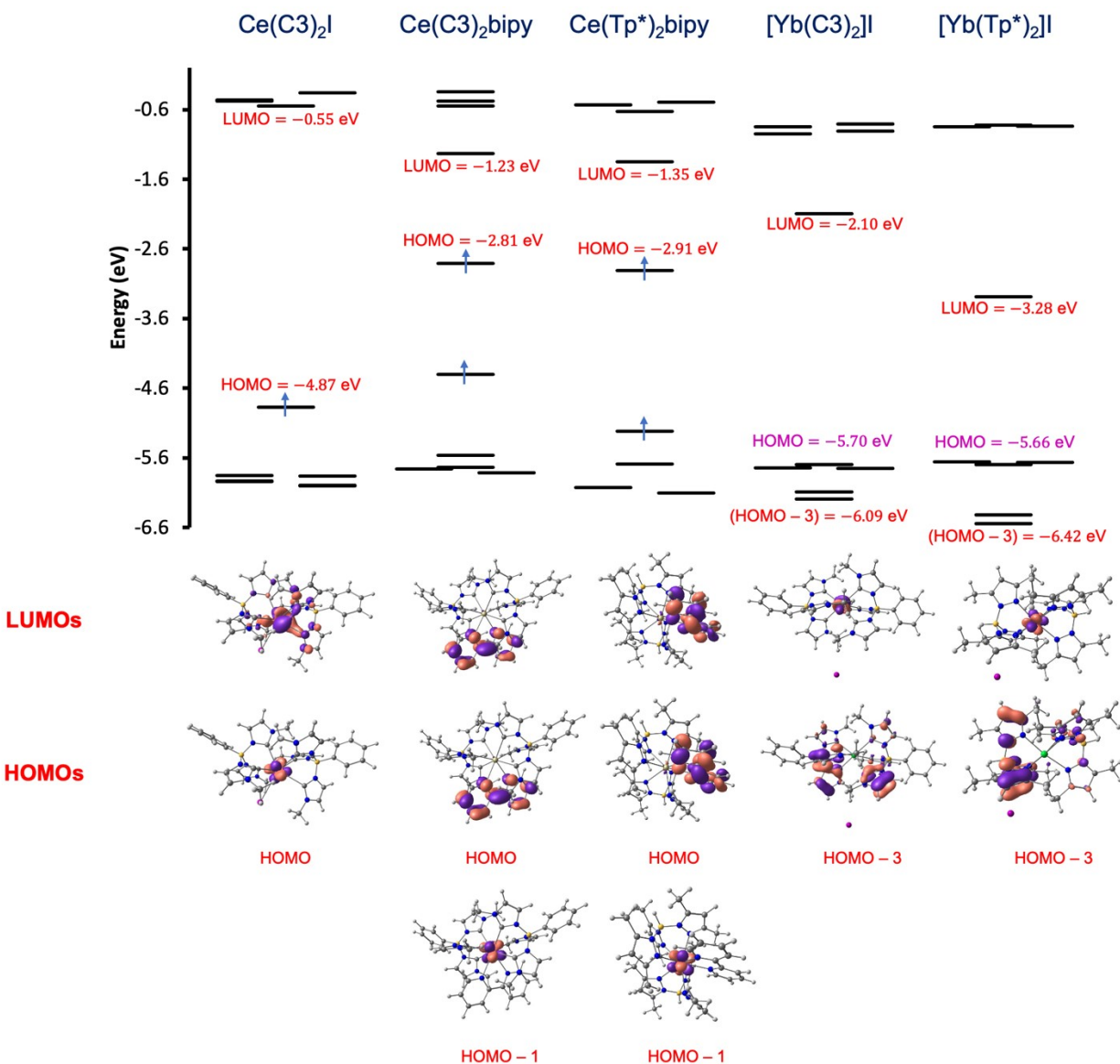


4)  $[\text{Yb}(\text{C3})_2]\text{I}$  (MOs localized on the Iodine ion were ignored)



5)  $[\text{Yb}(\text{Tp}^*)_2]\text{I}$  (MOs localized on the Iodine ion were ignored)





**Figure S5.** Calculated frontier molecular orbital diagrams for lanthanide borate complexes. The three nearly degenerate HOMOs for the Yb complexes (shown in magenta) are exclusively localized on the non-bonded iodine ion.

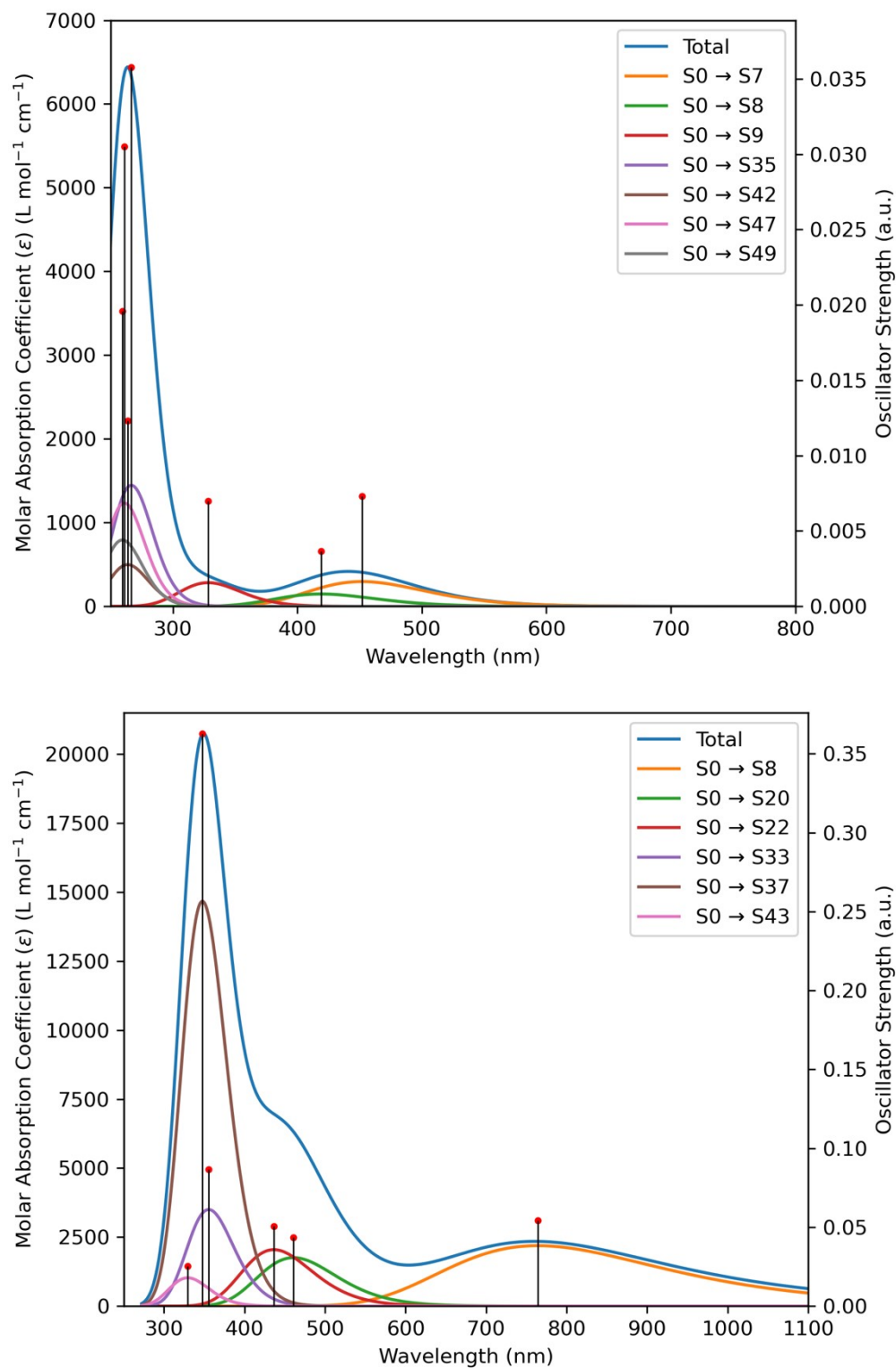
#### Additional discussion of electronic structure for Ce(C3)<sub>2</sub>I, Ce(C3)<sub>2</sub>bipy:

As shown in Figure 5, for **Ce(C3)<sub>2</sub>bipy** both the HOMO and LUMO are delocalized over the bipyridyl ligand with a predominantly p-character. The (HOMO-1) orbital, on the other hand, is entirely 4f in character, representing the unpaired electron on the metal center. As expected, the SOMO of **Ce(C3)<sub>2</sub>I** is the electron located in a cerium 4f-orbital. More interestingly, the LUMO is a hybrid of p (52%), d (34%), and f (10%) orbitals, with major contributions from the metal center and the carbene carbons. The Ce-I bond is primarily ionic, as there was no observed overlap between Ce and I in any occupied molecular orbitals.

## UV-Vis Spectra Analysis

The UV-Vis absorption spectra of  $\text{Ce}(\text{C3})_2\text{I}$  and  $\text{Ce}(\text{C3})_2\text{bipy}$  were obtained using the time-dependent density functional theory (TD-DFT) method and were compared with the experimental spectra. As illustrated in Figures 1 and 3, the TD-DFT computed spectra reproduce all the major peaks in the experimental spectra, validating the theoretical predictions. In this study, we further analyze each of the UV-Vis peaks to understand their origins. By identifying the contributions of the individual excited states or transitions, we gain a deeper insight into the electronic structure of the two complexes and the nature of the electronic transitions that occur upon excitation. Figure 6 illustrates the TD-DFT computed UV-Vis spectra of the two complexes, along with the individual transition curves, which provide insight into the contribution of each transition to a particular peak in the spectrum. The absorption spectrum of  $\text{Ce}(\text{C3})_2\text{I}$  exhibited two major peaks at 263.4 nm and 440.6 nm, as depicted in Figure 6a. The highly intense peak at 263.4 nm was found to have contributions from multiple excited states, specifically transitions S35, S47, S49, and S42, with a contribution percentage ranging from 7% to 22%. The transitions were found to be delocalized across multiple molecular orbitals. The second peak at 440.6 nm was observed to be mostly composed of the  $S_0 \rightarrow S_7$  transition (68.8%), which is mainly associated with the  $\alpha$ -HOMO to  $\alpha$ -LUMO transition. The remaining intensity (30.9%) was assigned to the S8 excited state, which mainly corresponds to the  $\alpha$ -HOMO to  $\alpha$ -(LUMO+1) transition (47.6%). A small shoulder peak at 328.3 nm in the absorption spectrum was observed and was found to be exclusively attributed to the  $S_0 \rightarrow S_9$  transition. This transition involves multiple molecular orbital transitions, with the primary contributions coming from the  $\alpha$ -HOMO to  $\alpha$ -(LUMO+2) transition (12.2%) and the  $\alpha$ -HOMO to  $\alpha$ -(LUMO+10) transition (13.7%).

The UV-Vis absorption spectrum of  $\text{Ce}(\text{C3})_2\text{bipy}$  was analyzed to reveal two major peaks at 348.8 nm and 760.8 nm. As illustrated in Figure 6b, the peak at 348.8 nm was found to be mostly composed of the  $S_0 \rightarrow S_{37}$  transition (70.6%), with a minor contribution from the  $S_0 \rightarrow S_{33}$  transition (16.4%). Further analysis revealed that the S37 excited state is primarily composed of a  $\beta$ -HOMO to  $\beta$ -LUMO transition (50%). The second peak at 760.8 nm was found to be almost exclusively associated with the S8 excited state (93.4%), which is predominantly characterized by a transition from  $\alpha$ -HOMO to  $\alpha$ -(LUMO+1) (83%). A broad peak was also observed at around 445 nm in the absorption spectrum, with almost equal contributions from the S20 and S22 excited states, primarily composed of the  $\alpha$ -HOMO to  $\alpha$ -(LUMO+12) (59%) and  $\alpha$ -HOMO to  $\alpha$ -(LUMO+15) (45%) transitions, respectively.



**Figure 6.** TD-DFT computed UV-Vis spectrum of **(a)** Ce(C3)<sub>2</sub>I **(b)** Ce(C3)<sub>2</sub>bipy with individual transition (or excited state) contributions.



## Optimized Cartesian Coordinates for the Lanthanide Borate Complexes

### 1) Ce(C3)2I

Ce	-0.157819	6.377283	11.522108	I	0.451971	5.375455	8.294702
C	0.800199	3.862642	11.625017	C	-4.192131	-0.021759	12.376656
N	1.086684	8.468456	14.102477	C	3.170704	4.223066	10.962207
N	1.070711	9.756535	11.862178	N	-3.007918	5.260010	9.413321
C	1.071261	7.163520	13.708698	C	-1.390404	5.003049	13.440790
C	0.102238	11.398382	15.311082	C	-1.446489	0.356523	12.602033
C	2.060432	11.721581	13.973597	C	-3.388916	-1.076357	12.821683
C	0.858616	11.018979	14.184032	H	-0.369864	0.486148	12.735947
C	0.492266	12.445910	16.151389	H	-1.370311	-1.687169	13.305579
C	1.674820	13.146608	15.896028	H	-3.834932	-2.040325	13.082578
B	0.484689	9.695052	13.315992	H	-5.275000	-0.154281	12.295005
C	2.464465	12.771167	14.805842	H	-4.272466	2.017997	11.721039
C	1.411761	8.695755	11.073240	H	2.716802	11.437843	13.147614
N	-1.718602	3.694649	13.231851	H	3.404337	13.293474	14.604227
N	-1.689072	5.239334	14.748401	H	1.984126	13.968434	16.547948
N	-2.961536	8.668823	12.500439	H	-0.126444	12.710025	17.014018
N	-1.069062	9.518858	13.113756	H	-0.806783	10.848316	15.565639
N	1.953489	3.437704	11.041913	H	-2.487334	6.745785	15.970198
N	-2.350656	3.680859	10.735914	H	-0.738690	6.448733	16.197412
N	-0.086986	2.846789	11.443710	H	-1.320936	7.291159	14.731525
N	1.691024	6.475264	14.702267	H	-0.037881	0.940329	10.398412
C	-1.547141	6.502051	15.452687	H	1.536697	4.607301	13.789685
C	-1.630831	8.392349	12.590217	H	2.944269	4.795257	14.884971
C	-2.225002	1.427686	12.123967	H	1.301200	4.592148	15.564638
B	-1.596725	2.905182	11.878372	H	-4.237708	10.375831	12.918294
C	0.495418	1.837946	10.695548	H	1.898607	11.265916	9.062867
N	1.796382	9.261194	9.890679	H	2.619096	6.970274	16.602872
C	1.879849	5.036038	14.739411	H	-2.519160	2.100719	14.484518
C	-3.233792	9.957696	12.919703	H	1.857965	9.514135	15.855375
C	1.645299	10.634622	9.911554	H	-2.721971	7.327823	9.427367
C	2.096800	7.322848	15.716669	H	-2.764302	6.590723	7.802256
C	-2.197773	3.133037	14.408036	H	-4.282194	6.794976	8.732861
C	1.716342	8.572944	15.337566	H	-3.103072	2.007307	9.566594
C	-3.613982	1.206381	12.040881	H	2.587248	1.689527	9.919375
C	-3.208278	6.563556	8.808779	H	0.911532	11.906425	11.572315
C	-2.321126	5.032304	10.565965	H	-3.974600	4.040121	7.898334
C	-2.991928	3.082614	9.663171	H	-3.516578	6.809095	11.737481
C	1.787390	2.200968	10.449784	H	-4.635561	7.479828	12.962069
C	1.171686	10.940786	11.150697	H	-4.619378	8.156838	11.306577
C	-3.419991	4.075743	8.833168	H	-2.481524	4.083073	16.408069
C	-3.992847	7.726832	12.102051	H	-1.815053	11.491234	13.652424
C	-2.181772	4.101018	15.362961	H	2.486620	7.498896	9.010815
C	-2.037069	10.493166	13.291261	H	1.728695	8.642840	7.871340
C	-2.010520	-0.878444	12.941068	H	3.361895	8.981740	8.521346
C	2.373608	8.557832	8.758883	H	3.070402	5.105436	11.607974
				H	4.032379	3.629683	11.303556

H 3.350311 4.555248 9.927693

## 2) Ce(C3)<sub>2</sub>bipy

Ce 18.374770 7.254596 7.934107  
N 20.186990 8.739720 5.229502  
N 15.389096 5.737608 8.919556  
N 21.479183 6.741312 6.177142  
N 15.479513 5.852386 6.350140  
N 20.157049 6.644735 9.893331  
N 20.735290 9.771288 9.372912  
N 21.369527 8.884881 7.508325  
N 15.711895 9.864616 7.878652  
N 20.800344 4.732445 6.597691  
N 16.768667 4.914580 10.362014  
N 17.006875 5.523425 4.855202  
N 17.755636 7.916732 10.473349  
N 14.822381 7.897541 7.753805  
N 18.145500 8.984663 4.560843  
C 20.227346 9.397922 4.006479  
H 21.149551 9.707251 3.527950  
C 19.933913 7.109836 11.182332  
C 18.893492 8.485636 5.584863  
C 20.392849 6.030615 6.586178  
C 16.678101 5.309712 9.059911  
C 18.944840 9.551785 3.581966  
H 18.536232 10.009942 2.684255  
C 18.662190 7.689341 11.498736  
C 13.170350 5.829471 7.491705  
C 21.336346 6.055287 9.635153  
H 21.474335 5.694717 8.618731  
C 20.263195 9.342643 8.167248  
C 22.758006 8.885609 5.261402  
C 16.811980 6.026688 6.106324  
C 23.338272 10.124504 5.591203  
H 22.966288 10.682224 6.453848  
C 15.586099 5.127468 11.041390  
H 15.459246 4.885793 12.094147  
C 22.559297 5.894301 5.992311  
H 23.543102 6.243434 5.696887  
C 19.940162 10.464115 10.369545  
H 20.124199 11.550276 10.322281  
H 20.192761 10.105135 11.376027  
H 18.879551 10.269949 10.178874  
C 18.303359 8.035935 12.840382  
H 19.000138 7.840199 13.654872  
C 22.486131 8.976405 8.323824

H 23.471168 8.641583 8.012084  
C 14.722826 5.660742 10.132303  
H 13.692573 5.979782 10.259645  
C 16.009517 8.557594 7.647069  
C 23.254871 8.248937 4.105696  
H 22.806203 7.310685 3.769568  
C 20.973644 6.996201 12.159469  
H 20.824229 7.404292 13.158819  
C 24.376819 10.683250 4.837412  
H 24.802426 11.648090 5.128799  
C 22.365095 5.875778 10.549276  
H 23.290085 5.381692 10.247176  
C 22.170466 6.387348 11.856741  
H 22.956789 6.311148 12.613173  
C 22.093194 9.550551 9.495245  
H 22.655275 9.814979 10.387756  
C 17.079046 8.596014 13.126178  
H 16.817470 8.851089 14.157125  
C 16.679803 10.946154 7.872829  
H 16.649451 11.491243 8.828716  
H 16.466902 11.654615 7.056607  
H 17.684510 10.528464 7.732440  
C 16.561443 8.443231 10.791605  
H 15.866919 8.578481 9.965877  
C 24.293125 8.793220 3.343835  
H 24.650519 8.265282 2.454773  
C 16.161882 8.814685 12.067524  
H 15.170141 9.239051 12.232565  
C 17.943318 4.315293 10.966631  
H 17.785835 3.237326 11.134677  
H 18.162806 4.795309 11.930522  
H 18.799462 4.457602 10.298412  
C 13.815999 8.784406 8.100332  
H 12.790297 8.478154 8.277046  
C 14.870919 5.238597 5.262218  
H 13.814962 4.995715 5.231290  
C 12.743632 4.597536 8.021646  
H 13.436755 3.995733 8.614382  
C 24.865922 10.014893 3.711877  
H 25.678859 10.445922 3.120610  
C 14.369399 10.029446 8.167590  
H 13.929855 10.998831 8.391009  
C 15.828746 5.030331 4.320031  
H 15.776650 4.579695 3.331655  
C 22.134238 4.622849 6.245618  
H 22.656132 3.669732 6.202918  
C 10.542576 4.828357 7.033086  
H 9.531199 4.447859 6.864023

C	16.698615	8.936024	4.451729	H	-0.266730	16.495197	14.180061
H	16.295963	8.423973	5.329742	H	0.124943	15.836303	15.777121
H	16.401320	8.392512	3.541475	C	5.953502	12.935746	15.126633
H	16.281384	9.954372	4.402117	C	5.971335	11.597869	15.508963
C	12.239442	6.524468	6.693497	H	6.564764	11.153635	16.305451
H	12.532460	7.460049	6.210638	C	5.064106	10.950054	14.650095
C	18.263375	5.501783	4.128868	C	6.701714	14.090878	15.702131
H	19.011160	6.054997	4.703950	H	7.375418	14.553416	14.962918
H	18.138027	5.971244	3.141053	H	7.307529	13.755663	16.555766
H	18.610702	4.466370	3.982705	H	6.017172	14.876756	16.058981
C	11.452953	4.101781	7.805241	C	4.740078	9.492200	14.589678
H	11.159677	3.141307	8.239290	H	3.790067	9.314721	14.073860
C	10.945791	6.043029	6.469484	H	4.671248	9.061727	15.599683
H	10.251903	6.615208	5.846565	H	5.531495	8.941312	14.052486
C	19.971175	3.614370	7.008060	C	5.285950	14.232118	10.646590
H	20.330431	3.190698	7.959495	C	4.563029	13.785338	9.547846
H	19.986594	2.823508	6.242736	H	4.839152	13.882048	8.499573
H	18.939883	3.964042	7.138587	C	3.396443	13.191994	10.074072
B	21.453140	8.313694	6.046792	C	6.599029	14.945171	10.671892
B	14.712425	6.327485	7.630910	H	6.508071	15.964965	11.079617

### 3) Ce(Tp\*)<sub>2</sub>bipy

Ce	1.940604	12.327705	13.486625	H	6.993829	15.024753	9.648725
N	3.770342	15.246251	13.762203	H	7.343940	14.414019	11.285285
N	2.496698	14.805093	13.948885	C	2.281787	12.597379	9.272302
N	5.083809	13.054095	14.090976	H	2.598154	11.661974	8.783256
N	4.521406	11.841568	13.807692	H	1.984230	13.292866	8.470945
N	4.570396	13.909592	11.755951	H	1.406590	12.383765	9.888109
N	3.417354	13.265674	11.412849	C	-1.948965	10.429513	14.060007
N	-1.156359	11.289718	13.370359	C	-1.913183	10.806407	15.398625
N	-0.590100	12.194517	14.224711	H	-2.439329	10.332786	16.224829
N	-0.825929	12.838949	11.383041	C	-1.054230	11.919538	15.452543
N	0.286248	13.549912	11.730900	C	-2.680380	9.296597	13.421981
N	0.088683	10.473565	11.258824	H	-3.439596	9.648606	12.704899
N	1.388660	10.638739	11.627949	H	-3.188847	8.700568	14.192935
N	2.515490	12.351764	16.052640	H	-1.995053	8.631203	12.873967
N	1.513830	10.096497	14.809241	C	-0.703765	12.747555	16.646447
C	3.854280	16.564668	14.075390	H	-0.565150	12.115497	17.536194
C	2.588180	16.978321	14.485569	H	-1.514353	13.461091	16.875119
H	2.300879	17.977942	14.805318	H	0.216628	13.318337	16.482031
C	1.767986	15.838659	14.387679	C	-1.593648	13.549004	10.514874
C	5.108468	17.368755	13.967906	C	-0.952248	14.761432	10.296567
H	5.911875	16.959122	14.599705	H	-1.287196	15.571724	9.651903
H	4.913457	18.401827	14.289301	C	0.223988	14.716661	11.073839
H	5.488095	17.399183	12.934286	C	-2.872134	13.050100	9.923772
C	0.311428	15.712818	14.697713	H	-2.714431	12.153927	9.302305
H	-0.086466	14.736050	14.392641	H	-3.312247	13.830735	9.286702
				H	-3.609555	12.784217	10.697605
				C	1.272065	15.781885	11.138986
				H	2.201448	15.409038	11.574485

H	0.931192	16.644394	11.734291	N	5.672778	9.998047	27.042964
H	1.485551	16.156803	10.125119	N	4.281126	11.368025	23.122056
C	-0.004639	9.491677	10.325277	N	4.176700	13.530410	23.045660
C	1.282223	9.008137	10.096764	N	6.231019	9.865507	22.696809
H	1.567646	8.217839	9.405453	N	8.262561	10.370339	22.140652
C	2.124990	9.761289	10.935584	C	7.317993	14.454592	26.023636
C	-1.286635	9.061549	9.690517	C	8.083644	13.855762	23.094480
H	-2.012787	8.704558	10.437023	C	9.365123	12.207912	25.586769
H	-1.091504	8.242492	8.983810	C	5.793822	10.523041	25.798271
H	-1.764271	9.884540	9.135592	C	4.775659	12.499799	23.698371
C	3.609804	9.670201	11.081795	C	7.328025	10.562689	23.109665
H	4.002455	10.450628	11.746246	C	8.425180	16.323140	26.581872
H	4.103224	9.774039	10.101764	H	9.236979	17.041081	26.608549
H	3.906220	8.689855	11.488968	C	7.212398	16.373911	27.201919
C	3.072349	13.421011	16.653847	H	6.773287	17.122182	27.857474
H	3.194471	14.304373	16.030820	C	5.206728	14.872310	27.277483
C	3.483062	13.467740	17.975595	H	5.164490	14.796595	28.374823
H	3.924962	14.379274	18.381424	H	4.922246	13.905867	26.841854
C	3.314063	12.296206	18.757331	H	4.488493	15.637796	26.946748
H	3.630215	12.268930	19.803702	C	9.905578	14.912372	22.309865
C	2.750998	11.184899	18.173851	H	10.852339	15.440938	22.340606
H	2.633293	10.277062	18.764361	C	9.194021	14.476649	21.230185
C	2.340786	11.198535	16.804853	H	9.378924	14.573182	20.163052
C	1.754095	10.052448	16.175501	C	7.047496	13.237978	20.904313
C	1.412574	8.875134	16.910774	H	6.388560	12.626778	21.528696
H	1.577249	8.841761	17.987240	H	7.504645	12.602042	20.133050
C	0.859608	7.782551	16.283794	H	6.449540	14.021767	20.414686
H	0.597136	6.890764	16.859532	C	11.500727	12.819315	25.244042
C	0.631348	7.839480	14.884946	H	12.332608	13.478554	25.018098
H	0.196846	7.004956	14.332156	C	11.500464	11.475475	25.480994
C	0.970360	9.010024	14.227113	H	12.313789	10.754746	25.523491
H	0.797470	9.080900	13.155664	C	9.731895	9.769706	25.958496
B	4.884905	14.316692	13.205756	H	10.219846	9.375064	26.862644
H	5.910866	14.945256	13.214358	H	9.970107	9.109754	25.110323
B	-1.044685	11.380184	11.821494	H	8.646181	9.777233	26.114153
H	-2.079573	10.984475	11.353246	C	10.842535	15.834973	25.130474

#### 4) [Yb(C3)<sub>2</sub>]I

Yb	7.007603	12.383248	24.784614	H	13.353793	16.699317	27.316018
N	8.482610	15.140315	25.858027	C	12.653905	17.957656	25.700345
N	6.550280	15.215096	26.842365	H	13.353347	18.770333	25.915491
N	9.201746	14.554692	23.446591	C	11.734298	18.073150	24.653971
N	8.081705	13.834111	21.736461	H	11.702792	18.984070	24.049308
N	10.193021	13.262541	25.339886	C	10.843081	17.029532	24.383840
N	10.181359	11.125740	25.693258	H	10.113557	17.172083	23.583451
N	5.031047	9.739179	24.986213	C	4.442585	8.733334	25.739972
				H	3.784564	7.983289	25.316091

C	4.843346	8.891855	27.032830
H	4.610494	8.323638	27.930270
C	6.328115	10.513319	28.233297
H	5.583669	10.737341	29.012227
H	6.865599	11.436779	27.981780
H	7.045512	9.778527	28.630074
C	3.425608	11.706423	22.087302
H	2.944845	10.969556	21.452261
C	3.343801	13.068485	22.046736
H	2.785097	13.735809	21.395059
C	4.361731	14.935616	23.370042
H	4.484187	15.521467	22.447570
H	5.256276	15.046300	23.995342
H	3.489264	15.321510	23.920625
C	6.474516	9.297062	21.458853
H	5.728969	8.730071	20.911596
C	7.758703	9.598212	21.112038
H	8.345681	9.331949	20.236292
C	9.617487	10.896361	22.161440
H	10.345563	10.081155	22.292853
H	9.718667	11.603678	22.990109
H	9.837305	11.416578	21.218310
C	3.824559	8.745826	22.947885
C	4.299350	7.450011	22.662838
H	5.373744	7.251030	22.673082
C	3.434930	6.384822	22.391984
H	3.844447	5.394550	22.172419
C	2.051138	6.582812	22.411397
H	1.370118	5.754296	22.197548
C	1.549476	7.849686	22.722587
H	0.469202	8.016797	22.762573
C	2.426201	8.905959	22.992408
H	1.998181	9.873665	23.263767
B	9.695950	14.707814	24.938654
B	4.829891	9.921729	23.425583
I	4.534695	16.156260	19.314176

### 5) [Yb(Tp\*)<sub>2</sub>]I

Yb	0.117627	0.063942	0.190567
N	1.303187	1.557786	-1.147480
N	2.143031	-0.064383	1.300396
N	2.581352	1.218900	-1.490797
N	3.270752	-0.177453	0.536280
B	3.225977	-0.108748	-1.014286
C	2.508552	-0.175425	2.590517
C	3.894421	-0.372445	2.658139
C	4.345046	-0.365743	1.336643

C	3.114052	2.183505	-2.276628
C	1.026894	2.743908	-1.717898
C	2.146588	3.175695	-2.443449
C	5.740919	-0.500966	0.828549
C	1.521617	-0.049249	3.705630
C	-0.311532	3.395584	-1.582575
C	4.506620	2.142878	-2.810021
H	4.342978	-0.173712	-1.439261
H	4.502830	-0.489960	3.551839
H	2.253483	4.098651	-3.008831
H	5.841436	-1.335395	0.117282
H	6.064418	0.418891	0.316268
H	0.511638	-0.361065	3.401000
H	1.458084	0.995560	4.053189
H	-0.886130	2.982924	-0.741801
H	-0.202983	4.479887	-1.429672
H	-0.909106	3.252510	-2.498672
H	4.684010	1.248028	-3.426857
H	4.689361	3.030937	-3.430948
H	5.245150	2.140785	-1.993117
N	-1.118096	-1.527831	1.392028
N	-1.157867	1.509398	1.520405
N	1.117967	-1.547202	-1.190719
N	-1.802246	0.094338	-1.147697
N	2.411041	-1.315214	-1.568602
H	6.424126	-0.680566	1.670250
H	1.828353	-0.662439	4.565555
N	-2.461271	-1.318199	1.525400
C	-0.839018	-2.735086	1.913513
N	-2.478426	1.216975	1.709151
C	-0.885521	2.635517	2.203214
C	0.693876	-2.644456	-1.843385
N	-3.014127	0.105211	-0.513773
C	-2.032792	0.185162	-2.469945
C	2.804255	-2.253117	-2.460892
B	-3.138182	-0.010549	1.031982
C	-3.035172	-2.388425	2.124217
C	-2.025909	-3.316145	2.387876
C	0.553332	-3.276875	1.961517
C	-3.043856	2.150599	2.510877
C	-2.053194	3.073641	2.848665
C	0.469326	3.262694	2.178536
C	1.729894	-3.121993	-2.661167
C	-0.670847	-3.221562	-1.645100
C	-4.007570	0.213463	-1.427403
C	-3.416703	0.268535	-2.690097
C	-0.936605	0.139859	-3.484818
C	4.160805	-2.286376	-3.083799

H	-4.299530	-0.041040	1.323408	H	0.029814	0.442242	-3.062331
C	-4.496281	-2.489131	2.414645	H	-0.821558	-0.881516	-3.885222
H	-2.142853	-4.287796	2.862792	H	-1.169192	0.799330	-4.334179
H	1.160262	-2.917269	1.118526	H	4.371021	-1.365413	-3.650138
H	0.540028	-4.376226	1.936822	H	4.228878	-3.137255	-3.776045
H	1.062424	-2.972701	2.891229	H	4.954238	-2.394515	-2.327589
C	-4.479217	2.128499	2.921233	H	-4.832424	-1.690596	3.094856
H	-2.168204	3.950374	3.482290	H	-4.713304	-3.456220	2.889324
H	1.249271	2.552468	1.873087	H	-5.099540	-2.414188	1.496157
H	0.500241	4.107164	1.470177	H	-4.730644	1.208556	3.472480
H	0.737809	3.661162	3.168035	H	-4.690587	2.987177	3.573656
H	1.707318	-3.988852	-3.318055	H	-5.153038	2.185322	2.051722
H	-1.406368	-2.453125	-1.373125	H	-5.685855	1.113303	-0.411780
H	-0.665324	-3.976731	-0.841298	H	-5.783028	-0.652967	-0.557219
H	-1.011683	-3.722003	-2.563456	H	-6.057016	0.371891	-1.988794
C	-5.457481	0.263562	-1.074142	I	4.377013	3.583633	1.176014
H	-3.929138	0.357673	-3.645545				

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