Electronic Supplementary Information (ESI) for Chemical Communication

Isolation and Crystal Structure of a Dithiophene Dication: Controlling Covalent Connection and Disconnction with Temperature and Phase

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Experimental Section

General Procedures

All experiments were carried out under a nitrogen atmosphere by using standard Schlenk techniques and a glovebox. Solvents were dried and degassed prior to use. $NOSbF_6$ (Alfa Aesar) was purchased and used upon arrival. $Li[Al(OR_F)_4]$ [1] and 1,2-Bis[5′-(4″-methoxyphenyl)-2′-methylthien-3′-yl]cyclopentene (**1o**)[2] were prepared by the published procedures. The NMR spectra were performed using a Bruker DRX-400 at variable-temperature in ppm downfield from internal Me_4Si. EPR spectra were obtained using Bruker EMX-10/12 variable-temperature apparatus. UV-vis spectra were recorded on the Lambda 750 spectrometer. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. X-ray crystal structures were obtained by using Bruker APEX DUO CCD detector.

Synthesis of $\mathbf{1c^{2+}}$•2$\mathbf{[Al(OR_F)_4]^-}$. A mixture of **1** (0.101 g, 1.13 mmol), $NOSbF_6$ (0.112 g, 0.420 mmol) and $Li[Al(OR_F)_4]$ (0.412 g, 0.420 mmol) in CH_2Cl_2 (~50 ml) were stirred at room temperature for 1d. The resultant bluish violet solution over a colorless precipitate of $LiSbF_6$ was filtered. The filtrate was then concentrated and stored at ca. -20 ^oC for 2d to afford violet crystals of the salt $\mathbf{1c^{2+}}$•2$[Al(OR_F)_4]^-$. Isolated Yield: 0.310 g, 63.4 %; elemental analysis calcd (%): C 30.12, H 1.27; found: C 30.23, H 1.23.

Reduction Reactions with Zn: Two identical solutions of $\mathbf{1c^{2+}}$•2$[Al(OR_F)_4]$ in THF with Zn powder (molar ratio $\mathbf{1c^{2+}}$•2$[Al(OR_F)_4]$: Zn = 1 : 98) were stirred about 10 h at 40 ^oC and -80 ^oC (in the dark), respectively. The unreacted solid was removed by filtration and the solvent was removed by vacuo. The residue was extracted with n-hexane and the identity of extractions was checked by UV-vis spectroscopy (Figures S3a,4a).

Computational details

All the geometry optimizations were carried out at the (U)B3LYP/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The spin densities were calculated at the level of UB3LYP/6-31G(d) at the optimized geometries. The UV absorption spectra were calculated using time-dependent DFT (TD-DFT) method at the (U)LC-wPBE/6-311+G(d,p) level, and polarized continuum model (PCM) was adopted to consider solvent (CH_3CN) effects. All calculations were performed with the Gaussian 09 program suite.

References:

1 I. Krossing, *Chem. –Eur. J.* **2001**, *7*, 490.

2 J. J. D. de Jong, L. N. Lucas, R. M. Kellogg, B. L. Feringa, J. H. van Esch, *Eur. J. Org. Chem.* **2003**, 1887.

Table S1. Crystal data and structure refinement for $\mathbf{1c}^{2+}\bullet 2[Al(OR_F)_4]^-\bullet CH_2Cl_2$.

	$\mathbf{1c}^{2+}\bullet 2[Al(OR_F)_4]^-\bullet CH_2Cl_2$
formula	$C_{62}H_{30}Al_2F_{72}Cl_2O_{10}S_2$
Mr [g mol^{-1}]	2491.84
crystal system	Monoclinic
space group	*P*2(1)/n
Z	4
Temp. (K)	123(2)
μ(mm^{-1})	0.361
a (Å)	11.7515(12)
b (Å)	24.273(3)
c (Å)	30.087(3)
α (°)	
β (°)	99.776(2)
γ (°)	
V [Å^3]	8457.5(15)
*R*1 ($I>2\sigma(I)$)	0.0754
*wR*2 (all data)	0.2025

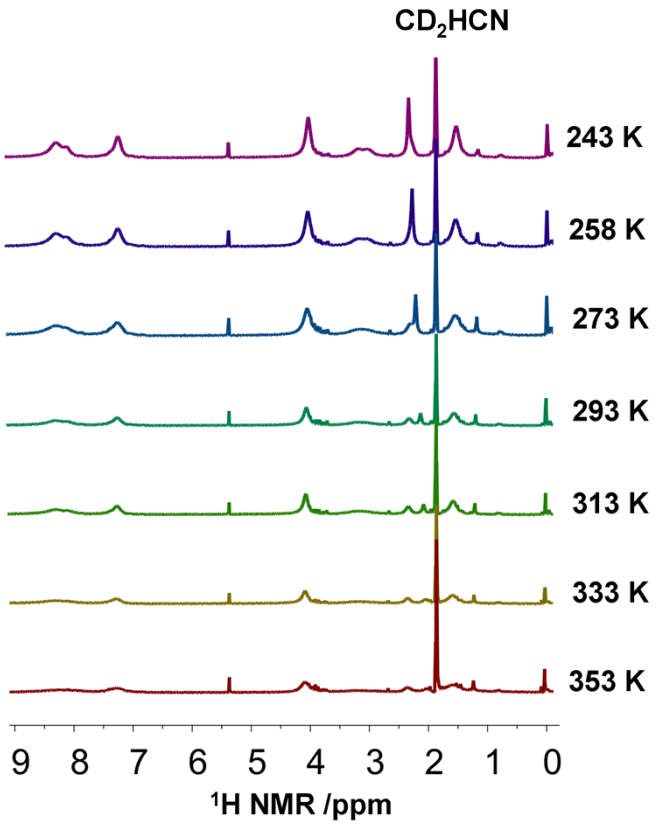


Fig. S1 ^{1}H NMR spectra of $\mathbf{1c}^{2+}$•2[Al(OR$_F$)$_4$]$^-$ in CD_3CN between 243 and 353 K.

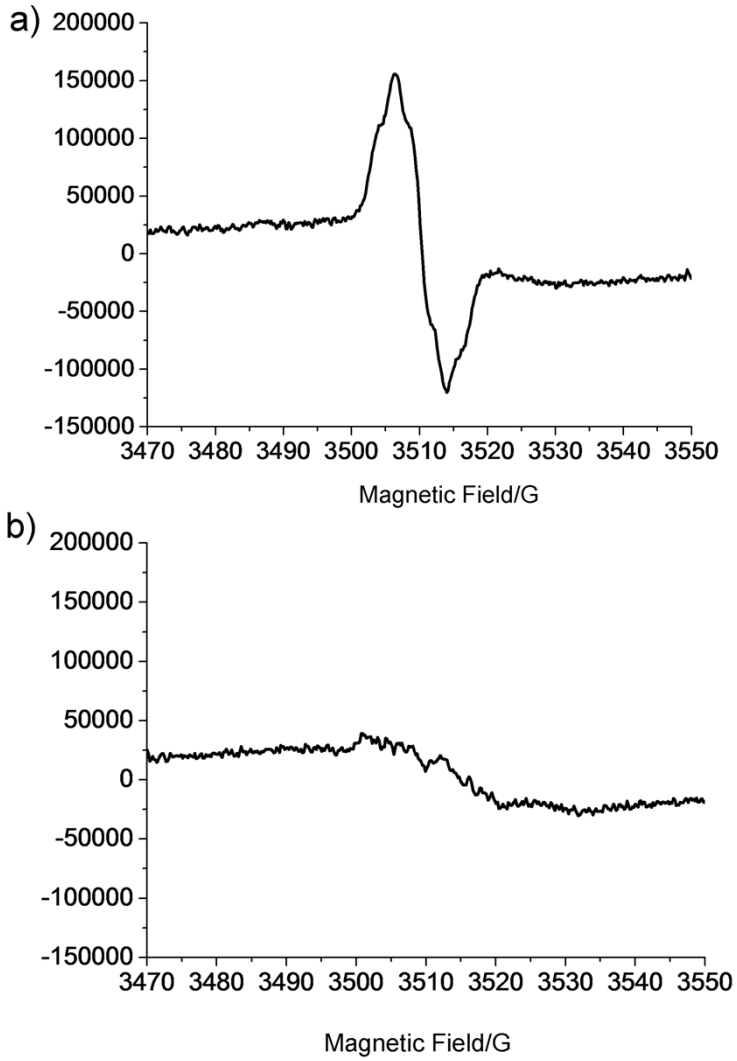


Fig.S2 EPR spectra of a) $\mathbf{1c^{2+}}$•2$[Al(OR_F)_4]^-$ in CH_2Cl_2 (1 x 10^{-3} M) and b) $\mathbf{1c^{2+}}$•2$[Al(OR_F)_4]^-$ in CH_2Cl_2 (1 x 10^{-3} M) with a small amount of $NO[Al(OR_F)_4]$.

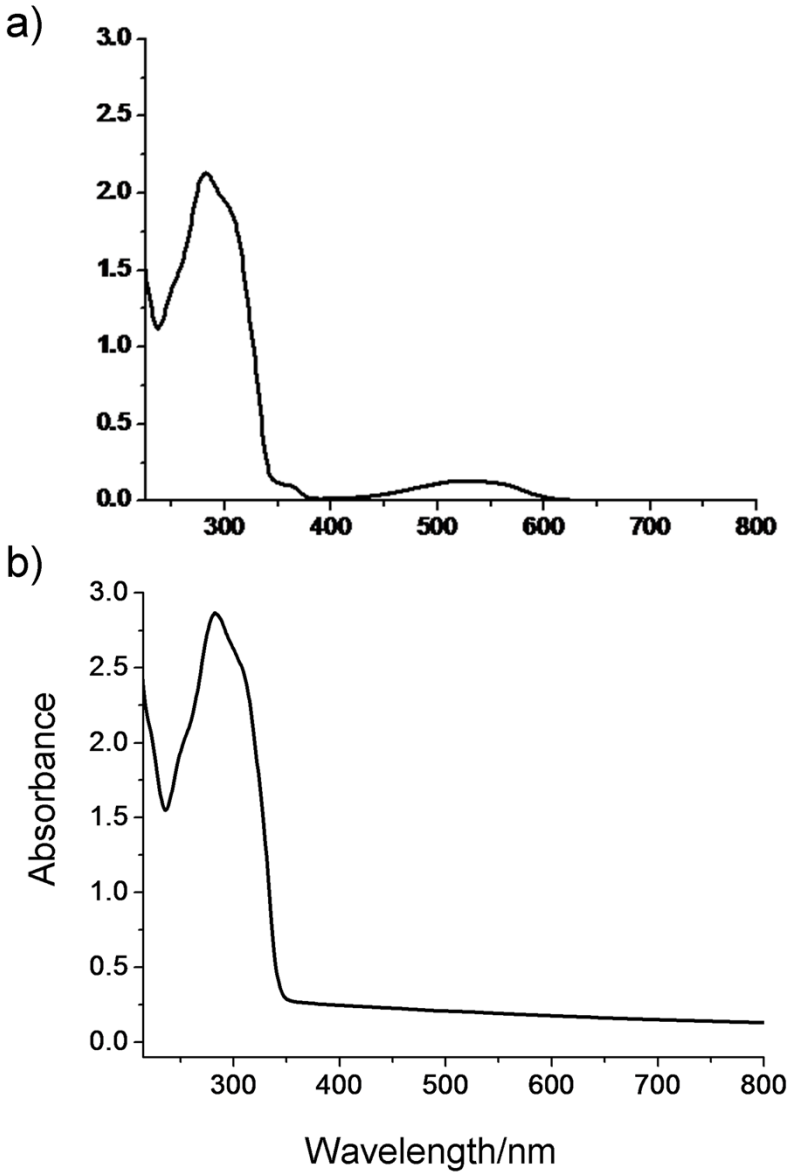


Fig.S3 a) UV-vis spectrum of hexane extraction of reduction reaction solution of **1c**$^{2+}$•2[Al(OR$_F$)$_4$]$^-$ with Zn in THF at 40 ^{o}C. b) UV-vis spectrum of **1o** in hexane.

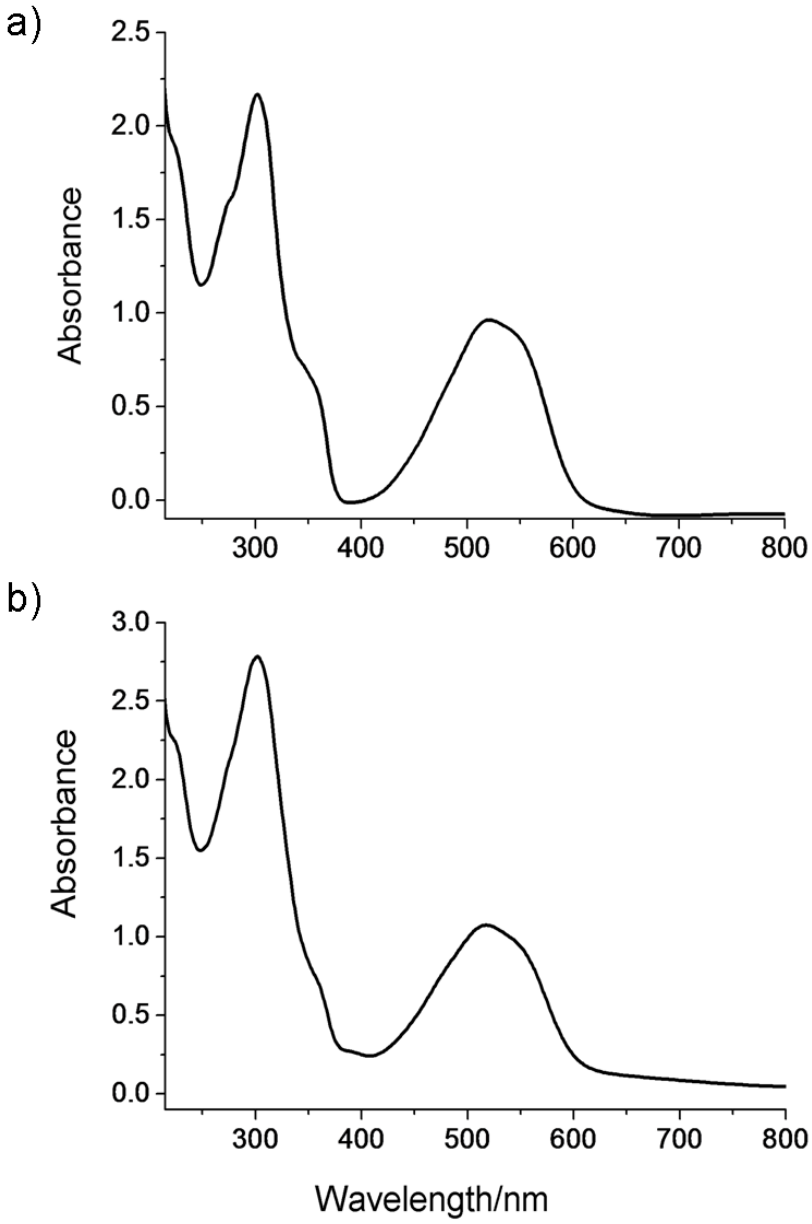
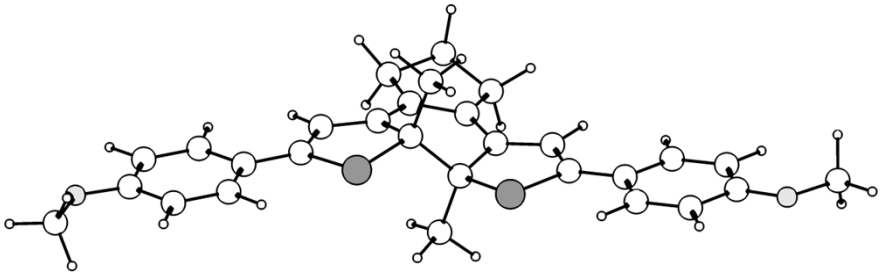
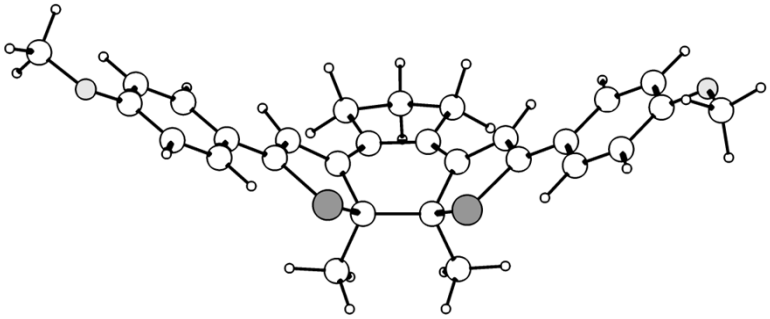


Fig.S4 a) UV-Vis spectrum of hexane extraction of reduction reaction solution of **1c**$^{2+}$•2[Al(OR$_F$)$_4$]$^-$ with Zn in THF at -80 ^{o}C (in the dark). b) UV-vis spectrum of **1c** in hexane obtained by irradiation of **1o** with UV-light.



Trans-, -2067.742277 a.u.



Cis-, -2067.717938 a.u.

Fig.S5 The geometry and energy of the *trans*- and *cis*-isomers of $\mathbf{1c}^{2+}$.

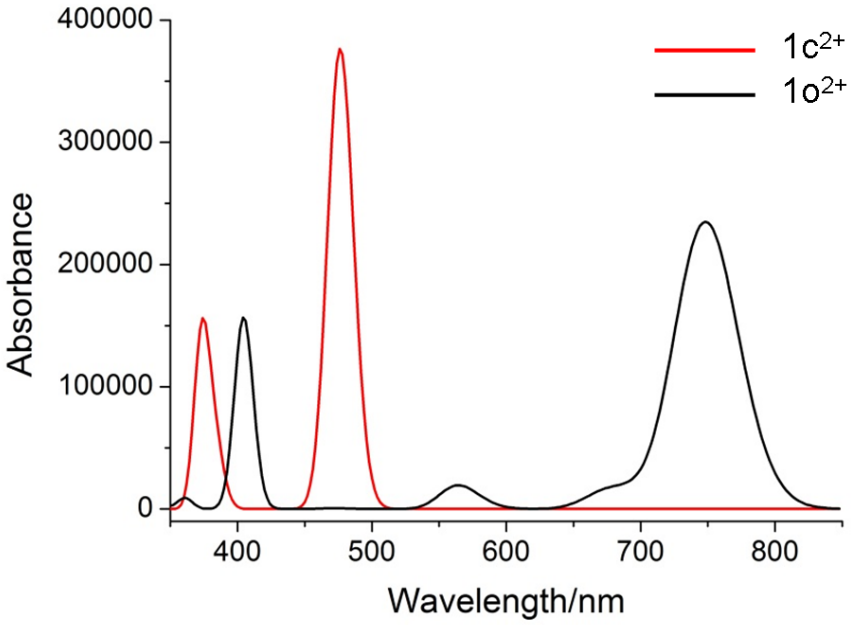


Fig. S6 The calculated UV spectra by at (U)LC-wPBE/6-311+G(d,p) with the PCM solvent model.

Table S2. TD-DFT calculated absorption wavelengths (λ), oscillator strengths (f), and assignments for four highest electronic transition configurations of $\mathbf{1c}^{2+}$.[a]

No.	λ (nm)	f	Assignment
1	476.4	1.7322	**HOMO->LUMO (79%)**, H-5->L+1 (2%), H-2->LUMO (7%), H-1->L+1 (8%)
2	383.5	0.217	H-1->LUMO (58%), HOMO->L+1 (30%), H-7->LUMO (2%), H-2->L+1 (5%), H-1->L+2 (2%)
3	373.4	0.6569	H-2->LUMO (59%), H-1->L+1 (28%), H-6->LUMO (2%), H-5->L+1 (4%), HOMO->L+2 (2%)
4	325.5	0.2195	H-5->LUMO (12%), H-2->L+1 (35%), HOMO->L+1 (36%), H-6->L+1 (2%), H-3->LUMO (2%), H-1->LUMO (6%)

[a] H represents HOMO and L represents LUMO.

Table S3. TD-DFT calculated absorption wavelengths (λ), oscillator strengths (f), and assignments for ten highest electronic transition configurations of $\mathbf{1o}^{2+}$.

No.	λ (nm)	f	Assignment
1	748.28	1.0797	**H-2(α)->LUMO(α) (13%), H-1(α)->LUMO(α) (28%), HOMO(α)->LUMO(α) (19%), H-2(β)->LUMO(β) (11%), H-1(β)->LUMO(β) (12%)**, H-3(α)->LUMO(α) (2%), **HOMO(β)->LUMO(β) (7%)**
2	679.99	0.079	H-1(α)->LUMO(α) (14%), H-2(β)->LUMO(β) (15%), H-1(β)->LUMO(β) (27%), HOMO(β)->LUMO(β) (16%), H-3(α)->LUMO(α) (2%), H-2(α)->LUMO(α) (2%), HOMO(α)->LUMO(α) (9%), H-3(β)->LUMO(β) (3%)
3	576.24	0.0209	H-2(α)->LUMO(α) (40%), H-2(β)->LUMO(β) (22%), H-3(α)->LUMO(α) (9%), H-3(β)->LUMO(β) (7%), HOMO(β)->L+1(β) (2%)
4	562.16	0.0758	H-2(α)->LUMO(α) (19%), H-3(β)->LUMO(β) (18%), H-2(β)->LUMO(β) (27%) H-3(α)->LUMO(α) (8%), HOMO(α)->LUMO(α) (2%), H-7(β)->LUMO(β) (2%), H-4(β)->LUMO(β) (3%), H-1(β)->LUMO(β) (2%), HOMO(β)->LUMO(β) (4%)
5	474.29	0.0014	H-6(β)->LUMO(β) (34%), H-5(β)->LUMO(β) (24%), H-4(β)->LUMO(β) (19%) H-7(β)->LUMO(β) (5%), H-6(β)->L+2(β) (2%), H-5(β)->L+2(β) (2%), H-3(β)->LUMO(β) (2%)
6	469.63	0.0016	H-6(α)->LUMO(α) (11%), H-5(α)->LUMO(α) (26%), H-4(α)->LUMO(α) (40%) H-7(α)->LUMO(α) (5%), H-5(α)->L+2(α) (2%), H-4(α)->L+2(α) (3%), H-3(α)->LUMO(α) (3%)
7	434.56	0.0004	H-7(α)->LUMO(α) (3%), H-3(α)->LUMO(α) (4%), H-2(α)->L+3(α) (2%), H-1(α)->L+3(α) (6%), H-1(α)->L+4(α) (3%), HOMO(α)->L+1(α) (7%), HOMO(α)->L+3(α) (7%), HOMO(α)->L+4(α) (3%), H-7(β)->LUMO(β) (2%), H-6(β)->LUMO(β) (2%), H-3(β)->LUMO(β) (4%), H-1(β)->L+3(β) (7%), H-1(β)->L+4(β) (2%), HOMO(β)->L+1(β) (9%), HOMO(β)->L+3(β) (7%), HOMO(β)->L+4(β) (2%)
8	404.62	0.715	H-1(α)->L+1(α) (10%), HOMO(α)->L+1(α) (29%), HOMO(β)->L+1(β) (26%) H-1(β)->L+1(β) (7%)
9	396.00	0.0154	HOMO(α)->L+1(α) (17%), HOMO(β)->L+1(β) (22%), H-5(α)->L+4(α) (2%), H-2(α)->LUMO(α) (2%), H-1(α)->L+1(α) (8%), HOMO(α)->LUMO(α) (2%), H-2(β)->LUMO(β) (2%), H-1(β)->L+1(β) (8%), HOMO(β)->LUMO(β) (4%)
10	360.75	0.0415	HOMO(α)->LUMO(α) (10%), H-3(β)->LUMO(β) (13%), HOMO(β)->LUMO(β) (26%), H-7(α)->LUMO(α) (3%), H-6(α)->LUMO(α) (2%), H-3(α)->LUMO(α) (6%), H-2(α)->LUMO(α) (3%), HOMO(α)->L+1(α) (3%), H-7(β)->LUMO(β) (4%), H-6(β)->LUMO(β) (4%), H-4(β)->LUMO(β) (4%), H-2(β)->LUMO(β) (5%)

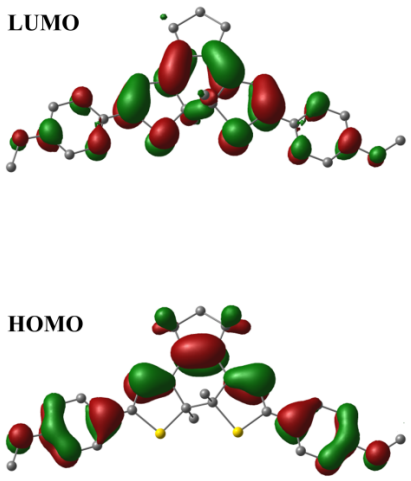


Fig. S7 The frontier molecular orbitals for $\mathbf{1c}^{2+}$.

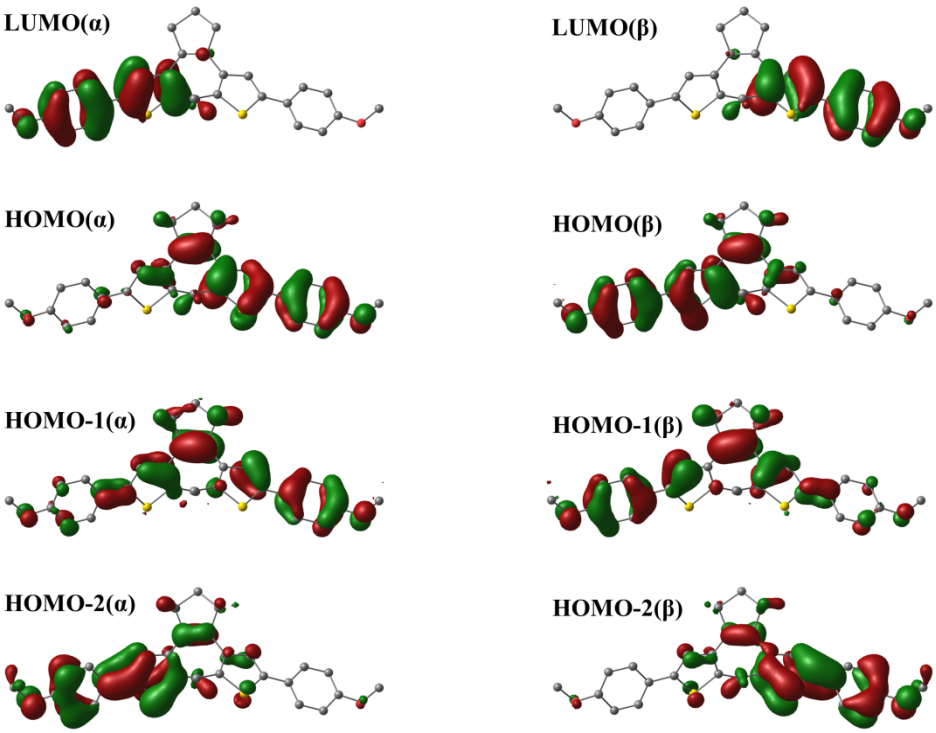


Fig. S8 The frontier molecular orbitals for **1o**$^{2+}$.

Coordinates for calculated geometries

trans-**1c**$^{2+}$

C	6.886199000	-0.255299000	-0.000831000
C	5.596230000	0.216266000	0.085913000
C	7.116978000	-1.652088000	-0.078789000
C	4.473385000	-0.665073000	0.103238000
C	6.014274000	-2.551095000	-0.064275000
O	8.306412000	-2.216778000	-0.167001000
C	3.151080000	-0.162506000	0.200244000
C	4.736488000	-2.069236000	0.024980000
C	9.511618000	-1.420738000	-0.191236000
C	2.763927000	1.217104000	0.233315000
S	1.756437000	-1.213231000	0.272456000
C	1.418316000	1.443328000	0.307701000
C	0.570450000	0.196773000	0.520605000
C	0.735212000	2.701581000	0.173653000
C	1.314873000	4.089728000	0.302266000
C	-0.606819000	0.251298000	-0.513193000
C	0.083887000	0.134318000	1.991785000
C	-0.616788000	2.746390000	-0.083539000
C	-1.122108000	4.169349000	-0.113177000
C	0.181061000	5.004239000	-0.232919000
S	-1.878107000	-1.091361000	-0.313971000
C	-1.375674000	1.537711000	-0.248537000
C	-0.124076000	0.212071000	-1.985978000
C	-2.732067000	1.393211000	-0.166925000
C	-3.204975000	0.040653000	-0.184829000

C	-4.557600000	-0.375199000	-0.096844000
C	-4.912509000	-1.756995000	-0.087308000
C	-5.622412000	0.579289000	-0.020869000
C	-6.930334000	0.180209000	0.056054000
C	-6.221239000	-2.170868000	-0.009325000
C	-7.257193000	-1.202427000	0.063842000
O	-8.544551000	-1.481934000	0.141682000
H	0.366155000	5.241270000	-1.284948000
H	0.119857000	5.949569000	0.309591000
H	3.486390000	2.018561000	0.142805000
H	7.714548000	0.442359000	-0.007142000
H	5.449303000	1.288341000	0.149847000
H	6.220067000	-3.614179000	-0.125123000
H	3.912831000	-2.777105000	0.034371000
H	9.606660000	-0.848393000	0.735879000
H	9.511195000	-0.758089000	-1.061354000
H	-0.446301000	-0.800626000	2.185755000
H	-0.588411000	0.969705000	2.207416000
H	0.935398000	0.194460000	2.673713000
H	0.344433000	-0.747438000	-2.216062000
H	0.600454000	1.010191000	-2.171430000
H	-0.969631000	0.352571000	-2.663538000
H	-4.135928000	-2.514549000	-0.143105000
H	-5.408153000	1.641614000	-0.029859000
H	-7.741523000	0.897964000	0.110608000
H	-6.452793000	-3.228914000	-0.004572000
H	-3.401880000	2.234522000	-0.039503000

C	-9.013988000	-2.848028000	0.157360000
H	-10.097703000	-2.772423000	0.225012000
H	-8.619262000	-3.374905000	1.030703000
H	-8.730243000	-3.357426000	-0.767868000
H	-1.822343000	4.355121000	-0.934315000
H	2.253154000	4.212479000	-0.250935000
H	1.546204000	4.295626000	1.357046000
H	-1.661354000	4.390372000	0.819919000
H	10.323535000	-2.141314000	-0.270437000

cis-**1c**$^{2+}$

C	-5.986480000	-1.293555000	-1.064724000
C	-4.919927000	-0.457196000	-0.823620000
C	-6.045766000	-2.555180000	-0.421237000
C	-3.865450000	-0.821822000	0.065998000
C	-5.003894000	-2.943732000	0.465896000
O	-7.016873000	-3.436471000	-0.574543000
C	-2.785183000	0.062266000	0.320265000
C	-3.951470000	-2.100689000	0.700730000
C	-8.140744000	-3.165196000	-1.440023000
C	-2.562598000	1.335834000	-0.298391000
S	-1.502797000	-0.330208000	1.438163000
C	-1.426057000	1.979337000	0.102423000
C	-0.769584000	1.391002000	1.341359000
C	-0.783802000	3.078865000	-0.567223000
C	-1.392925000	4.112655000	-1.485550000

C	0.822038000	1.462271000	1.283370000
C	-1.366871000	2.153548000	2.565324000
C	0.587616000	3.090121000	-0.647528000
C	1.068811000	4.131246000	-1.631210000
C	-0.184909000	5.021821000	-1.830759000
S	1.710820000	-0.177342000	1.432803000
C	1.331090000	2.022654000	-0.032988000
C	1.430808000	2.363623000	2.402757000
C	2.459594000	1.423434000	-0.513899000
C	2.836140000	0.213505000	0.156339000
C	3.953951000	-0.603653000	-0.153415000
C	4.237537000	-1.790330000	0.585164000
C	4.850855000	-0.257971000	-1.214169000
C	5.940013000	-1.035822000	-1.506500000
C	5.327878000	-2.579267000	0.302648000
C	6.202203000	-2.211267000	-0.753482000
O	7.277490000	-2.888783000	-1.111129000
H	-0.149742000	5.864723000	-1.133880000
H	-0.247892000	5.432911000	-2.840124000
H	-3.198347000	1.710562000	-1.090771000
H	-6.773038000	-0.980825000	-1.740350000
H	-4.903877000	0.504934000	-1.322832000
H	-5.074987000	-3.914344000	0.944507000
H	-3.172435000	-2.418910000	1.387364000
H	-7.802195000	-3.029207000	-2.471149000
H	-8.686080000	-2.284526000	-1.088944000
H	-2.455661000	2.074615000	2.548636000

H	-1.105510000	3.213816000	2.528842000
H	-1.012410000	1.733500000	3.508539000
H	1.198998000	1.980040000	3.397673000
H	1.057551000	3.387542000	2.320512000
H	2.517304000	2.391642000	2.296497000
H	3.585734000	-2.086692000	1.402123000
H	4.682481000	0.634600000	-1.805234000
H	6.624635000	-0.777530000	-2.306961000
H	5.513947000	-3.471176000	0.888295000
H	2.996415000	1.794253000	-1.378073000
C	7.662271000	-4.097793000	-0.421222000
H	8.570815000	-4.429871000	-0.920256000
H	6.881021000	-4.856817000	-0.520164000
H	7.868947000	-3.884996000	0.631470000
H	1.938994000	4.686551000	-1.264808000
H	-2.222006000	4.655343000	-1.018683000
H	-1.799858000	3.623352000	-2.382895000
H	1.375130000	3.645967000	-2.569825000
H	-8.772112000	-4.048880000	-1.367604000

1o^{2+}-CS

C	-0.651562000	2.550820000	-0.179819000
C	0.648163000	2.551743000	0.249285000
C	1.167010000	3.966536000	0.413355000
H	2.153280000	4.115859000	-0.041981000
H	1.292010000	4.185073000	1.483961000

C	0.068394000	4.840899000	-0.237770000
H	-0.074918000	5.789359000	0.283998000
H	0.345224000	5.073778000	-1.270872000
C	-1.206592000	3.961385000	-0.234300000
H	-1.825807000	4.157292000	0.654483000
H	-1.846885000	4.128561000	-1.106623000
C	-1.420170000	1.364907000	-0.521770000
C	-2.771532000	1.179838000	-0.170060000
H	-3.327223000	1.914404000	0.400070000
C	-3.313662000	-0.047847000	-0.551744000
S	-2.087694000	-0.981507000	-1.437662000
C	-0.909741000	0.269753000	-1.281509000
C	0.329170000	0.194109000	-2.117844000
H	0.842848000	1.155169000	-2.130830000
H	0.074742000	-0.073004000	-3.149706000
H	1.027403000	-0.570279000	-1.752032000
C	1.421840000	1.360624000	0.573212000
C	2.770707000	1.177966000	0.210449000
H	3.324661000	1.918985000	-0.352712000
C	3.313168000	-0.056265000	0.569603000
S	2.091569000	-1.000780000	1.448112000
C	0.913625000	0.253414000	1.315555000
C	-0.322488000	0.162593000	2.155021000
H	-0.852746000	1.114506000	2.166346000
H	-0.060982000	-0.095253000	3.187623000
H	-1.008306000	-0.615341000	1.794778000
C	-4.625956000	-0.568156000	-0.335467000

C	-5.657453000	0.264641000	0.191694000
C	-4.962200000	-1.920247000	-0.648987000
C	-6.934434000	-0.206805000	0.395187000
H	-5.445999000	1.302564000	0.424184000
C	-6.228983000	-2.404028000	-0.448356000
H	-4.206326000	-2.590592000	-1.047401000
C	-7.242193000	-1.555848000	0.077409000
H	-7.696576000	0.455178000	0.787926000
H	-6.490711000	-3.430160000	-0.682503000
C	4.623833000	-0.574804000	0.336080000
C	5.652536000	0.264455000	-0.185632000
C	4.960383000	-1.931744000	0.626498000
C	6.927454000	-0.205525000	-0.405837000
H	5.441086000	1.306149000	-0.400577000
C	6.225073000	-2.414129000	0.409172000
H	4.206594000	-2.607031000	1.020511000
C	7.235602000	-1.559497000	-0.111007000
H	7.687579000	0.461480000	-0.793956000
H	6.487033000	-3.444014000	0.625953000
O	-8.429351000	-2.115606000	0.228387000
O	8.421047000	-2.118576000	-0.278969000
C	-9.550858000	-1.365634000	0.742886000
H	-10.379348000	-2.071394000	0.757000000
H	-9.339125000	-1.013870000	1.756717000
H	-9.782400000	-0.527387000	0.079453000
C	9.539769000	-1.362005000	-0.789472000
H	10.367202000	-2.068461000	-0.820851000

H	9.321399000	-0.993709000	-1.796019000
H	9.777323000	-0.534723000	-0.114480000

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C	-0.656293000	2.154962000	-0.168433000
C	0.647607000	2.164562000	0.218538000
C	1.147443000	3.592223000	0.401100000
H	2.137502000	3.755715000	-0.040502000
H	1.255858000	3.803900000	1.475031000
C	0.051401000	4.457876000	-0.253736000
H	-0.089184000	5.415291000	0.253036000
H	0.321359000	4.671998000	-1.293080000
C	-1.212912000	3.573577000	-0.224132000
H	-1.819781000	3.772841000	0.672501000
H	-1.866595000	3.732187000	-1.088397000
C	-1.528635000	1.021662000	-0.507971000
C	-2.877522000	0.960756000	-0.104292000
H	-3.324219000	1.712132000	0.535428000
C	-3.588428000	-0.149091000	-0.579050000
S	-2.528294000	-1.130134000	-1.595206000
C	-1.194261000	-0.051117000	-1.365478000
C	0.075608000	-0.291094000	-2.116354000
H	0.630230000	0.643467000	-2.227065000
H	-0.124588000	-0.699553000	-3.111786000
H	0.720600000	-1.009195000	-1.593560000
C	1.534147000	1.037286000	0.555707000

C	2.873680000	0.967668000	0.124287000
H	3.307793000	1.706458000	-0.538265000
C	3.592728000	-0.137311000	0.599971000
S	2.552303000	-1.101987000	1.650571000
C	1.215003000	-0.024191000	1.431430000
C	-0.044263000	-0.259514000	2.201543000
H	-0.615310000	0.667508000	2.286995000
H	0.171478000	-0.631471000	3.208132000
H	-0.680311000	-1.006234000	1.708639000
C	-4.952402000	-0.503072000	-0.349512000
C	-5.817576000	0.361717000	0.390298000
C	-5.508985000	-1.718537000	-0.857536000
C	-7.138410000	0.049657000	0.609388000
H	-5.435805000	1.296893000	0.783890000
C	-6.821683000	-2.043855000	-0.644371000
H	-4.886455000	-2.405616000	-1.422461000
C	-7.665687000	-1.164529000	0.093161000
H	-7.768056000	0.731365000	1.168258000
H	-7.250755000	-2.964007000	-1.026073000
C	4.951329000	-0.495636000	0.347449000
C	5.802029000	0.357151000	-0.423195000
C	5.517477000	-1.704003000	0.862587000
C	7.117748000	0.040679000	-0.664252000
H	5.412981000	1.286576000	-0.823184000
C	6.825165000	-2.033710000	0.627812000
H	4.906055000	-2.381667000	1.450510000
C	7.654754000	-1.166166000	-0.140128000

H	7.736416000	0.713145000	-1.246133000
H	7.261503000	-2.948275000	1.014694000
O	-8.913448000	-1.567924000	0.237884000
O	8.898683000	-1.572657000	-0.303587000
C	-9.884249000	-0.771862000	0.954830000
H	-10.806779000	-1.347642000	0.911447000
H	-9.570775000	-0.639404000	1.994051000
H	-10.018878000	0.193869000	0.459878000
C	9.856360000	-0.789024000	-1.051913000
H	10.778734000	-1.365630000	-1.017759000
H	9.522266000	-0.672285000	-2.086544000
H	10.001685000	0.183855000	-0.574373000

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C	-0.658452000	2.098611000	-0.165693000
C	0.648309000	2.111181000	0.212147000
C	1.144774000	3.541267000	0.390967000
H	2.133717000	3.706566000	-0.052366000
H	1.254423000	3.754861000	1.464425000
C	0.046208000	4.403225000	-0.262686000
H	-0.092330000	5.363356000	0.239568000
H	0.310725000	4.611470000	-1.304652000
C	-1.215958000	3.517794000	-0.221107000
H	-1.815816000	3.718954000	0.679862000
H	-1.876460000	3.673425000	-1.080733000
C	-1.542665000	0.971425000	-0.498225000

C	-2.894992000	0.937105000	-0.102027000
H	-3.332873000	1.702608000	0.526824000
C	-3.622799000	-0.164536000	-0.571276000
S	-2.574823000	-1.172579000	-1.571780000
C	-1.222606000	-0.115888000	-1.341820000
C	0.052770000	-0.392096000	-2.069740000
H	0.606514000	0.537216000	-2.224578000
H	-0.136802000	-0.854329000	-3.043208000
H	0.695655000	-1.077441000	-1.502001000
C	1.549478000	0.994072000	0.548536000
C	2.890356000	0.946601000	0.117841000
H	3.312679000	1.692402000	-0.544360000
C	3.628495000	-0.145642000	0.595534000
S	2.604948000	-1.126449000	1.645939000
C	1.248412000	-0.072828000	1.422934000
C	-0.013342000	-0.336569000	2.178780000
H	-0.582083000	0.588309000	2.300645000
H	0.195796000	-0.752980000	3.168933000
H	-0.650656000	-1.057366000	1.649874000
C	-4.994242000	-0.491444000	-0.345368000
C	-5.844716000	0.390351000	0.391559000
C	-5.572641000	-1.696609000	-0.853707000
C	-7.171761000	0.103675000	0.607633000
H	-5.446069000	1.317967000	0.786245000
C	-6.891765000	-1.996723000	-0.643529000
H	-4.961968000	-2.395667000	-1.416853000
C	-7.720720000	-1.100798000	0.091260000

H	-7.789691000	0.797448000	1.164728000
H	-7.337311000	-2.908922000	-1.025438000
C	4.993411000	-0.479181000	0.343114000
C	5.825400000	0.381949000	-0.438914000
C	5.584394000	-1.671048000	0.869070000
C	7.146264000	0.088541000	-0.680564000
H	5.417085000	1.298876000	-0.848358000
C	6.897479000	-1.977781000	0.633878000
H	4.987883000	-2.353935000	1.466158000
C	7.707985000	-1.102296000	-0.145663000
H	7.750151000	0.766440000	-1.271595000
H	7.352574000	-2.879663000	1.028841000
O	-8.976094000	-1.480585000	0.233653000
O	8.958754000	-1.486712000	-0.309107000
C	-9.933401000	-0.666202000	0.948287000
H	-10.866337000	-1.224841000	0.903389000
H	-9.619530000	-0.539032000	1.988048000
H	-10.049075000	0.301563000	0.452543000
C	9.899175000	-0.693556000	-1.069462000
H	10.832076000	-1.252790000	-1.032694000
H	9.559135000	-0.594129000	-2.103952000
H	10.028217000	0.286829000	-0.602763000