Electronic Supplementary Information for the paper

Entitled

Dicationic Ditelluride Salts Stabilized by *N*-Heterocyclic Carbene

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Table S2. NPA charges and WBI of **1**, $\mathbf{3}^{2+}$, and **4**.

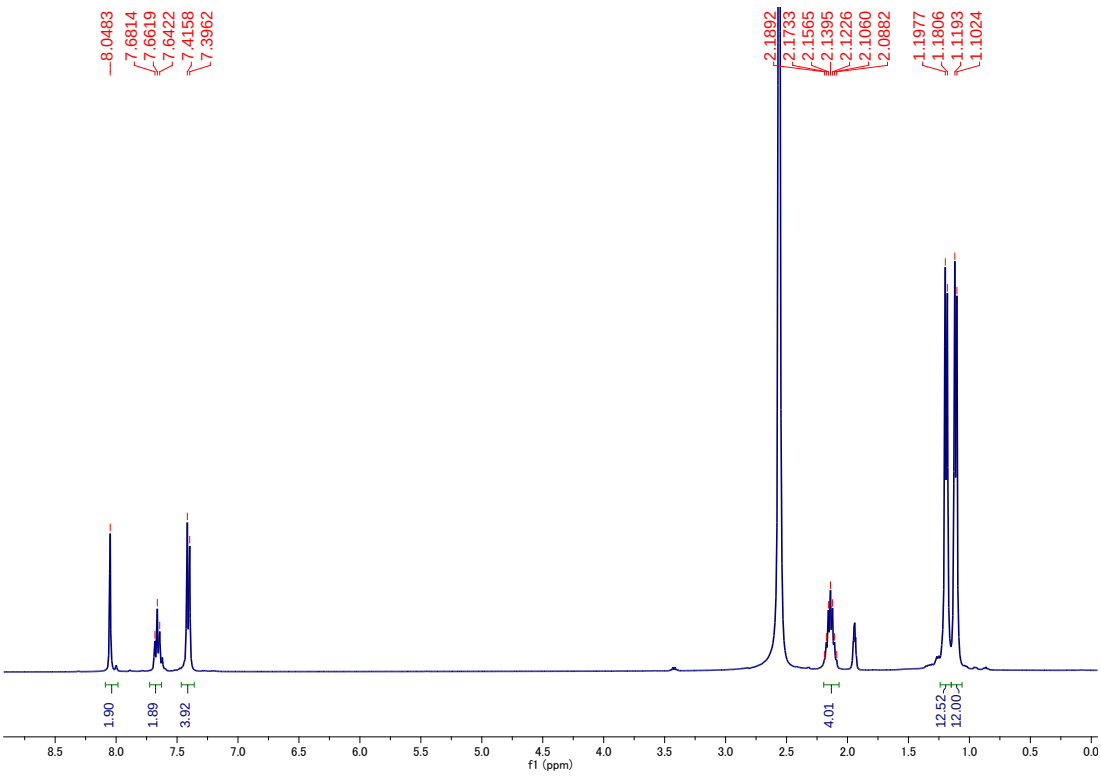


Figure S1. ^{1}H NMR (400 MHz, 25 °C, CD_3CN) of $\mathbf{2}^{2+}$ 2 $(OTf)^{-}$.

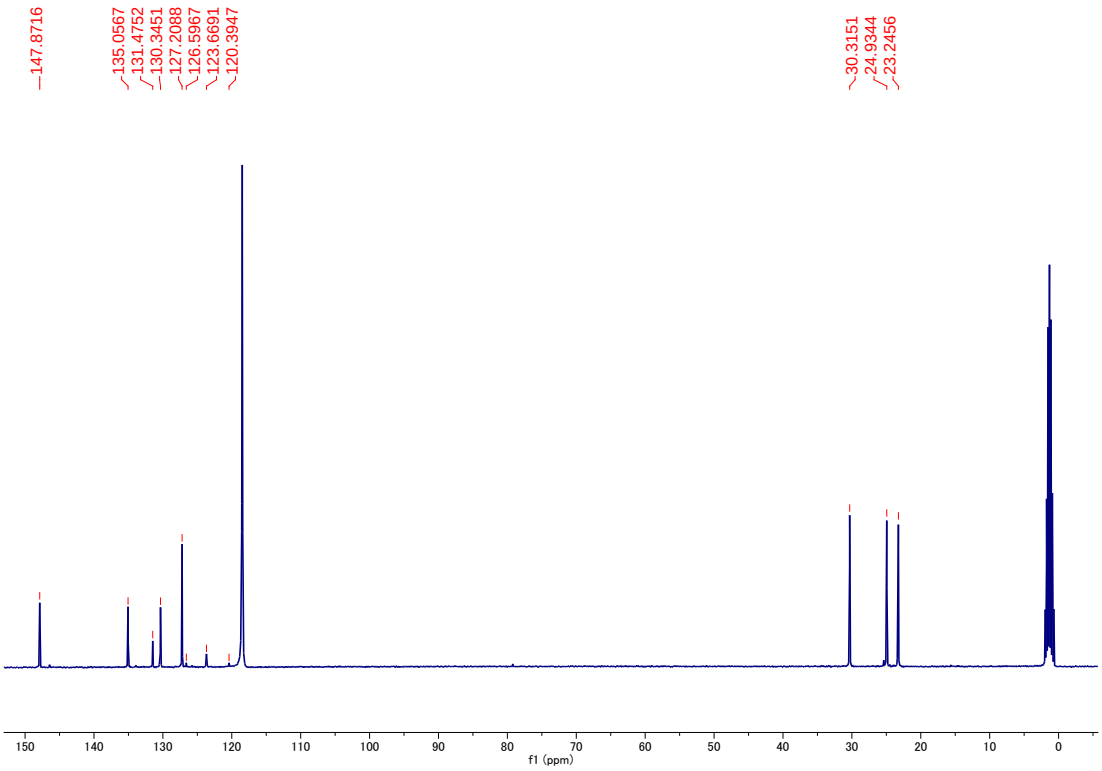


Figure S2. $^{13}C\{^{1}H\}$ NMR (100.7 MHz, 25 °C, CD_3CN) of $\mathbf{2}^{2+}$ 2 $(OTf)^{-}$.

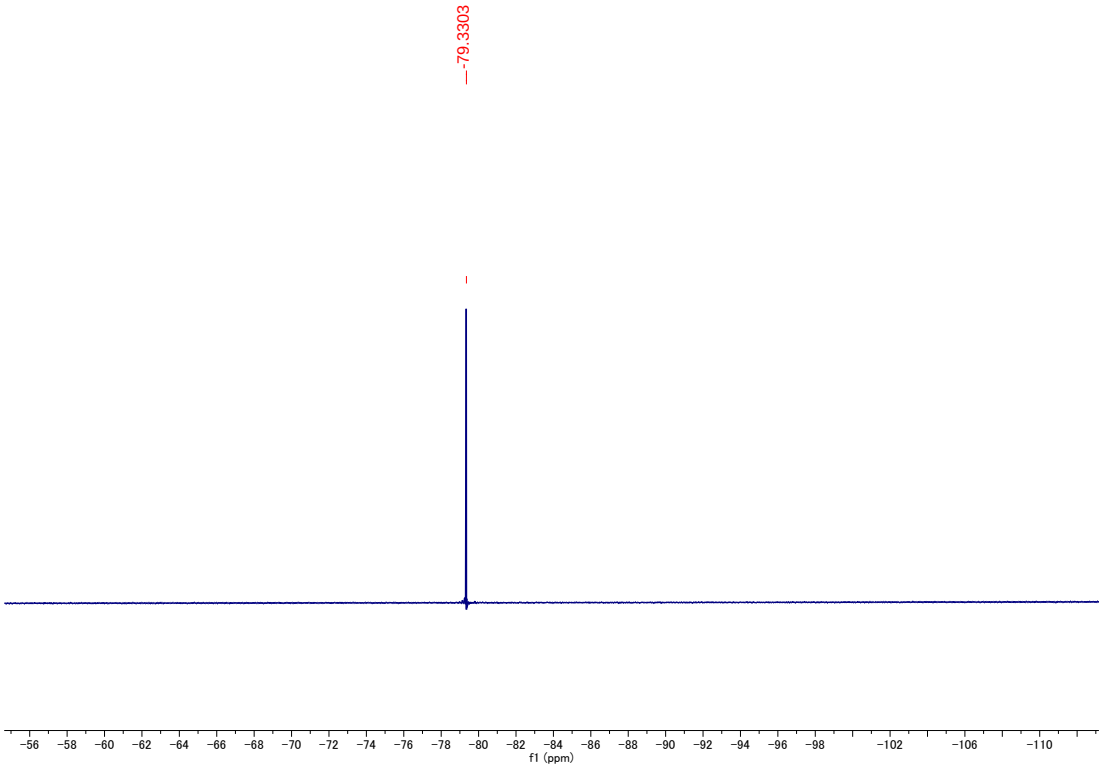


Figure S3. $^{19}F\{^{1}H\}$ NMR (470.5 MHz, 25 °C, CD_3CN) of $\mathbf{2}^{2+}$ 2 $(OTf)^-$.

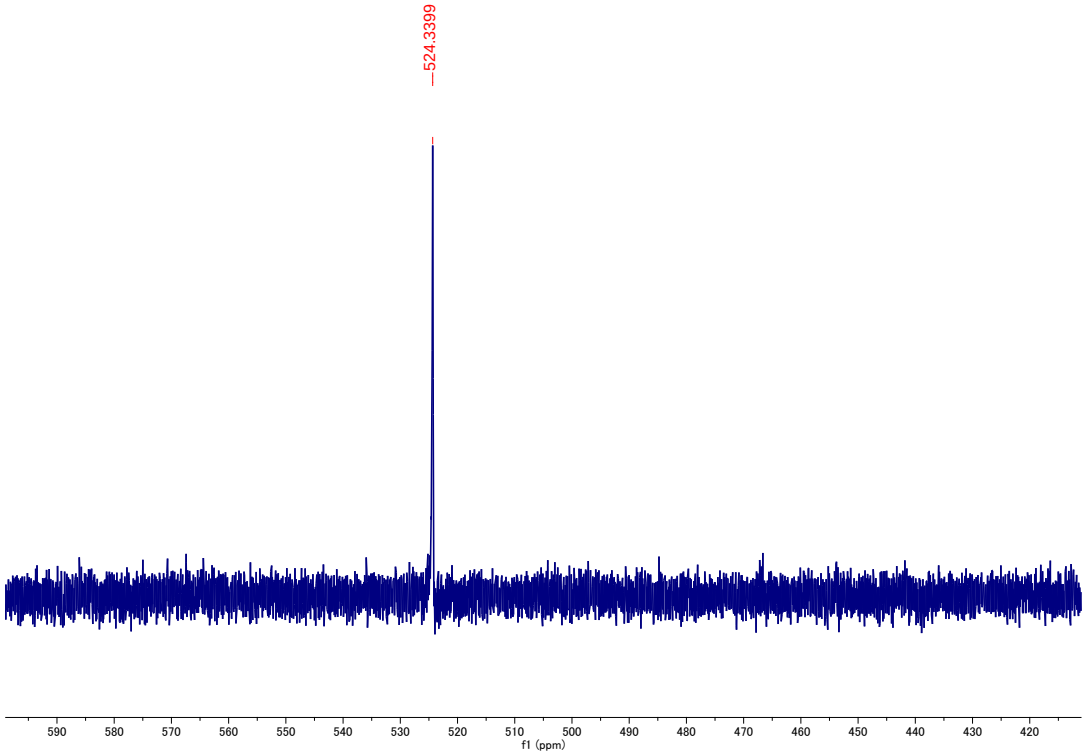


Figure S4. $^{125}Te\{^{1}H\}$ NMR (94 MHz, 25 °C, CD_3CN) of $\mathbf{2}^{2+}$ 2 $(OTf)^-$.

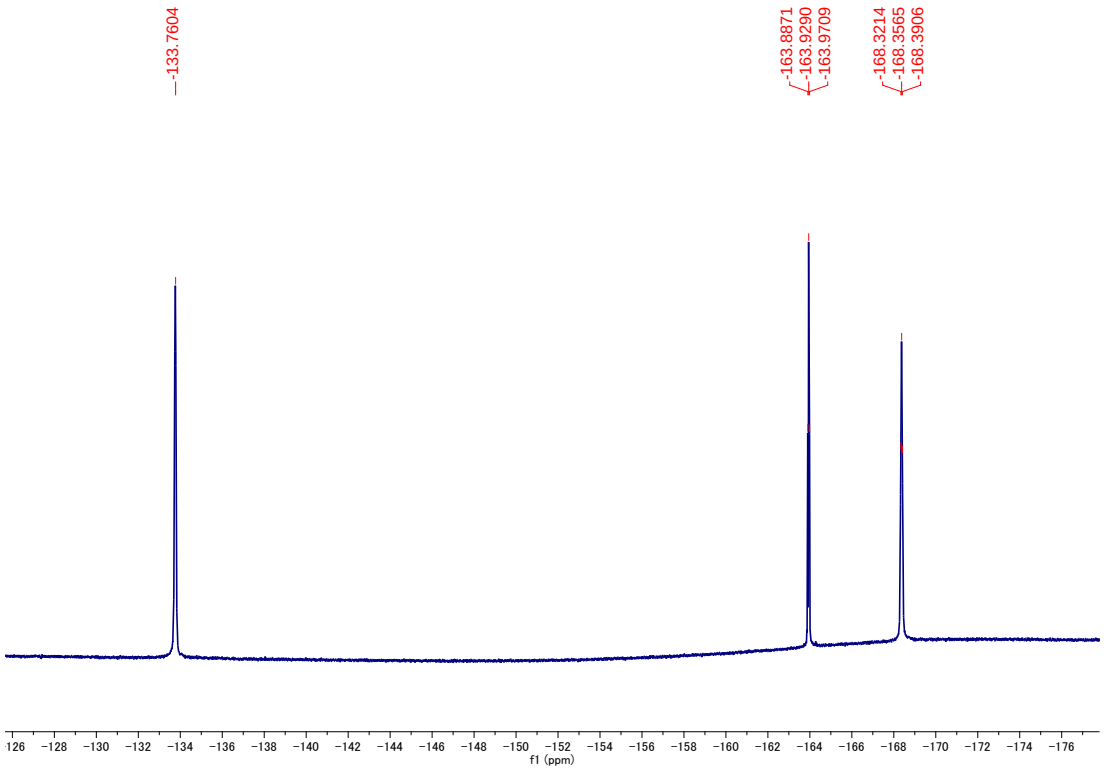
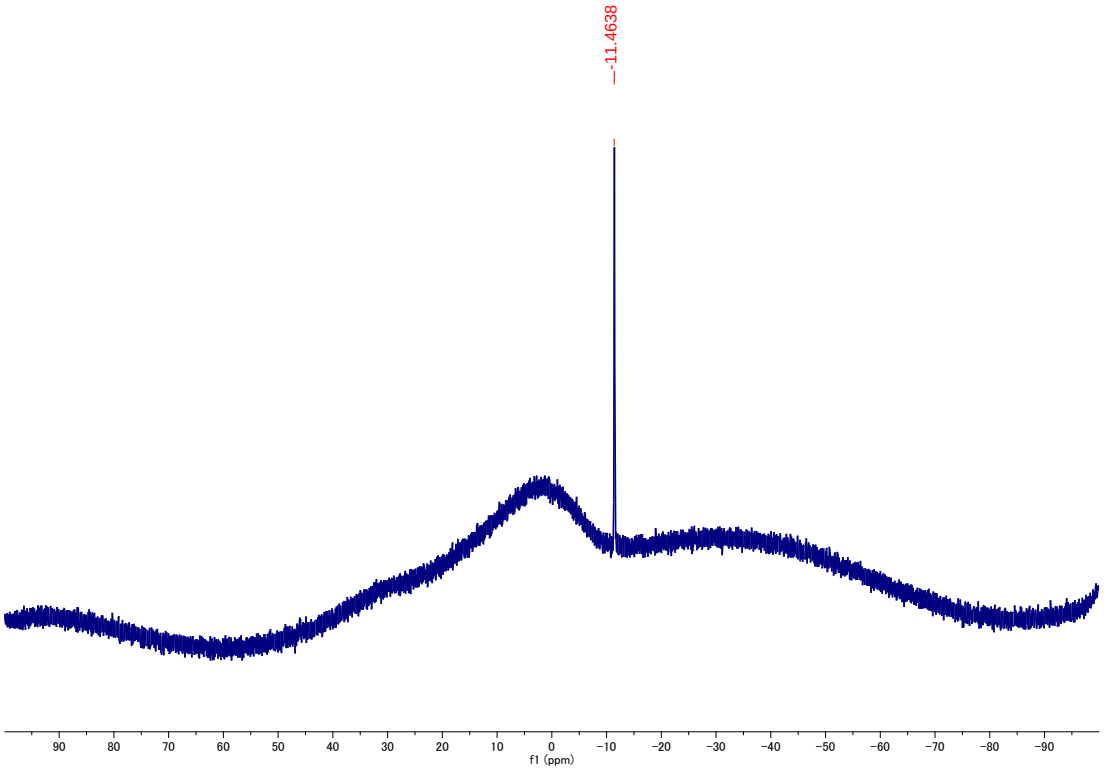


Figure S5. $^{19}F\{^{1}H\}$ NMR (470.5 MHz, 25 °C, CD_3CN) of $\mathbf{2}^{2+}$ 2 $[B(C_6F_5)_4]^-$



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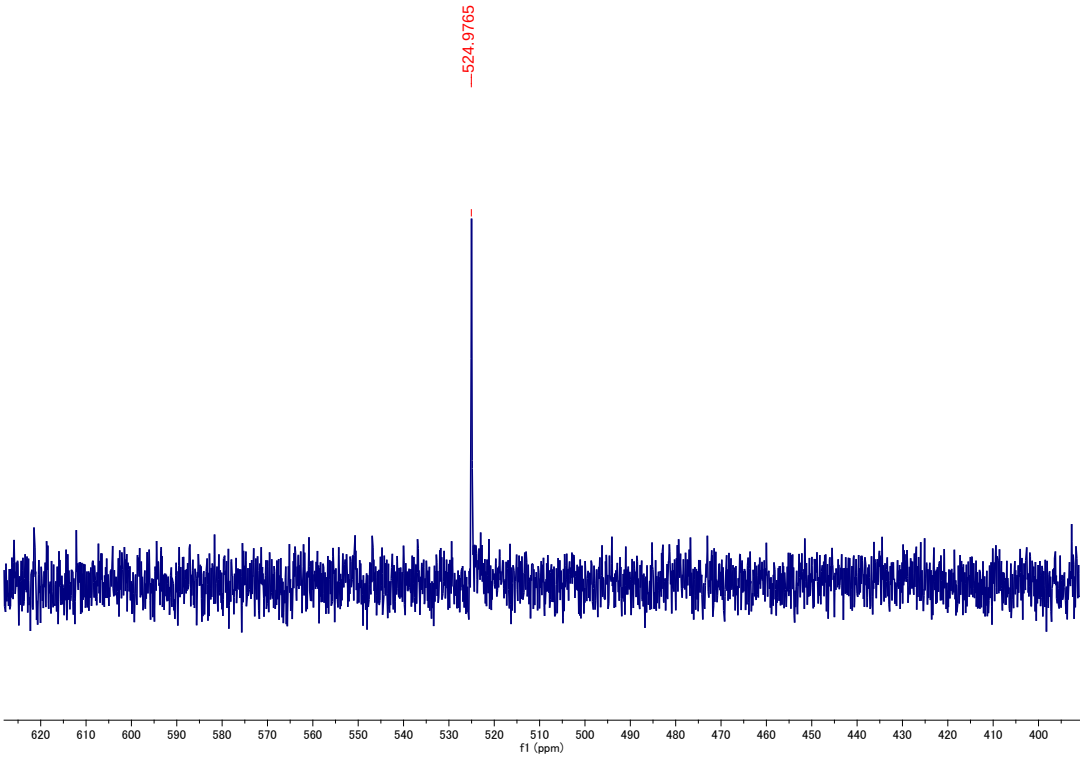

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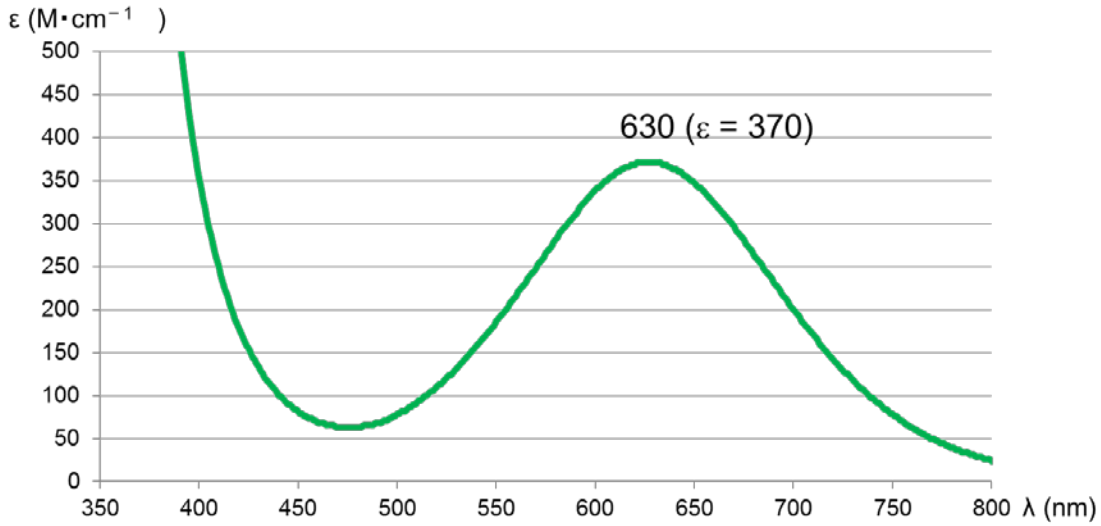

Figure S8. UV/Vis spectrum of $\mathbf{2}^{2+}$ 2 $(TfO)^-$ in CD_3CN.

Table S1. Crystallographic data and details of refinement for $\mathbf{2}^{2+}$ 2 $(OTf)^-$ and $\mathbf{2}^{2+}$ 2 $[B(C_6F_5)_4]^-$.

	$\mathbf{2}^{2+}$ 2 $(OTf)^-$	$\mathbf{2}^{2+}$ 2 $[B(C_6F_5)_4]^-$
Formula	$C_{56}H_{72}F_6N_4O_6S_2Te_2$	$C_{106}H_{78}B_2F_{40}N_6Te_2$
Formula weight	1330.50	2472.56
Color	green	blue
Crystal size / mm	0.30 × 0.28 × 0.17	0.20 × 0.09 × 0.07
Temperature / K	90	90
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/n$
a /Å	11.9321(11)	11.0816(8)
b /Å	12.2008(12)	18.5142(13)
c /Å	12.6710(10)	25.3460(18)
a / deg.	89.3920(10)	90
b / deg.	64.7660(10)	101.5380(10)
g / deg.	64.8090(10)	90
V /Å^3	1469.7(2)	5095.1(6)
Z	1	2
D_{calcd} / g cm^{-3}	1.496	1.612
No. of unique data	5367	11440
No. of parameters	398	712
No. of restraints	0	0
R_1 ($I > 2s(I)$)	0.0468	0.0278
wR_2 (all data)	0.1230	0.0748
GOF	1.010	1.029

Computational details

Atomic Coordinates for $\mathbf{3}^{2+}$ in C_i symmetry.
Total Energy: –1706.23776716 hartree

Te	0.050951	1.407219	0.404624
N	0.083300	1.716410	-2.810013
N	0.092636	3.563098	-1.666140
C	0.078230	0.335078	-3.228578
C	1.317649	5.823059	1.006946
H	2.257542	6.184218	1.416214
C	1.342417	4.900462	-0.042355
C	-2.464593	0.456601	-3.287730
H	-2.547329	1.355977	-3.909505
C	0.097593	4.472901	-0.543045
C	2.622971	0.397979	-3.164433
H	2.720288	0.635575	-2.097614
C	1.286322	-1.579477	-4.001382
H	2.223456	-2.091508	-4.203352
C	0.102256	2.769029	-3.717553
H	0.110781	2.587661	-4.782344
C	0.108562	3.920929	-3.002143
H	0.123439	4.955803	-3.311619
H	2.727158	1.337310	-3.719799
C	-2.447403	4.519132	-0.680091
H	-2.554921	3.428693	-0.710279
C	-1.103375	5.865935	0.983486
H	-2.037770	6.259989	1.374654
C	-1.163243	-0.262718	-3.518929
H	-3.310362	-0.190155	-3.533736
C	-1.140295	4.945884	-0.067757
C	1.318428	-0.289146	-3.463796
H	3.489228	4.873578	-0.098348
C	0.110126	6.300714	1.512811

H	0.115254	7.030790	2.317877
C	-1.134850	-1.554999	-4.052764
H	-2.072713	-2.047759	-4.295236
H	-2.549453	4.887511	-1.708345
C	2.645237	4.416507	-0.620842
H	2.739264	4.673502	-1.682656
C	0.075034	-2.203227	-4.295815
H	0.074108	-3.200214	-4.728098
H	2.753621	3.328404	-0.535518
C	0.077060	2.218628	-1.558856
H	3.465918	-0.241059	-3.438638
H	-2.578773	0.770464	-2.242951
H	-3.287630	4.919209	-0.107115
Te	-0.050951	-1.407219	-0.404624
N	-0.083300	-1.716410	2.810013
N	-0.092636	-3.563098	1.666140
C	-0.078230	-0.335078	3.228578
C	-1.317649	-5.823059	-1.006946
H	-2.257542	-6.184218	-1.416214
C	-1.342417	-4.900462	0.042355
C	2.464593	-0.456601	3.287730
H	2.547329	-1.355977	3.909505
C	-0.097593	-4.472901	0.543045
C	-2.622971	-0.397979	3.164433
H	-2.720288	-0.635575	2.097614
C	-1.286322	1.579477	4.001382
H	-2.223456	2.091508	4.203352
C	-0.102256	-2.769029	3.717553
H	-0.110781	-2.587661	4.782344
C	-0.108562	-3.920929	3.002143
H	-0.123439	-4.955803	3.311619
H	-2.727158	-1.337310	3.719799
C	2.447403	-4.519132	0.680091

H	2.554921	-3.428693	0.710279
C	1.103375	-5.865935	-0.983486
H	2.037770	-6.259989	-1.374654
C	1.163243	0.262718	3.518929
H	3.310362	0.190155	3.533736
C	1.140295	-4.945884	0.067757
C	-1.318428	0.289146	3.463796
H	-3.489228	-4.873578	0.098348
C	-0.110126	-6.300714	-1.512811
H	-0.115254	-7.030790	-2.317877
C	1.134850	1.554999	4.052764
H	2.072713	2.047759	4.295236
H	2.549453	-4.887511	1.708345
C	-2.645237	-4.416507	0.620842
H	-2.739264	-4.673502	1.682656
C	-0.075034	2.203227	4.295815
H	-0.074108	3.200214	4.728098
H	-2.753621	-3.328404	0.535518
C	-0.077060	-2.218628	1.558856
H	-3.465918	0.241059	3.438638
H	2.578773	-0.770464	2.242951
H	3.287630	-4.919209	0.107115

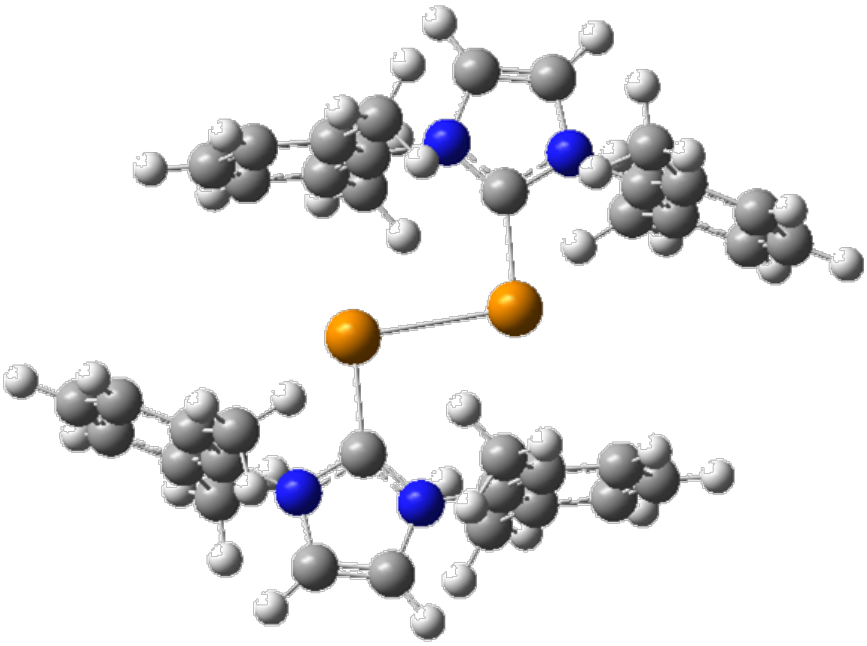

Figure S8. Optimized geometry of $\mathbf{3}^{2+}$ [B3LYP/6-31G+(d) for C, H, N and LanL2DZ for Te level].

Atomic Coordinates for **4**.

Total Energy: –95.95396251 hartree

Te	-1.37099594	-0.24038776	-0.29659056
Te	1.37098525	-0.24036257	0.29661296
C	1.98065381	1.30609668	-1.10359577
H	1.71249427	1.01200638	-2.11930448
H	1.51348553	2.25652789	-0.84211988
H	3.06804146	1.39374208	-1.01946693
C	-1.98060345	1.30622098	1.10348289
H	-1.71251784	1.01222119	2.11923255
H	-1.51328183	2.25655218	0.84189316
H	-3.06796779	1.39406170	1.01927762

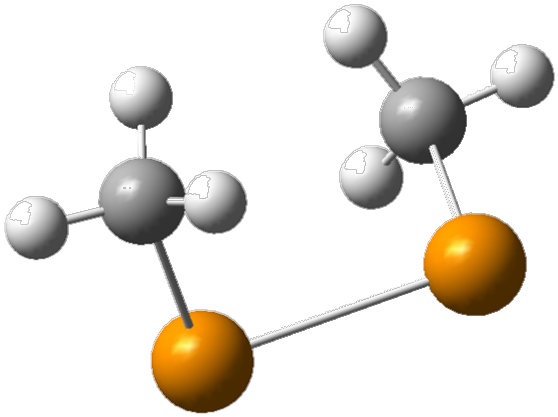

Figure S9. Optimized geometry of **4** [B3LYP/6-31G+(d) for C, H and LanL2DZ for Te level].

Atomic Coordinates for **1**.

Total Energy: –853.35994074 hartree

Te	-0.14762400	-0.19810500	1.87156700
N	1.13548900	0.11241300	-0.97541100
N	-1.03418600	0.12378300	-1.08109500
C	2.51036100	0.05906700	-0.53931500
C	-4.41636000	-1.19195000	-0.31741000
H	-4.94935000	-2.13903800	-0.30062900
C	-3.06131800	-1.17989500	-0.65880000
C	2.45296200	2.59751300	-0.34641800
H	2.06565200	2.80551200	-1.35093500
C	-2.42068200	0.07405200	-0.67579900
C	2.41307700	-2.46848900	-0.83218800
H	1.61164300	-2.65278600	-0.10571400
C	4.52096800	-1.20201000	-0.24034800
H	5.05382000	-2.14920300	-0.23132000
C	0.78382900	0.25859500	-2.31218400
H	1.53743900	0.34168900	-3.08154300
C	-0.57062000	0.26502100	-2.37661000
H	-1.24708200	0.35521000	-3.21400200
H	1.95451300	-2.44966800	-1.82767500
C	-2.37187500	2.61688500	-0.50392600
H	-1.45655900	2.64801800	0.09836800
C	-4.42969800	1.21643300	-0.06589300
H	-4.97280400	2.13381900	0.14582400
C	3.17177000	1.27675700	-0.28894200
H	3.12810000	3.41456400	-0.08042100
C	-3.07543000	1.29009100	-0.40279200
C	3.15337400	-1.19374800	-0.53121200
H	-3.01507400	-3.30714800	-0.95087500
C	-5.09241700	-0.00871800	-0.02573500
H	-6.15044300	-0.04031800	0.22074400
C	4.53862500	1.20793800	-0.00128200

H	5.08529600	2.12714200	0.19212600
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H	-1.94850400	-2.42151800	-2.04201900
C	5.20595400	-0.01574800	0.01762300
H	6.27215200	-0.04417400	0.22562900
H	-1.49213600	-2.64537500	-0.34878600
C	0.01193200	0.03185200	-0.23461000
H	3.09183200	-3.32424800	-0.79923900
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H	-3.02345900	3.42337500	-0.15844600

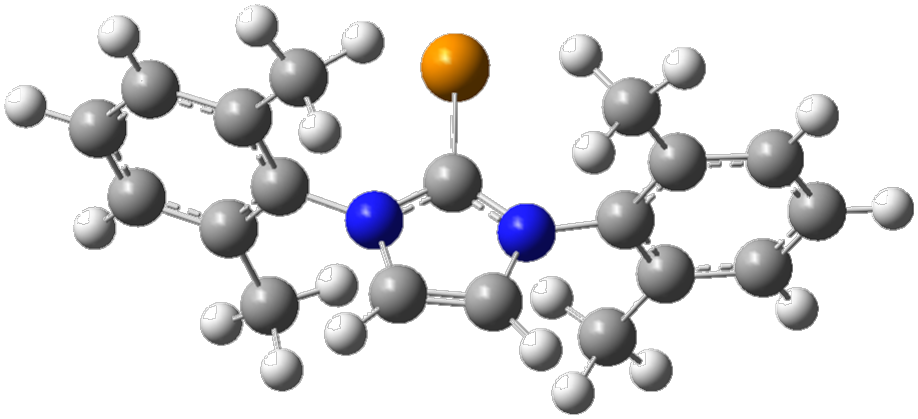

Figure S10. Optimized geometry of **1** [B3LYP/6-31G+(d) for C, H, N and LanL2DZ for Te level].

Table S2. NPA charges and WBI of **1**, $\mathbf{3}^{2+}$, and **4**.

Compounds	NPA	WBI
1	$C_{carbene}$: +0.190	C–Te: 1.155
	N: –0.453, –0.453	
	Te: –0.212	
	$C_{NHC\text{-}backbone}$: -0.086, -0.082	
$\mathbf{3}^{2+}$	$C_{carbene}$: +0.157	C–Te: 0.945
	N: –0.366, –0.366	Te–Te: 0.885
	Te: +0.463	
	$C_{NHC\text{-}backbone}$: -0.046, -0.055	
4	Te: +0.227	C–Te: 1.041
	C: –0.1.013	Te–Te: 0.949