**Supporting Information**

# Chemical Oxidation of a Double-Twisted Nanographene

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## Contents

## 1. General

The $^{1}H$ and $^{13}C$ NMR measurements were carried out with a Bruker AVANCE NEO 600 MHz instrument. The NMR chemical shifts are reported in ppm with reference to residual protons and carbons of $CD_2Cl_2$ ($\delta$ 5.32 ppm in $^{1}H$ NMR, $\delta$ 53.84 ppm in $^{13}C$ NMR) and $CD_3CN$ ($\delta$ 118.26 ppm in $^{13}C$ NMR). Centrifugation was performed on a Herexi TD5A centrifuge. The UV-vis-NIR absorption spectra were measured with a Shimadzu UV-3600i Plus spectrometer. The circular dichroism (CD) spectrum was recorded on a JASCO-J-1700 Circular Dichroism Spectrophotometer.

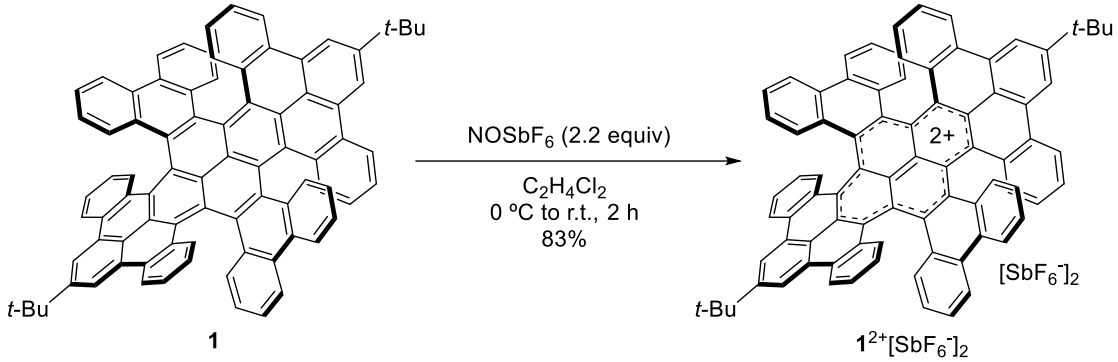
Dry $C_2H_4Cl_2$ (1,2-dichloroethane) was purchased from Beijing InnoChem Science & Technology Co. $NOSbF_6$ was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. *n*-Hexane was purchased from Shanghai Titan Scientific Co., Ltd. Unless otherwise noted, all commercial reagents and solvents were used as received and no further purification was performed.

A double-twisted nanographene (**1**)[1] was prepared according to literature procedures. The reaction was carried out under a nitrogen atmosphere.

## 2. Computational Methods

All calculations were performed using the Gaussian 09 program. All structures at the stationery states were optimized at the B3LYP-D3 level of theory with basis sets of SDD for Sb and 6-31G(d) for the rest without any symmetry assumptions and confirmed by frequency analysis at the same level of theory. The NMR chemical shifts were calculated at the GIAO-B3LYP-D3/6-311+G(2d,p) level of theory using the structure optimized at the aforementioned level. The NICS (nucleus-independent chemical shift) and ICSS (iso-chemical shielding surfaces) calculations were performed at the HF/6-31+G(d,p) level of theory using structures optimized at the aforementioned level, the latter of which was computed by Multiwfn 3.8-dev program.[2,3] ACID (anisotropy of current-induced density) plots were generated at the B3LYP-D3/6-31G(d) level of theory using structures optimized at the aforementioned level. Optical transitions were calculated at the TD-CAM-B3LYP-D3 level of theory with basis sets of SDD for Sb and 6-31G(d) for the rest using the structure optimized at the aforementioned level.

## 3. Synthesis of $\mathbf{1}^{2+}[SbF_6^-]_2$




Powdery **1** (10 mg, 9.4 μmol) and $NOSbF_6$ (5.5 mg, 0.021 mmol, 2.2 equiv) were added into a 50 mL two-neck flask and degassed through three vacuum–$N_2$ cycles. Dry $C_2H_4Cl_2$ (10 mL) was added at 0 °C. During the process that the solution was allowed to warm up to room temperature for 2 h, the compounds were mostly precipitated. The resulting solid was collected by centrifugation (3000 rpm, 10 min) using $C_2H_4Cl_2$/*n*-hexane (1:20) for three times (21 mL × 3) to give $\mathbf{1}^{2+}[SbF_6^-]_2$ (12 mg, 7.8 μmol, 83%) as a brown powder.

(*MM*,*MMMM*)-$\mathbf{1}^{2+}[SbF_6^-]_2$ was prepared in a similar manner using (*MM*,*MMMM*)-**1**.

$\mathbf{1}^{2+}[SbF_6^-]_2$: $^1$H NMR (600 MHz, $CD_2Cl_2$) $\delta$ 9.10 (s, 4H), 8.77 (d, $J$ = 8.0 Hz, 4H), 8.29 (d, $J$ = 7.9 Hz, 4H), 7.77 (t, $J$ = 8.0 Hz, 4H), 7.56 (d, $J$ = 8.0 Hz, 4H), 7.46 (t, $J$ = 7.9 Hz, 4H), 7.17 (d, $J$ = 8.0 Hz, 4H), 7.11 (d, $J$ = 7.9 Hz, 4H), 6.95 (t, $J$ = 7.9 Hz, 4H), 1.73 (s, 18H); $^{13}$C NMR (151 MHz, $CD_2Cl_2$/$CD_3CN$ (5:1)) $\delta$ 155.67, 158.53, 144.35, 139.89, 137.32, 136.43, 136.36, 135.71, 133.51, 132.13, 130.62, 130.32, 130.06,129.87, 129.77, 128.56, 128.52, 127.78, 125.77, 125.39, 125.15, 36.26, 31.00 (The sum of carbon signals must be 23 in theory. Observed 23).

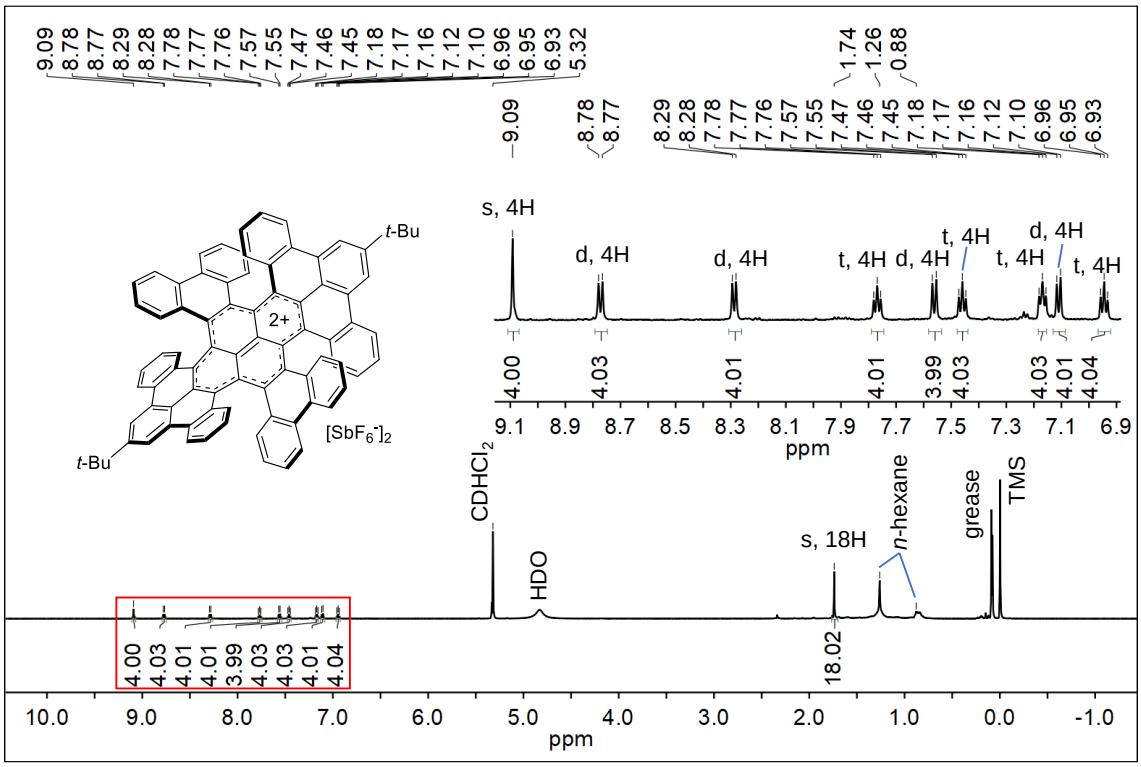



**Figure S1.** $^{1}$H NMR spectra (600 MHz, $CD_2Cl_2$) of $\mathbf{1}^{2+}[SbF_6^-]_2$.

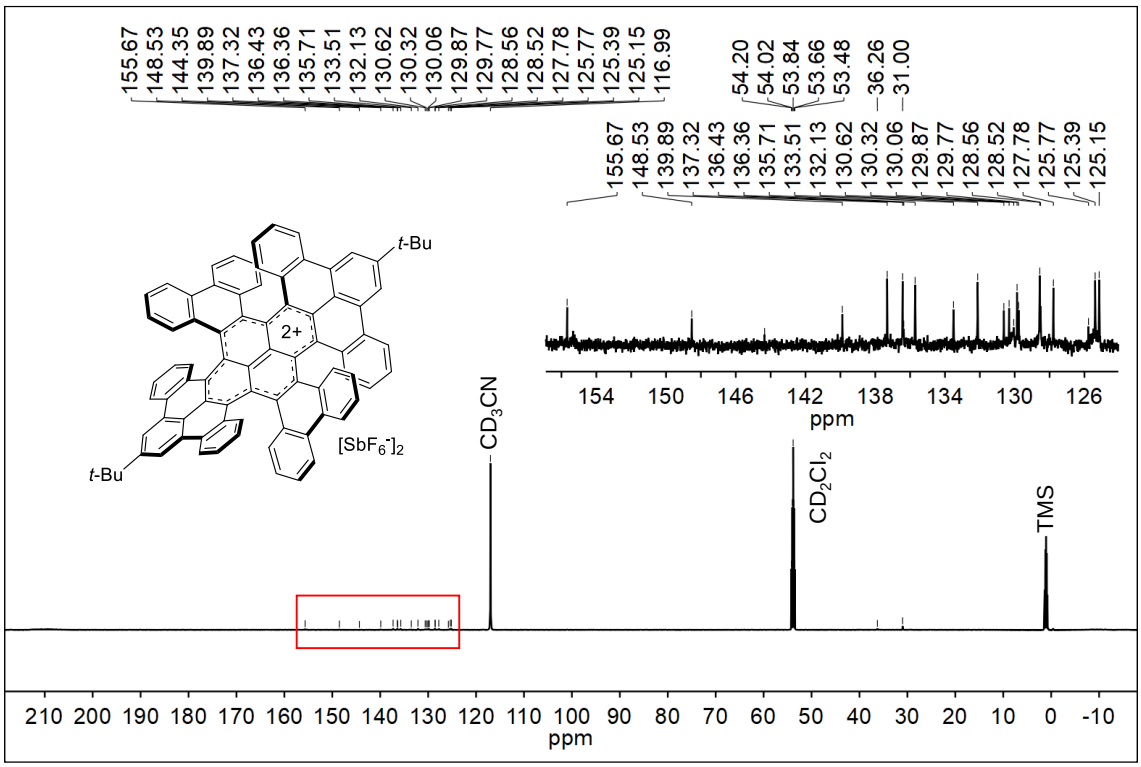



**Figure S2.** $^{13}$C NMR spectra (151 MHz, $CD_2Cl_2$/$CD_3CN$ (5:1)) of $\mathbf{1}^{2+}[SbF_6^-]_2$.

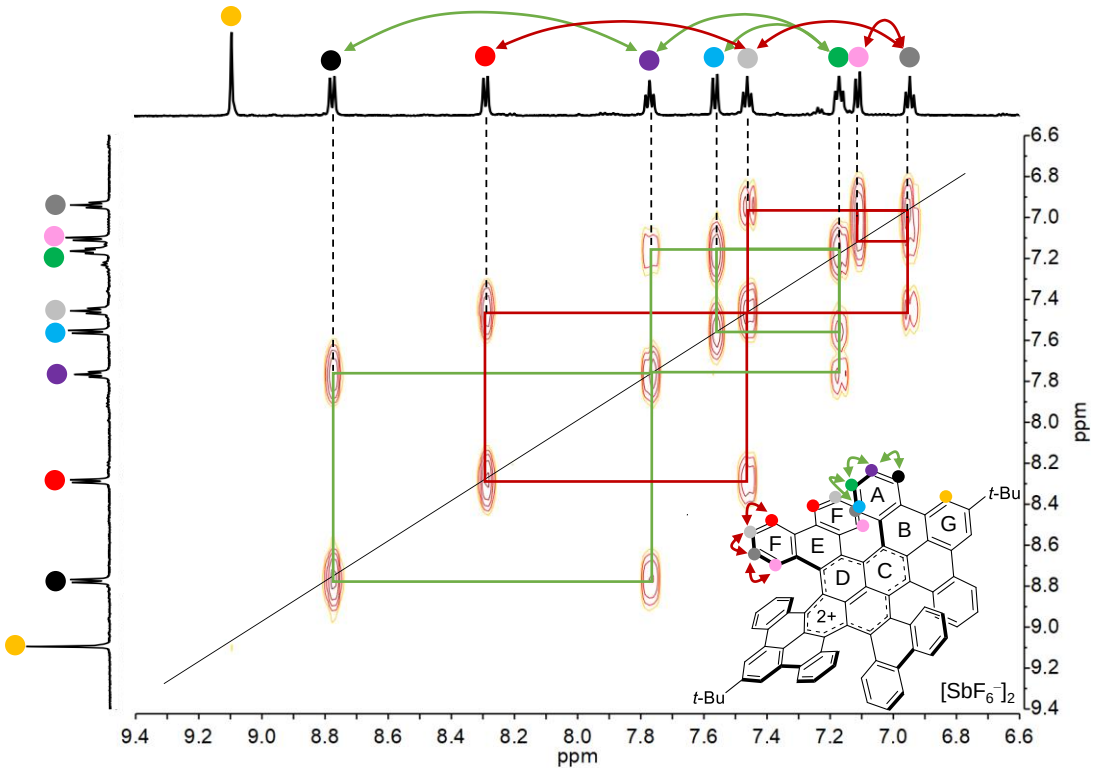



**Figure S3.** COSY spectrum (600 MHz, $CD_2Cl_2$, 298K) of $\mathbf{1}^{2+}[SbF_6^-]_2$.

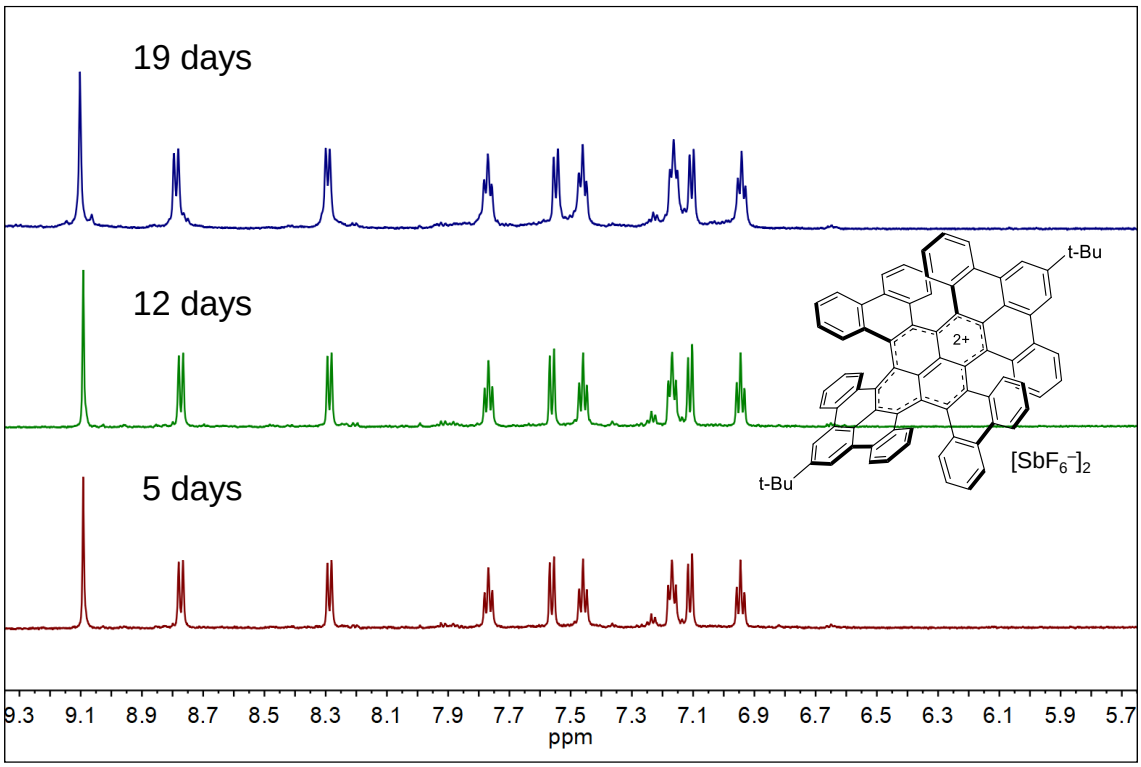



**Figure S4.** Spectral change in $^1H$ NMR spectra (600 MHz, $CD_2Cl_2$) of $\mathbf{1}^{2+}[SbF_6^-]_2$.

## 4. Simulated $^{13}$C NMR Spectrum

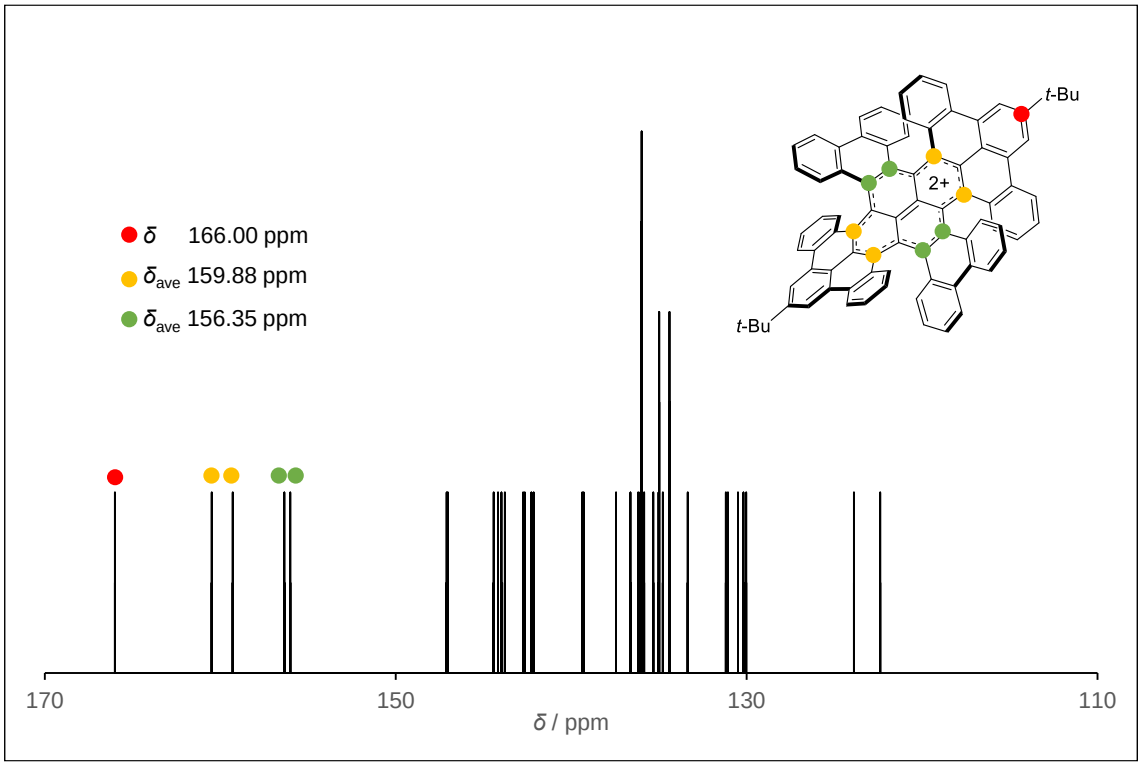
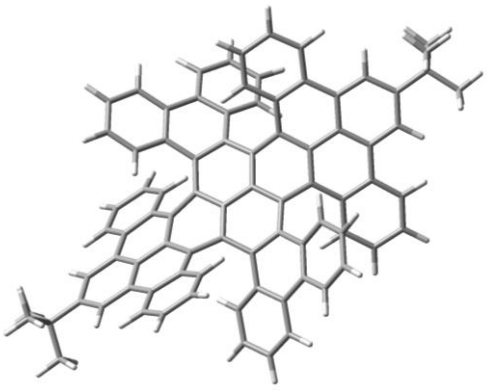



**Figure S5.** Simulated $^{13}$C NMR spectrum of $\mathbf{1}^{2+}$ (GIAO-B3LYP-D3/6-311+G(2d,p)// B3LYP-D3/6-31G(d)).

**Table S1.** Optimized structure of $\mathbf{1}^{2+}$ (B3LYP-D3/6-31G(d))



Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.855519 | 7.017146 | 0.790952 |
| 2 | 6 | 0 | -0.878824 | 5.617953 | 0.831776 |
| 3 | 6 | 0 | 0.026528 | 4.913970 | -0.007922 |
| 4 | 6 | 0 | 0.932460 | 5.603793 | -0.853531 |
| 5 | 6 | 0 | 0.916775 | 7.008643 | -0.831553 |
| 6 | 6 | 0 | 0.033072 | 7.732707 | -0.026250 |
| 7 | 6 | 0 | -1.726073 | 4.852540 | 1.753152 |
| 8 | 6 | 0 | 1.776971 | 4.827065 | -1.765950 |
| 9 | 6 | 0 | -2.452192 | 5.447777 | 2.800069 |
| 10 | 6 | 0 | -3.152898 | 4.675428 | 3.719440 |
| 11 | 6 | 0 | -3.139175 | 3.272689 | 3.643755 |
| 12 | 6 | 0 | -2.476291 | 2.653240 | 2.604163 |
| 13 | 6 | 0 | -1.796000 | 3.426866 | 1.632612 |
| 14 | 6 | 0 | 1.836531 | 3.400987 | -1.636912 |
| 15 | 6 | 0 | 2.514548 | 2.617082 | -2.602410 |
| 16 | 6 | 0 | 3.185099 | 3.225559 | -3.642900 |
| 17 | 6 | 0 | 3.210003 | 4.628209 | -3.726063 |
| 18 | 6 | 0 | 2.512335 | 5.410830 | -2.813968 |
| 19 | 6 | 0 | -1.036942 | 2.779468 | 0.608509 |
| 20 | 6 | 0 | -1.211235 | 1.402028 | 0.181553 |
| 21 | 6 | 0 | 0.004372 | 0.703359 | 0.000629 |
| 22 | 6 | 0 | 1.228539 | 1.386799 | -0.180520 |
| 23 | 6 | 0 | 1.071152 | 2.765870 | -0.611094 |
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| 26 | 6 | 0 | -2.456242 | -0.701579 | -0.012988 |
| 27 | 6 | 0 | -1.228539 | -1.386799 | -0.180520 |
| 28 | 6 | 0 | -0.004372 | -0.703359 | 0.000629 |
| 29 | 6 | 0 | -1.071152 | -2.765870 | -0.611094 |
| 30 | 6 | 0 | -0.021641 | -3.482882 | -0.002013 |
| 31 | 6 | 0 | 1.036942 | -2.779468 | 0.608509 |
| 32 | 6 | 0 | 1.211235 | -1.402028 | 0.181553 |
| 33 | 6 | 0 | 2.447588 | -0.730974 | 0.017575 |
| 34 | 6 | 0 | 2.456242 | 0.701579 | -0.012988 |
| 35 | 6 | 0 | -3.696232 | 1.426826 | -0.289183 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | -4.931060 | 0.727221 | -0.218988 |
| 37 | 6 | 0 | -4.939209 | -0.667795 | 0.227692 |
| 38 | 6 | 0 | -3.713093 | -1.382792 | 0.294267 |
| 39 | 6 | 0 | -3.689615 | 2.740087 | -0.810739 |
| 40 | 6 | 0 | -4.863981 | 3.383466 | -1.162145 |
| 41 | 6 | 0 | -6.086209 | 2.710955 | -1.040472 |
| 42 | 6 | 0 | -6.110194 | 1.396920 | -0.595289 |
| 43 | 6 | 0 | -6.125737 | -1.322641 | 0.606990 |
| 44 | 6 | 0 | -6.117225 | -2.637148 | 1.051225 |
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| 46 | 6 | 0 | -3.721810 | -2.696722 | 0.813776 |
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| 48 | 6 | 0 | 4.931060 | -0.727221 | -0.218988 |
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| 52 | 6 | 0 | 6.117225 | 2.637148 | 1.051225 |
| 53 | 6 | 0 | 4.903311 | 3.325294 | 1.168271 |
| 54 | 6 | 0 | 3.721810 | 2.696722 | 0.813776 |
| 55 | 6 | 0 | 3.689615 | -2.740087 | -0.810739 |
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| 57 | 6 | 0 | 6.086209 | -2.710955 | -1.040472 |
| 58 | 6 | 0 | 6.110194 | -1.396920 | -0.595289 |
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| 65 | 6 | 0 | -1.776971 | -4.827065 | -1.765950 |
| 66 | 6 | 0 | 1.726073 | -4.852540 | 1.753152 |
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| 68 | 6 | 0 | -2.514548 | -2.617082 | -2.602410 |
| 69 | 6 | 0 | -3.185099 | -3.225559 | -3.642900 |
| 70 | 6 | 0 | -3.210003 | -4.628209 | -3.726063 |
| 71 | 6 | 0 | -2.512335 | -5.410830 | -2.813968 |
| 72 | 6 | 0 | 2.452192 | -5.447777 | 2.800069 |
| 73 | 6 | 0 | 3.152898 | -4.675428 | 3.719440 |
| 74 | 6 | 0 | 3.139175 | -3.272689 | 3.643755 |
| 75 | 6 | 0 | 2.476291 | -2.653240 | 2.604163 |
| 76 | 6 | 0 | 1.796000 | -3.426866 | 1.632612 |
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| 85 | 1 | 0 | -1.544209 | 7.571325 | 1.417803 |
| 86 | 1 | 0 | 1.609793 | 7.544227 | -1.465486 |
| 87 | 1 | 0 | -2.433637 | 6.524153 | 2.931554 |
| 88 | 1 | 0 | -3.677014 | 5.166885 | 4.534523 |
| 89 | 1 | 0 | -3.602024 | 2.667630 | 4.416113 |
| 90 | 1 | 0 | -2.382050 | 1.574806 | 2.593462 |
| 91 | 1 | 0 | 2.411872 | 1.539491 | -2.586392 |
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| 94 | 1 | 0 | 2.503359 | 6.486465 | -2.951647 |
| 95 | 1 | 0 | -2.747266 | 3.240302 | -0.992986 |
| 96 | 1 | 0 | -4.827148 | 4.389842 | -1.568021 |
| 97 | 1 | 0 | -7.011479 | 3.198750 | -1.333520 |
| 98 | 1 | 0 | -7.058477 | 0.872139 | -0.571846 |
| 99 | 1 | 0 | -7.067319 | -0.785803 | 0.586592 |
| 100 | 1 | 0 | -7.047737 | -3.113404 | 1.346632 |
| 101 | 1 | 0 | -4.878101 | -4.332629 | 1.572674 |
| 102 | 1 | 0 | -2.785499 | -3.209660 | 0.991706 |
| 103 | 1 | 0 | 7.067319 | 0.785803 | 0.586592 |
| 104 | 1 | 0 | 7.047737 | 3.113404 | 1.346632 |
| 105 | 1 | 0 | 4.878101 | 4.332629 | 1.572674 |
| 106 | 1 | 0 | 2.785499 | 3.209660 | 0.991706 |
| 107 | 1 | 0 | 2.747266 | -3.240302 | -0.992986 |
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| 111 | 1 | 0 | -1.609793 | -7.544227 | -1.465486 |
| 112 | 1 | 0 | 1.544209 | -7.571325 | 1.417803 |
| 113 | 1 | 0 | -2.411872 | -1.539491 | -2.586392 |
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| 121 | 1 | 0 | 1.318818 | 9.428769 | 1.743846 |
| 122 | 1 | 0 | 0.307820 | 10.861177 | 1.462596 |
| 123 | 1 | 0 | -0.401825 | 9.397474 | 2.158229 |
| 124 | 1 | 0 | -1.435287 | 10.860177 | -0.407039 |
| 125 | 1 | 0 | -1.647515 | 9.426015 | -1.432593 |
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| 127 | 1 | 0 | 0.846817 | 9.601723 | -2.007242 |
| 128 | 1 | 0 | 2.061246 | 9.604804 | -0.707674 |
| 129 | 1 | 0 | 0.976175 | 10.983894 | -0.913501 |
| 130 | 1 | 0 | -0.846817 | -9.601723 | -2.007242 |
| 131 | 1 | 0 | -0.976175 | -10.983894 | -0.913501 |
| 132 | 1 | 0 | -2.061246 | -9.604804 | -0.707674 |
| 133 | 1 | 0 | -0.307820 | -10.861177 | 1.462596 |
| 134 | 1 | 0 | 0.401825 | -9.397474 | 2.158229 |
| 135 | 1 | 0 | -1.318818 | -9.428769 | 1.743846 |
| 136 | 1 | 0 | 1.647515 | -9.426015 | -1.432593 |
| 137 | 1 | 0 | 2.179160 | -9.399294 | 0.256445 |
| 138 | 1 | 0 | 1.435287 | -10.860177 | -0.407039 |
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| 140 | 51 | 0 | 0.000000 | 0.000000 | -4.404251 |
| 141 | 9 | 0 | -1.899453 | -0.077402 | -4.327786 |
| 142 | 9 | 0 | 0.000000 | 0.000000 | -2.498909 |
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| 148 | 9 | 0 | 0.000000 | 0.000000 | 6.286119 |
| 149 | 9 | 0 | -1.898202 | 0.103962 | 4.331260 |
| 150 | 9 | 0 | -0.074524 | -1.887480 | 4.329408 |
| 151 | 9 | 0 | 1.898202 | -0.103962 | 4.331260 |
| 152 | 9 | 0 | 0.074524 | 1.887480 | 4.329408 |

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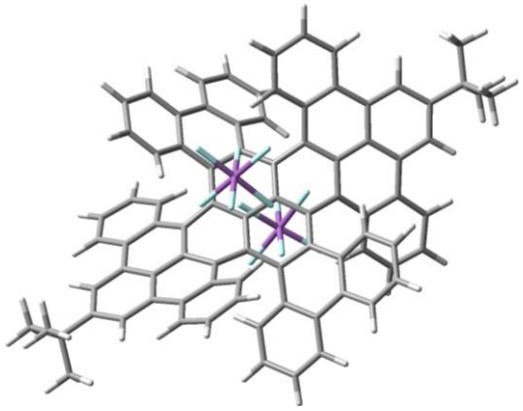
The total electronic energy was calculated to be –3233.366415 Hartree.

**Table S2.** Optimized structure of $\mathbf{1}^{2+}[SbF_6^-]_2$ (B3LYP-D3 with SDD for Sb and 6-31G(d) for the rest)



Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -7.770102 | -0.114799 | -0.577357 |
| 2 | 6 | 0 | -7.024684 | 0.950968 | -1.081345 |
| 3 | 6 | 0 | -5.621791 | 0.997890 | -0.993338 |
| 4 | 6 | 0 | -7.076961 | -1.153693 | 0.058448 |
| 5 | 6 | 0 | -5.685619 | -1.152496 | 0.205547 |
| 6 | 6 | 0 | -4.947491 | -0.071417 | -0.350630 |
| 7 | 6 | 0 | -3.515365 | -0.061142 | -0.255652 |
| 8 | 6 | 0 | -2.784340 | 1.091021 | -0.617794 |
| 9 | 6 | 0 | -3.414066 | 2.088277 | -1.444812 |
| 10 | 6 | 0 | -4.836109 | 2.071398 | -1.600532 |
| 11 | 6 | 0 | -5.424915 | 3.091160 | -2.377618 |
| 12 | 6 | 0 | -4.655139 | 4.048190 | -3.018055 |
| 13 | 6 | 0 | -3.252496 | 3.998877 | -2.943473 |
| 14 | 6 | 0 | -2.642360 | 3.028664 | -2.176336 |
| 15 | 6 | 0 | -0.706041 | -0.067080 | -0.063513 |
| 16 | 6 | 0 | -1.409023 | 1.161071 | -0.169816 |
| 17 | 6 | 0 | -0.709267 | 2.364413 | 0.066837 |
| 18 | 6 | 0 | -1.314737 | 3.593620 | 0.550614 |
| 19 | 6 | 0 | -2.479661 | 3.536700 | 1.342427 |
| 20 | 6 | 0 | -3.019709 | 4.699401 | 1.873390 |
| 21 | 6 | 0 | -2.387638 | 5.928342 | 1.647264 |
| 22 | 6 | 0 | -1.199781 | 5.986090 | 0.922605 |
| 23 | 6 | 0 | -0.632598 | 4.826865 | 0.372361 |
| 24 | 6 | 0 | 0.632856 | 4.826738 | -0.373325 |
| 25 | 6 | 0 | 1.200107 | 5.985792 | -0.923854 |
| 26 | 6 | 0 | 2.387929 | 5.927792 | -1.648556 |
| 27 | 6 | 0 | 3.019894 | 4.698754 | -1.874436 |
| 28 | 6 | 0 | 2.479785 | 3.536215 | -1.343174 |
| 29 | 6 | 0 | 1.314909 | 3.593404 | -0.551310 |
| 30 | 6 | 0 | 0.709375 | 2.364353 | -0.067213 |
| 31 | 6 | 0 | 1.409099 | 1.161046 | 0.169717 |
| 32 | 6 | 0 | 2.784398 | 1.091056 | 0.617712 |
| 33 | 6 | 0 | 3.414169 | 2.088471 | 1.444525 |
| 34 | 6 | 0 | 4.836200 | 2.071526 | 1.600314 |
| 35 | 6 | 0 | 5.425032 | 3.091321 | 2.377323 |
| 36 | 6 | 0 | 4.655283 | 4.048504 | 3.017582 |
| 37 | 6 | 0 | 3.252650 | 3.999315 | 2.942876 |
| 38 | 6 | 0 | 2.642488 | 3.029037 | 2.175825 |
| 39 | 6 | 0 | -9.897894 | 1.039370 | -1.407600 |
| 40 | 6 | 0 | -9.303086 | -0.184136 | -0.685631 |
| 41 | 6 | 0 | -9.914193 | -0.249478 | 0.734199 |
| 42 | 6 | 0 | -9.700715 | -1.451609 | -1.478129 |
| 43 | 6 | 0 | 7.770140 | -0.114814 | 0.577261 |
| 44 | 6 | 0 | 7.076969 | -1.153751 | -0.058440 |
| 45 | 6 | 0 | 5.685619 | -1.152560 | -0.205468 |
| 46 | 6 | 0 | 7.024751 | 0.951016 | 1.081169 |
| 47 | 6 | 0 | 5.621858 | 0.997920 | 0.993243 |
| 48 | 6 | 0 | 4.947522 | -0.071459 | 0.350699 |
| 49 | 6 | 0 | 3.515386 | -0.061217 | 0.255832 |
| 50 | 6 | 0 | 2.830694 | -1.195861 | -0.238663 |
| 51 | 6 | 0 | 3.550517 | -2.139257 | -1.050475 |
| 52 | 6 | 0 | 4.977115 | -2.159172 | -0.998154 |
| 53 | 6 | 0 | 5.648637 | -3.121331 | -1.777209 |
| 54 | 6 | 0 | 4.954923 | -3.974198 | -2.622961 |
| 55 | 6 | 0 | 3.560299 | -3.870341 | -2.753763 |
| 56 | 6 | 0 | 2.867083 | -2.963325 | -1.979371 |
| 57 | 6 | 0 | 0.706085 | -0.067104 | 0.063670 |
| 58 | 6 | 0 | 1.410459 | -1.292180 | 0.038080 |
| 59 | 6 | 0 | 0.697134 | -2.518790 | 0.134947 |
| 60 | 6 | 0 | 1.291807 | -3.763853 | 0.610192 |
| 61 | 6 | 0 | 2.450192 | -3.749902 | 1.416713 |
| 62 | 6 | 0 | 2.982289 | -4.921794 | 1.927373 |
| 63 | 6 | 0 | 2.344807 | -6.143450 | 1.672161 |
| 64 | 6 | 0 | 1.173083 | -6.171969 | 0.928681 |
| 65 | 6 | 0 | 0.620802 | -4.995771 | 0.388358 |
| 66 | 6 | 0 | -0.620986 | -4.995770 | -0.387621 |
| 67 | 6 | 0 | -1.173317 | -6.171974 | -0.927874 |
| 68 | 6 | 0 | -2.344998 | -6.143440 | -1.671427 |
| 69 | 6 | 0 | -2.982371 | -4.921762 | -1.926799 |
| 70 | 6 | 0 | -2.450227 | -3.749863 | -1.416203 |
| 71 | 6 | 0 | -1.291911 | -3.763832 | -0.609583 |
| 72 | 6 | 0 | -0.697205 | -2.518768 | -0.134394 |
| 73 | 6 | 0 | -1.410475 | -1.292106 | -0.037633 |
| 74 | 6 | 0 | -2.830703 | -1.195722 | 0.239042 |
| 75 | 6 | 0 | -3.550576 | -2.139098 | 1.050808 |
| 76 | 6 | 0 | -4.977169 | -2.159107 | 0.998285 |
| 77 | 6 | 0 | -5.648722 | -3.121390 | 1.777157 |
| 78 | 6 | 0 | -4.955060 | -3.974291 | 2.622921 |
| 79 | 6 | 0 | -3.560468 | -3.870307 | 2.753963 |
| 80 | 6 | 0 | -2.867217 | -2.963143 | 1.979770 |
| 81 | 6 | 0 | 9.914213 | -0.249532 | -0.734341 |
| 82 | 6 | 0 | 9.303127 | -0.184127 | 0.685494 |
| 83 | 6 | 0 | 9.700807 | -1.451549 | 1.478064 |
| 84 | 6 | 0 | 9.897915 | 1.039429 | 1.407388 |
| 85 | 1 | 0 | -7.542779 | 1.764689 | -1.567595 |
| 86 | 1 | 0 | -7.647311 | -1.980542 | 0.463370 |
| 87 | 1 | 0 | -6.500426 | 3.124012 | -2.506243 |
| 88 | 1 | 0 | -5.141318 | 4.813679 | -3.616557 |
| 89 | 1 | 0 | -2.647179 | 4.700894 | -3.508460 |
| 90 | 1 | 0 | -1.564856 | 2.932994 | -2.189045 |
| 91 | 1 | 0 | -2.894924 | 2.569289 | 1.601962 |
| 92 | 1 | 0 | -3.906029 | 4.645568 | 2.498080 |
| 93 | 1 | 0 | -2.799312 | 6.838537 | 2.074531 |
| 94 | 1 | 0 | -0.692517 | 6.939227 | 0.813139 |
| 95 | 1 | 0 | 0.692924 | 6.938996 | -0.814589 |
| 96 | 1 | 0 | 2.799646 | 6.837864 | -2.076043 |
| 97 | 1 | 0 | 3.906176 | 4.644706 | -2.499163 |
| 98 | 1 | 0 | 2.894960 | 2.568712 | -1.602510 |
| 99 | 1 | 0 | 6.500534 | 3.124081 | 2.506049 |
| 100 | 1 | 0 | 5.141486 | 4.814013 | 3.616037 |
| 101 | 1 | 0 | 2.647340 | 4.701462 | 3.507707 |
| 102 | 1 | 0 | 1.564973 | 2.933460 | 2.188483 |
| 103 | 1 | 0 | -9.524920 | 1.127354 | -2.434503 |
| 104 | 1 | 0 | -10.987657 | 0.940770 | -1.460118 |
| 105 | 1 | 0 | -9.676957 | 1.972651 | -0.876925 |
| 106 | 1 | 0 | -9.644076 | 0.638174 | 1.317157 |
| 107 | 1 | 0 | -11.007868 | -0.299990 | 0.673501 |
| 108 | 1 | 0 | -9.571167 | -1.129916 | 1.287668 |
| 109 | 1 | 0 | -9.344059 | -2.366220 | -0.992856 |
| 110 | 1 | 0 | -10.792027 | -1.521691 | -1.558567 |
| 111 | 1 | 0 | -9.283890 | -1.424950 | -2.491315 |
| 112 | 1 | 0 | 7.647289 | -1.980631 | -0.463343 |
| 113 | 1 | 0 | 7.542878 | 1.764813 | 1.567262 |
| 114 | 1 | 0 | 6.730964 | -3.177942 | -1.758980 |
| 115 | 1 | 0 | 5.504497 | -4.691618 | -3.226137 |
| 116 | 1 | 0 | 3.030774 | -4.473223 | -3.484388 |
| 117 | 1 | 0 | 1.807530 | -2.810777 | -2.137856 |
| 118 | 1 | 0 | 2.905092 | -2.801725 | 1.676811 |
| 119 | 1 | 0 | 3.869603 | -4.885150 | 2.552248 |
| 120 | 1 | 0 | 2.744279 | -7.065266 | 2.085474 |
| 121 | 1 | 0 | 0.661922 | -7.118610 | 0.791079 |
| 122 | 1 | 0 | -0.662230 | -7.118640 | -0.790168 |
| 123 | 1 | 0 | -2.744506 | -7.065268 | -2.084677 |
| 124 | 1 | 0 | -3.869627 | -4.885103 | -2.551756 |
| 125 | 1 | 0 | -2.905025 | -2.801672 | -1.676429 |
| 126 | 1 | 0 | -6.731040 | -3.178103 | 1.758772 |
| 127 | 1 | 0 | -5.504665 | -4.691834 | 3.225921 |
| 128 | 1 | 0 | -3.030999 | -4.473223 | 3.484603 |
| 129 | 1 | 0 | -1.807728 | -2.810410 | 2.138515 |

| | | | | | |
|---|---|---|---|---|---|
| 130 | 1 | 0 | 9.644040 | 0.638067 | -1.317354 |
| 131 | 1 | 0 | 11.007893 | -0.299982 | -0.673662 |
| 132 | 1 | 0 | 9.571221 | -1.130025 | -1.287740 |
| 133 | 1 | 0 | 9.344197 | -2.366202 | 0.992836 |
| 134 | 1 | 0 | 10.792121 | -1.521574 | 1.558512 |
| 135 | 1 | 0 | 9.283972 | -1.424854 | 2.491244 |
| 136 | 1 | 0 | 9.525017 | 1.127414 | 2.434318 |
| 137 | 1 | 0 | 10.987690 | 0.940902 | 1.459818 |
| 138 | 1 | 0 | 9.676876 | 1.972686 | 0.876710 |
| 139 | 51 | 0 | 1.057964 | 0.196806 | -3.717732 |
| 140 | 9 | 0 | -0.359558 | 0.037354 | -4.939825 |
| 141 | 9 | 0 | 2.086266 | -1.140584 | -4.554743 |
| 142 | 9 | 0 | 1.852409 | 1.582958 | -4.707302 |
| 143 | 9 | 0 | 0.064192 | 1.467679 | -2.697248 |
| 144 | 9 | 0 | 0.272903 | -1.171370 | -2.636678 |
| 145 | 9 | 0 | 2.439836 | 0.397360 | -2.410250 |
| 146 | 51 | 0 | -1.058050 | 0.197795 | 3.717952 |
| 147 | 9 | 0 | 0.359326 | 0.038427 | 4.940222 |
| 148 | 9 | 0 | -2.086397 | -1.139125 | 4.555626 |
| 149 | 9 | 0 | -1.852080 | 1.584685 | 4.706815 |
| 150 | 9 | 0 | -2.439974 | 0.397840 | 2.410446 |
| 151 | 9 | 0 | -0.273239 | -1.170785 | 2.637241 |
| 152 | 9 | 0 | -0.064103 | 1.468207 | 2.697054 |

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The total electronic energy was calculated to be –4442.9477363 Hartree.

## 5. References

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