Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Reaction of imidazoline-2-selone derivatives with mesityltellurenyl iodide: a unique example of a 3c-4e Se→Te←Se three-body system embedding a tellurenyl cation

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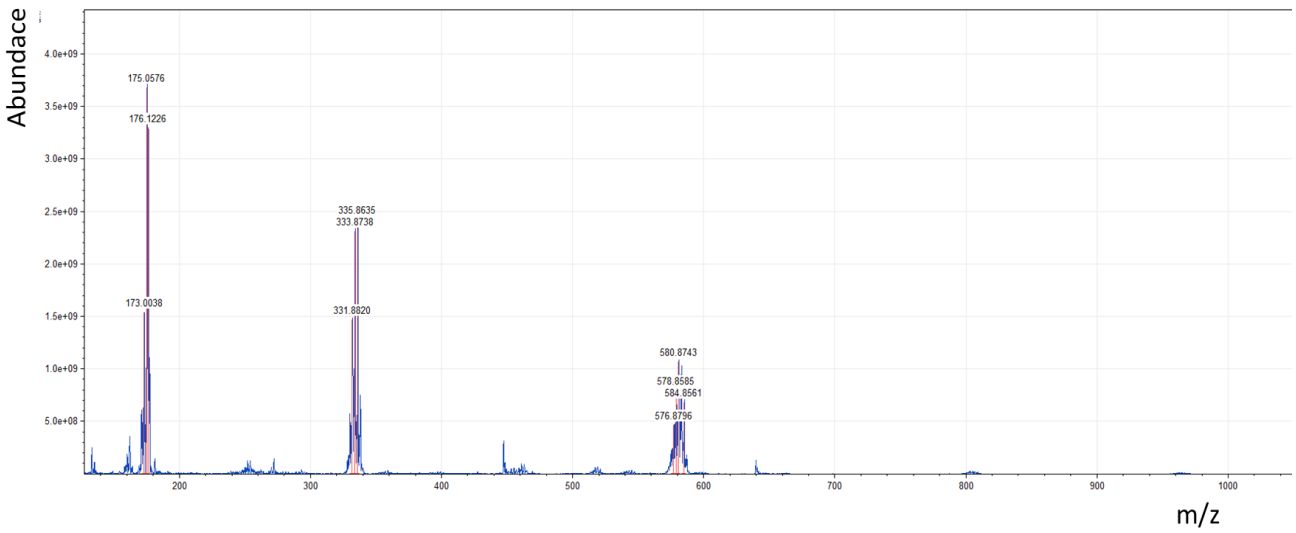


Figure S1. ESI(+) Mass Spectrum of **I**.

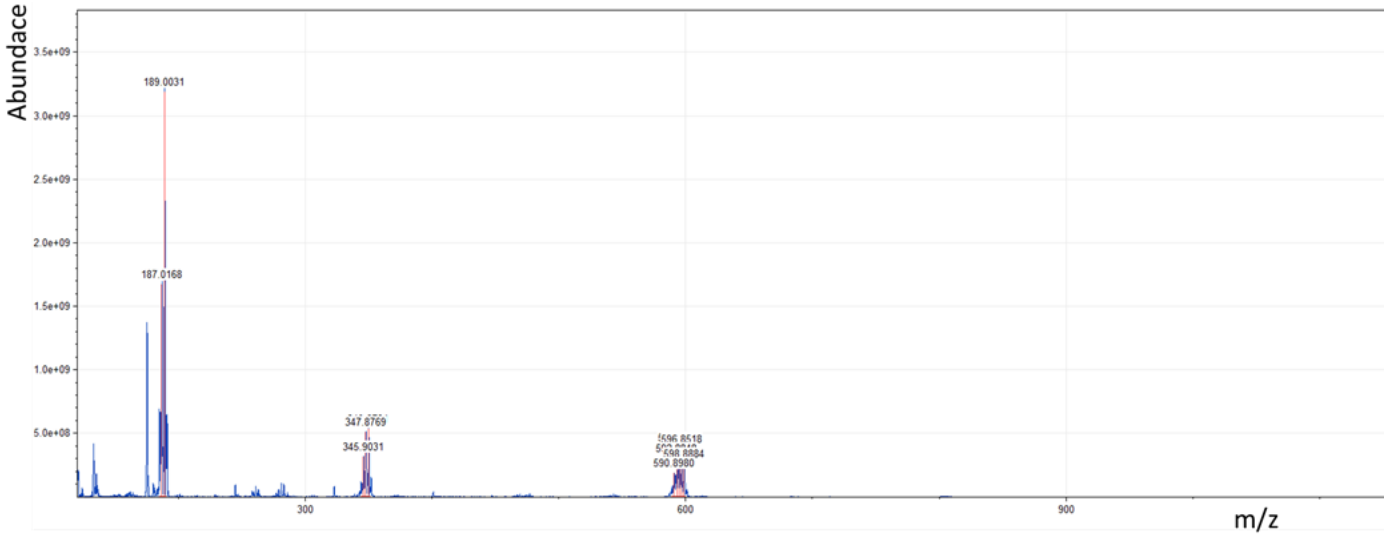


Figure S2. ESI(+) Mass Spectrum of compound **II.**

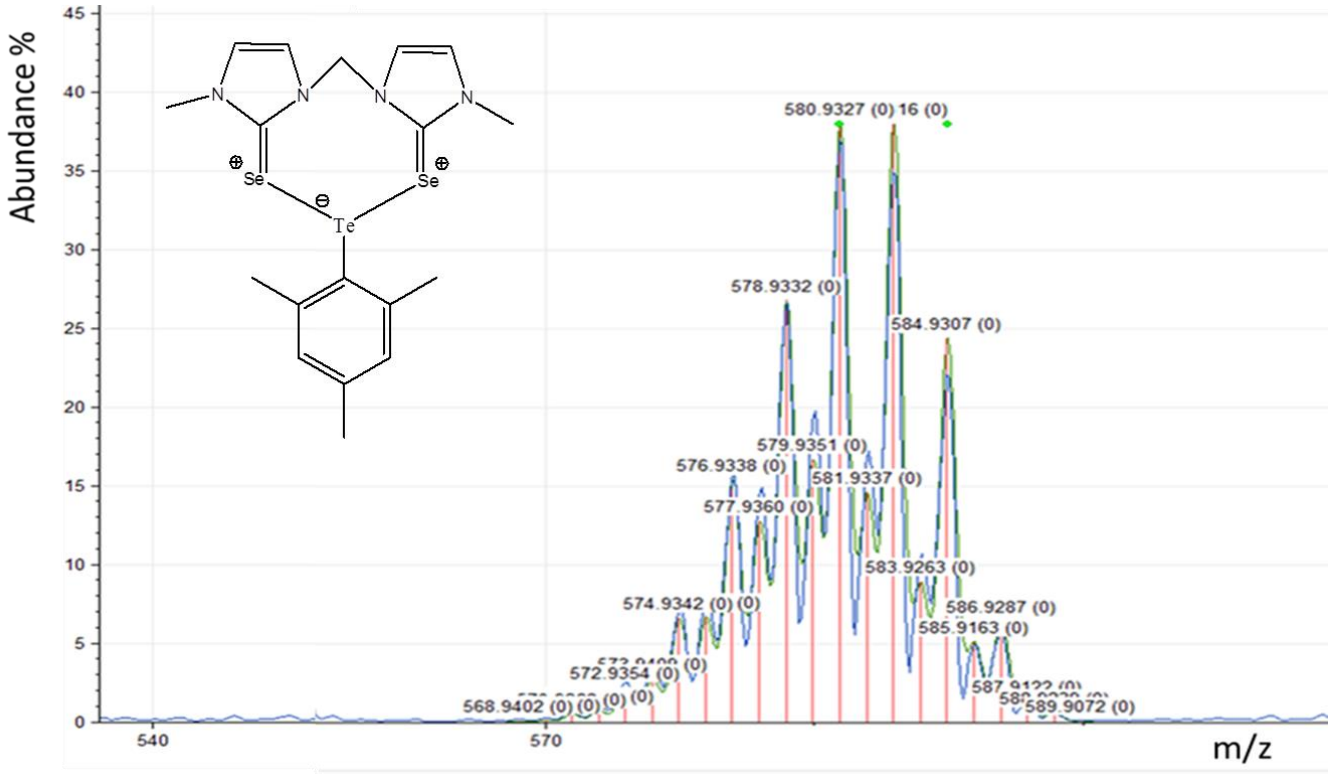


Figure S3. Isotopic ion distribution for the peak at m/z = 580.9, ($[C_{18}H_{23}N_4Se_2Te]^+$) in the ESI(+) Mass Spectrum of **I** (blue experimental line, green calculated line).

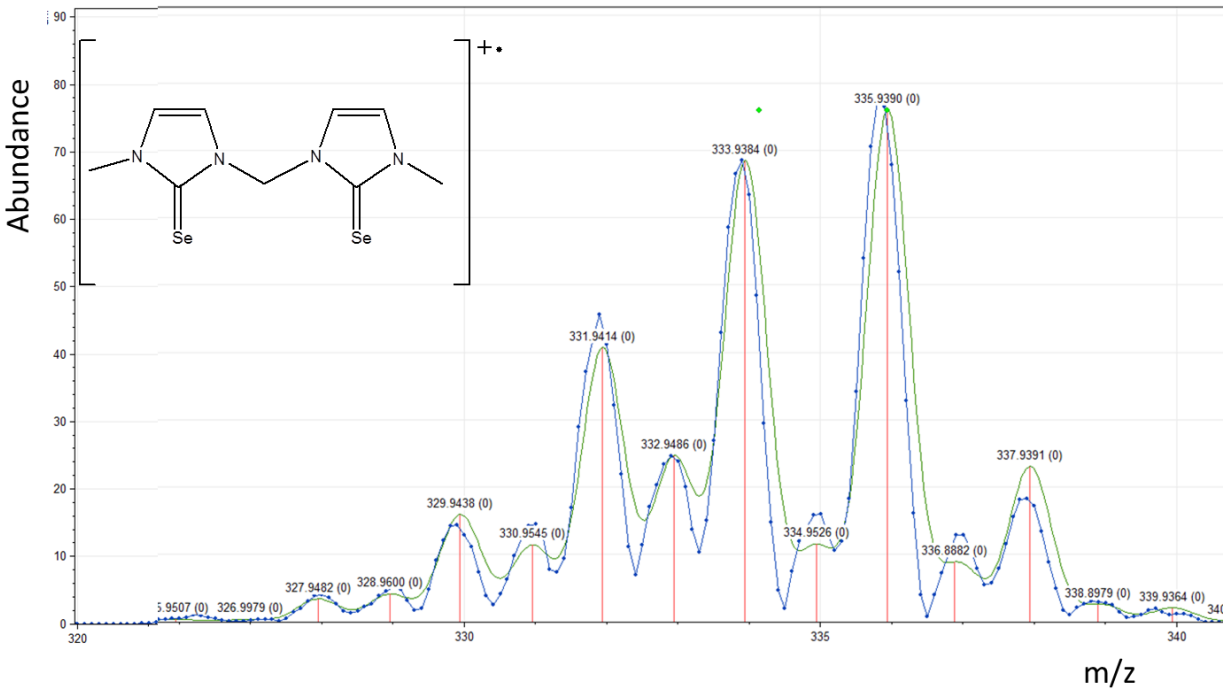


Figure S4. Isotopic ion distribution for the peak at m/z = 335.9, ($[C_9H_{12}N_4Se_2]^+$) in the ESI(+) Mass Spectrum of **I** (blue experimental line, green calculated line).

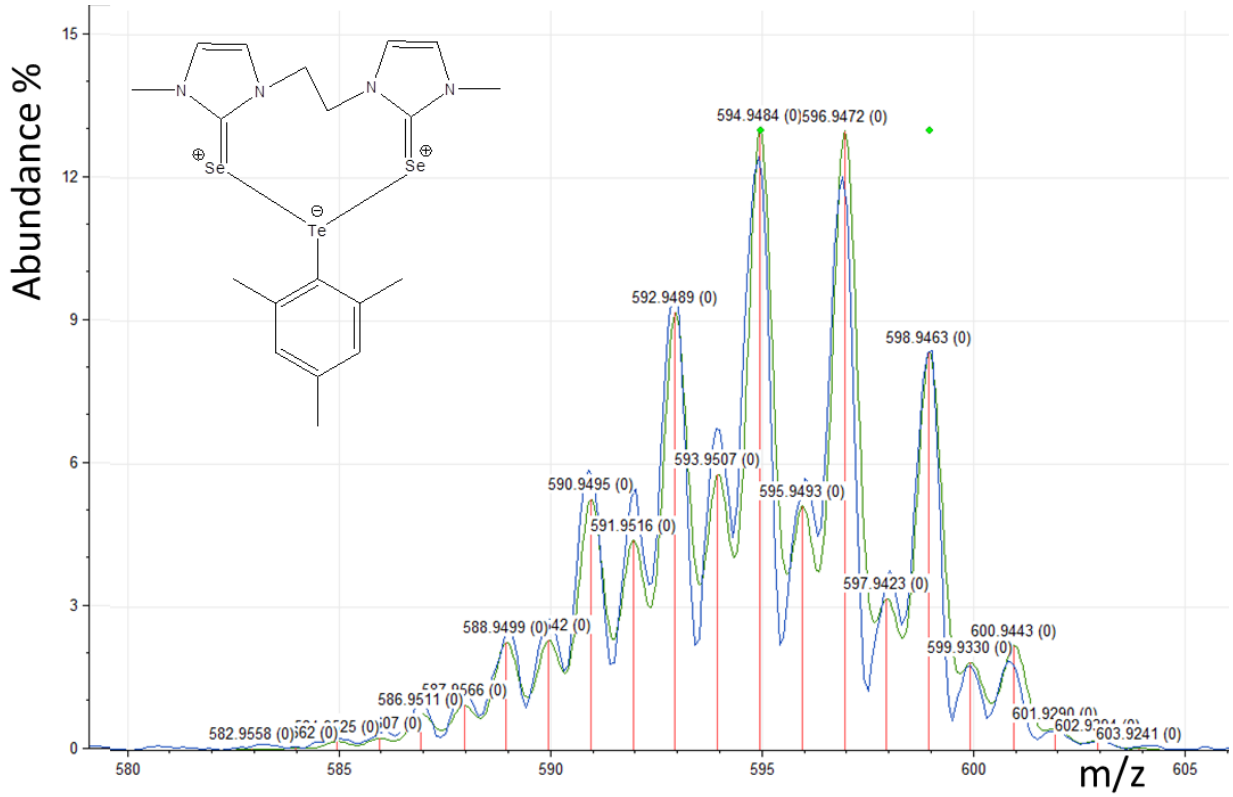


Figure S5. Isotopic ion distribution for the peak at m/z = 594.9, ($[C_{19}H_{25}N_4Se_2Te]^+$) in the ESI(+) Mass Spectrum of **II** (blue experimental line, green calculated line).

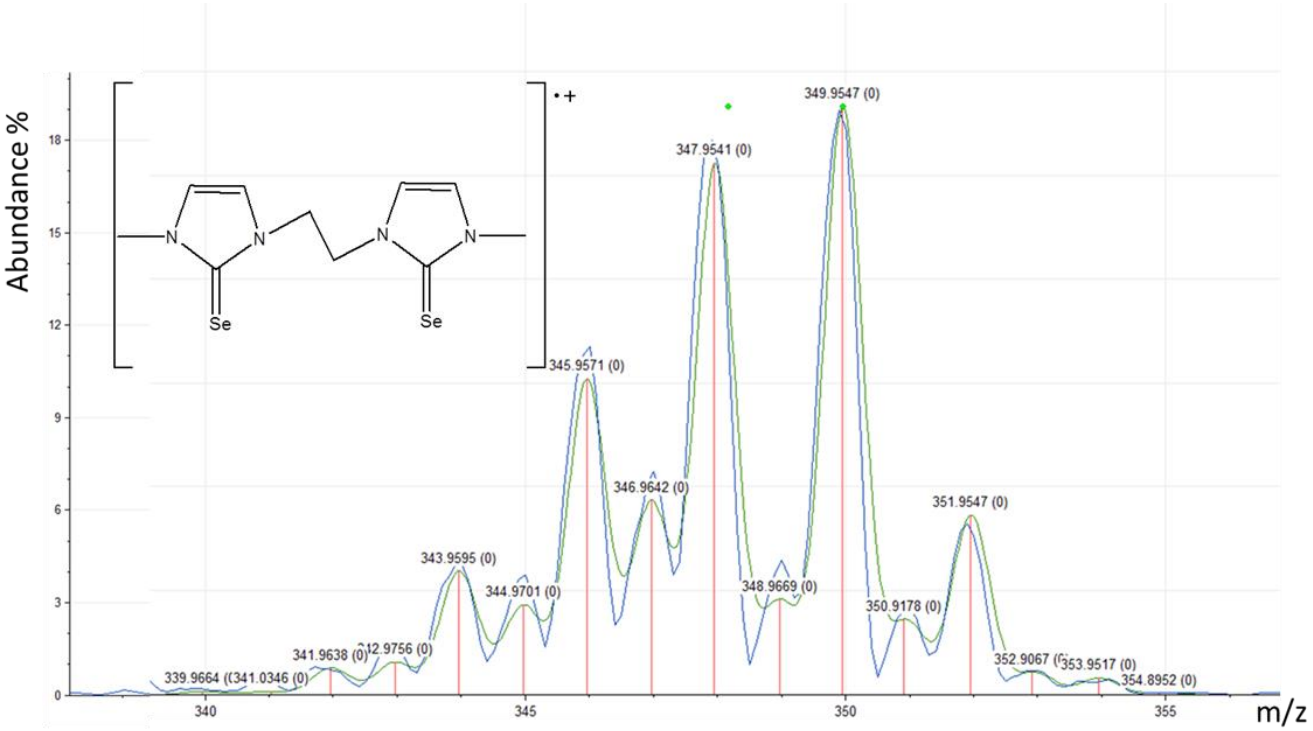


Figure S6. Isotopic ion distribution for the peak at m/z = 349.9 ($[C_{10}H_{14}N_4Se_2]^+$) in the ESI(+) Mass Spectrum of **II** (blue experimental line, green calculated line).

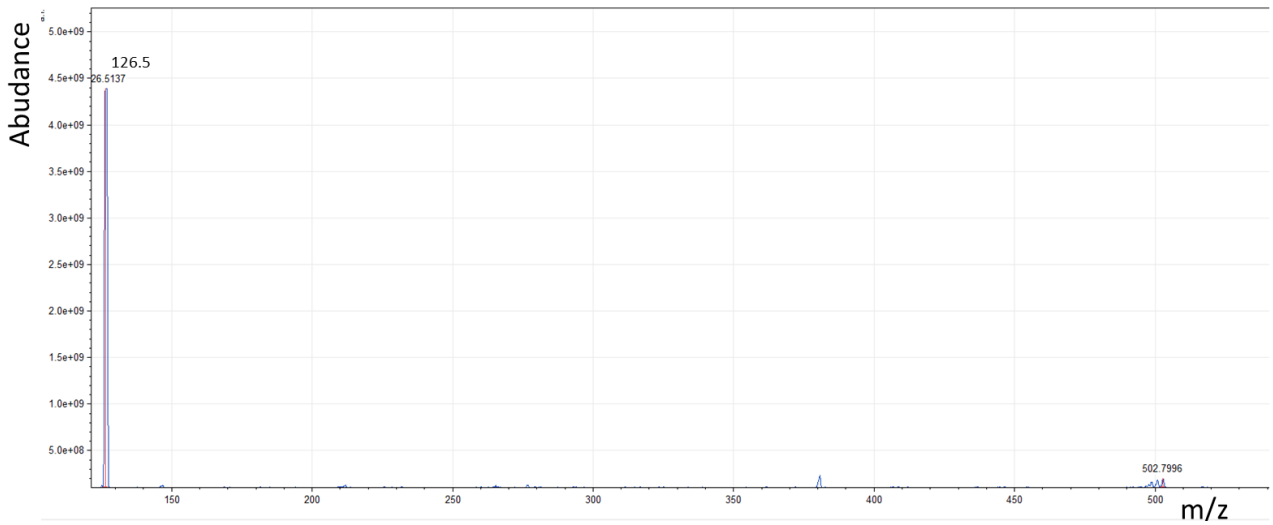


Figure S7. ESI(-) Mass Spectrum of compound **II.**

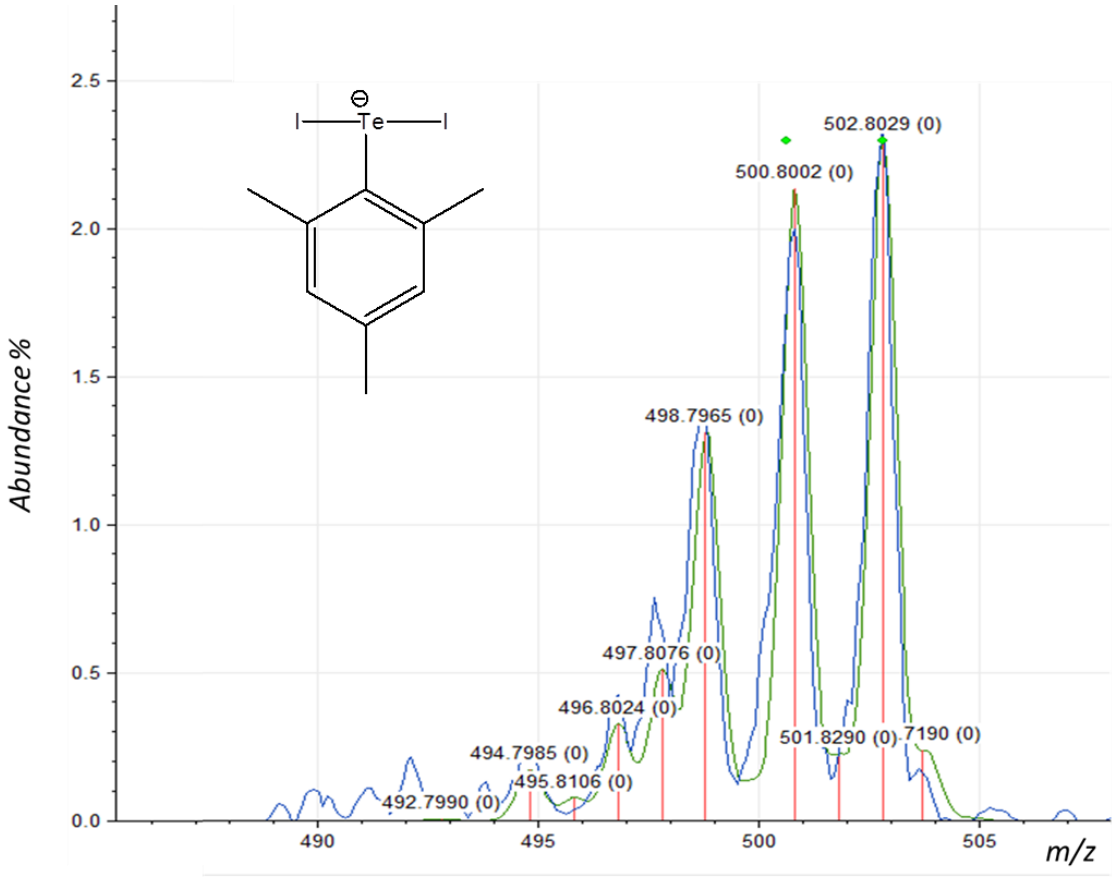


Figure S8. Isotopic ion distribution for the peak at m/z = 502.8 $(C_9H_{11}TeI_2)^-$ in the ESI(-) Mass Spectrum of **II** (blue experimental line, green calculated line).

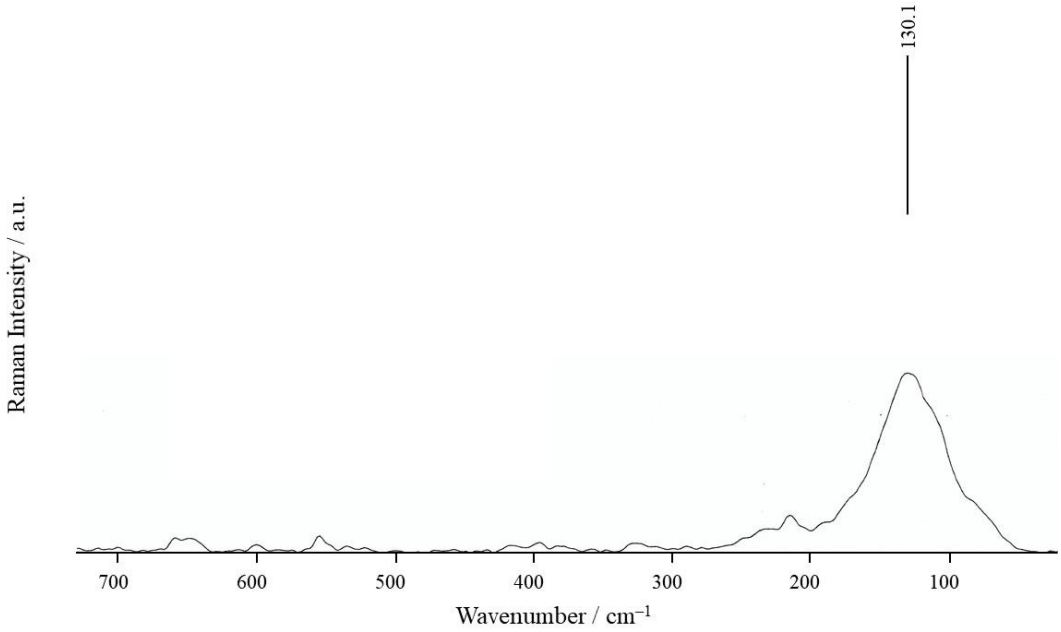


Figure S9. Solid state FT-Raman spectrum (750–50 cm^{-1}) recorded at r.t. for **1**·$2CH_2Cl_2$ (**I**).

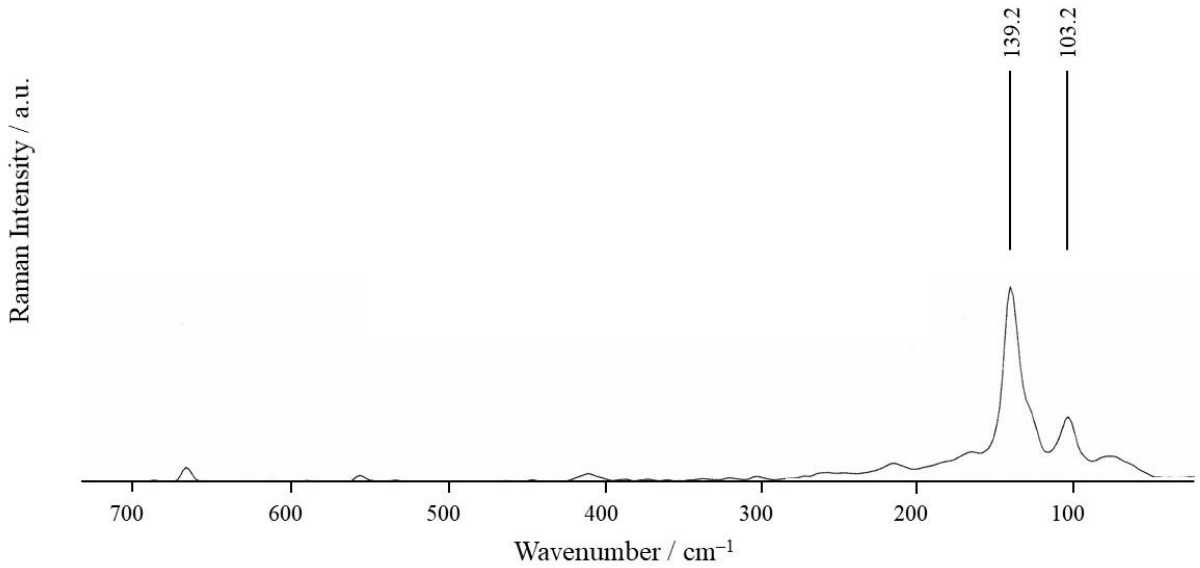


Figure S10. Solid state FT-Raman spectrum (750–50 cm^{-1}) recorded at r.t. for [**2**]$(MesTeI_2)_2$ (**II**).

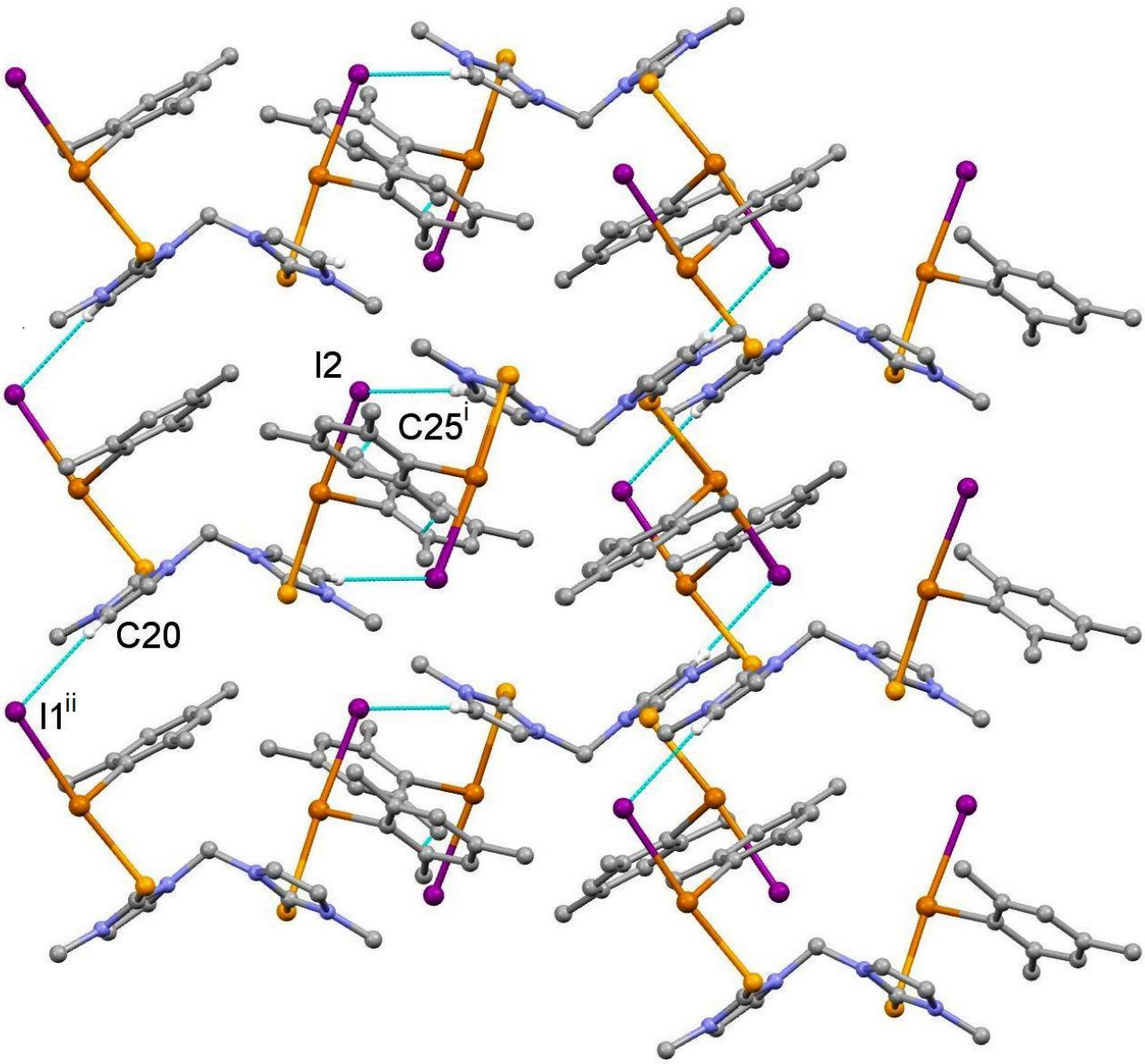
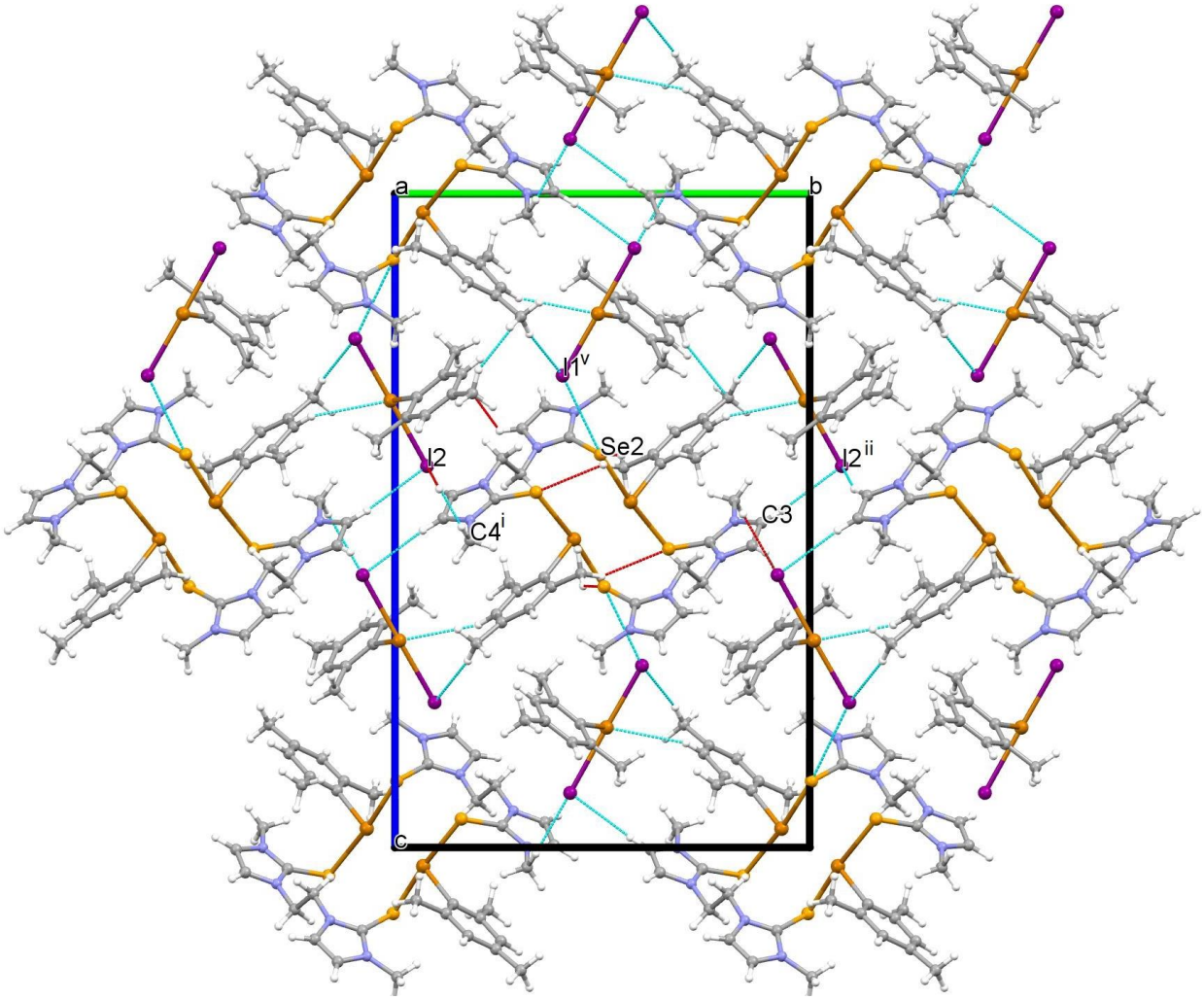


Figure S11. Crystal packing view of **I** along 010 direction, showing the weak I···H contacts I2···H25^{i}, 3.06, and I1^{ii}···H20, 3.10 Å. Symmetry codes: ^{i} = 2-x, -0.5+y, 0.5-z; ^{ii} = x, 0.5+y, -0.5+z. Hydrogen atoms not involved in showed interactions have been omitted for clarity.

a



b

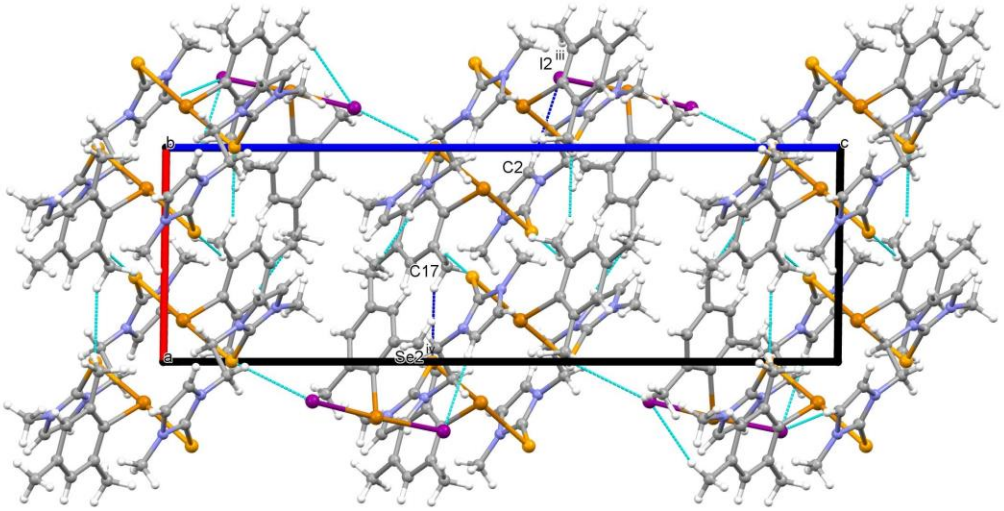


Figure S12. Crystal packing view of **II** along 100 (***a***) and 010 (***b***), showing the weak contacts: I2···C4H4A[i], 2.898; C3H3···I2[ii], 3.072; C2H2···I2[iii], 3.086; Se2iv···C17H17B, 2.969; I1[v]···Se2, 3.794 Å. Symmetry codes: [i] =-x, 1-y, 1-z; [ii] = 1+x, 1+y, z; [iii] = -1-x, 1-y, 1-z; [iv] = 1+x, y, z; [v] = -1-x, 0.5+y, 0.5-z.

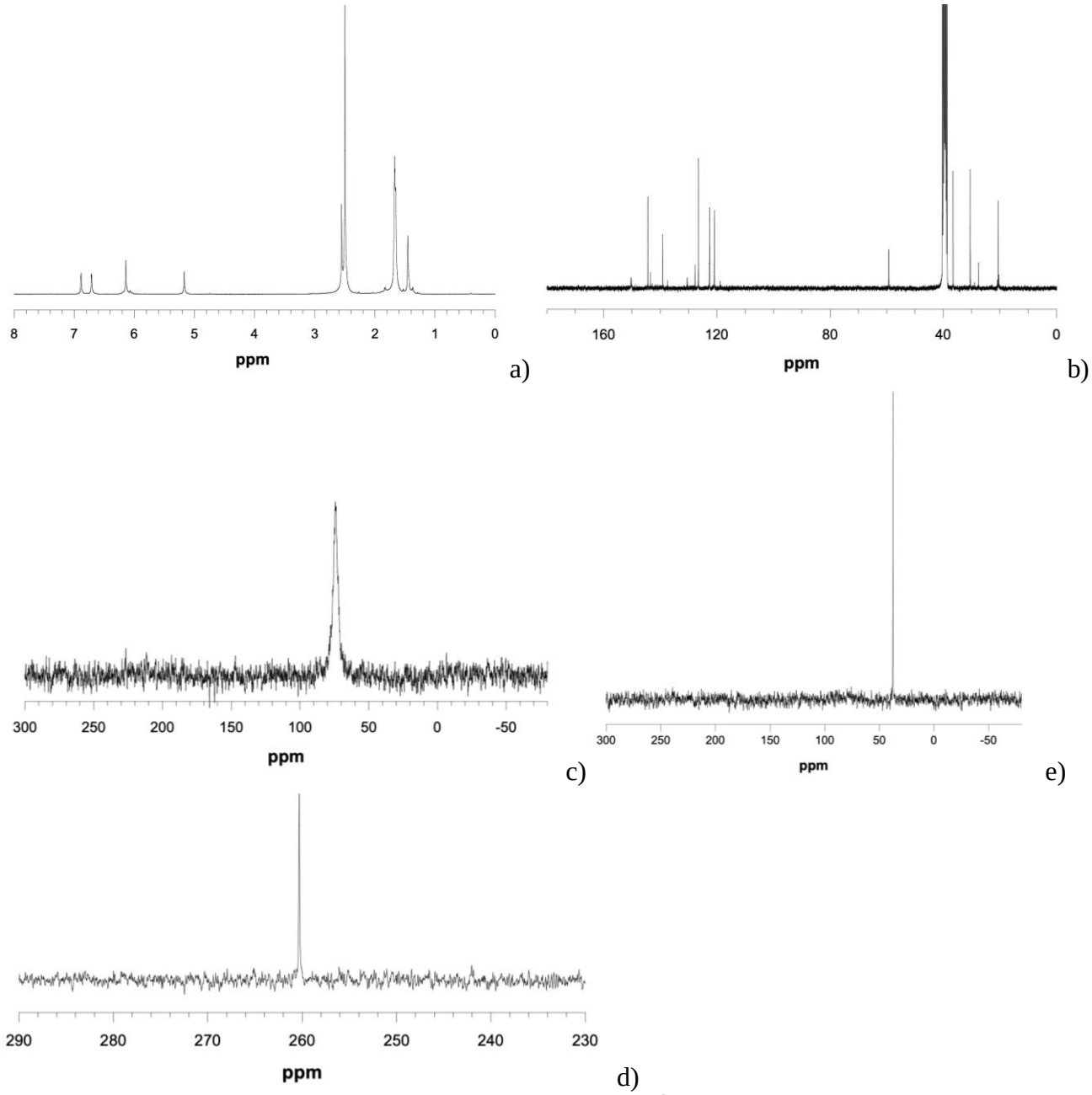


Figure S13. a) ^{1}H-NMR (300.1 MHz, DMSO-d_6, TMS); b) ^{13}C-NMR (75.5 MHz, DMSO-d_6); c) ^{77}Se-NMR (57.3 MHz, DMSO-d_6, H_2SeO_3); d) ^{125}Te-NMR (94.74 MHz, DMSO-d_6, Ph_2Te_2) for compound **I**; e) ^{77}Se-NMR (57.3 MHz, DMSO-d_6, H_2SeO_3) for $\mathbf{L^1}$.

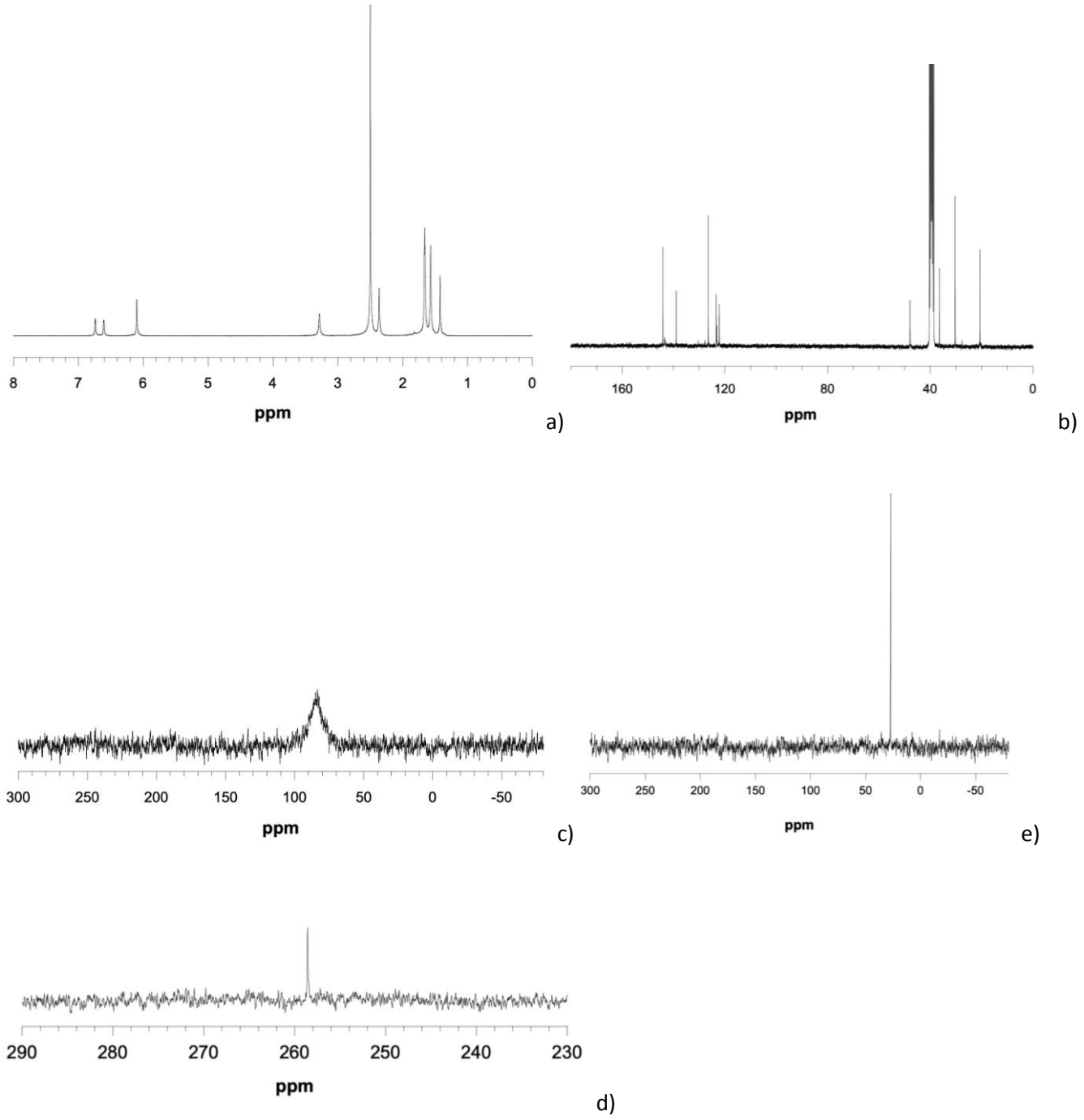


Figure S14. a) ^{1}H-NMR (300.1 MHz, DMSO-d_6, TMS); b) ^{13}C-NMR (75.5 MHz, DMSO-d_6); c) ^{77}Se-NMR (57.3 MHz, DMSO-d_6, H_2SeO_3); d) ^{125}Te-NMR (94.74 MHz, DMSO-d_6, Ph_2Te_2) for compound **II**; e) ^{77}Se-NMR (57.3 MHz, DMSO-d_6, H_2SeO_3) for $\mathbf{L^2}$.

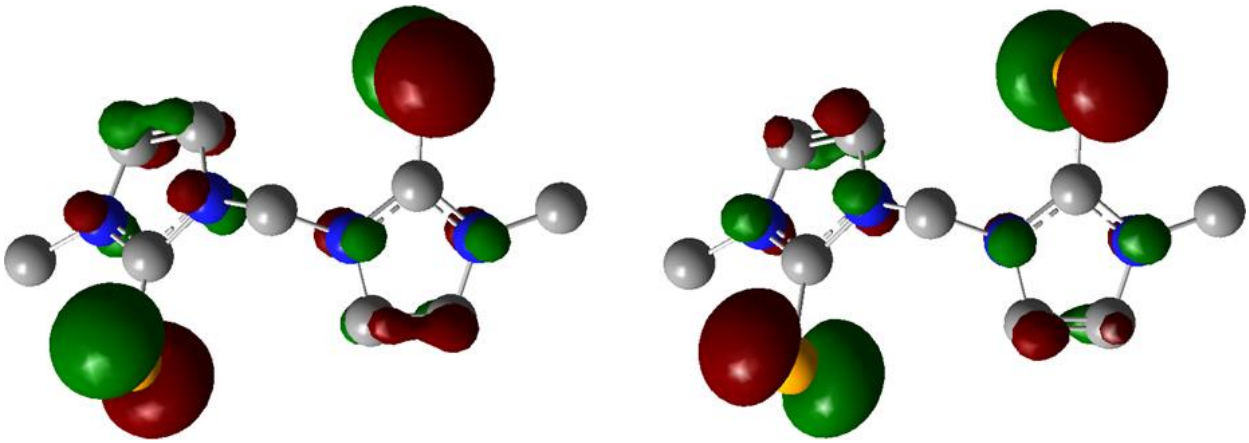


Figure S15. Isosurfaces of Kohn-Sham HOMO (left) and HOMO–1 (right) calculated for $\mathbf{L^1}$ at DFT level at the fully relaxed geometry. Cutoff value = 0.05 |e|. Hydrogen atoms have been omitted for clarity.

Table S1 - Crystal Data and Details of the Structure Determination
for: **I** P 21/c R = 0.09

Crystal Data			
Formula	C29 H34 Cl4 I2 N4 Se2 Te2		
Formula Weight	1251.35		
Crystal System	monoclinic		
Space group	P21/c (No. 14)		
a, b, c [Angstrom]	16.2052(17)	15.2199(16)	16.6992(17)
alpha, beta, gamma [deg]	90	99.016(2)	90
V [Ang**3]	4067.8(7)		
Z	4		
D(calc) [g/cm**3]	2.043		
Mu(MoKa) [/mm]	5.030		
F(000)	2344		
Crystal Size [mm]	0.17 x	0.19 x	0.29
Data Collection			
Temperature (K)	297		
Radiation [Angstrom]	MoKa 0.71073		
Theta Min-Max [Deg]	1.8, 25.0		
Dataset	-19: 19 ; -18: 18 ; -19: 19		
Tot., Uniq. Data, R(int)	28895, 7157, 0.061		
Observed Data [I > 2.0 sigma(I)]	6283		
Refinement			
Nref, Npar	7157, 330		
R, wR2, S	0.0903, 0.1968, 1.21		
w = ^2^(FO^2^)+(0.0557P)^2^+66.9394P] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error	0.00, 0.00		
Min. and Max. Resd. Dens. [e/Ang^3]	-0.87, 1.95		

Table S2 - Bond Distances (Angstrom)
for: **I** P 21/c R = 0.09

I1	-Te1	3.0222(15)	C6	-C9	1.50(2)
I2	-Te2	2.9283(14)	C10	-C11	1.390(13)
Te1	-Se1	2.757(2)	C10	-C15	1.390(13)
Te1	-C1	2.125(13)	C11	-C12	1.390(14)
Te2	-Se2	2.8719(18)	C11	-C16	1.50(2)
Te2	-C10	2.129(9)	C12	-C13	1.390(17)
Se1	-C19	1.895(15)	C13	-C14	1.389(16)
Se2	-C24	1.862(14)	C13	-C17	1.53(3)
N1	-C19	1.321(18)	C14	-C15	1.390(16)
N1	-C20	1.37(2)	C15	-C18	1.49(2)
N1	-C22	1.48(2)	C20	-C21	1.31(2)
N2	-C19	1.323(18)	C25	-C26	1.31(2)
N2	-C21	1.380(19)	C3	-H3	0.9300
N2	-C23	1.434(18)	C5	-H5	0.9300
N3	-C24	1.345(18)	C7	-H7A	0.9600
N3	-C25	1.36(2)	C7	-H7B	0.9600
N3	-C27	1.47(2)	C7	-H7C	0.9600
N4	-C23	1.457(18)	C8	-H8A	0.9600
N4	-C24	1.337(17)	C8	-H8B	0.9600
N4	-C26	1.380(19)	C8	-H8C	0.9600
C1	-C2	1.373(18)	C9	-H9A	0.9600
C1	-C6	1.43(2)	C9	-H9B	0.9600
C2	-C3	1.41(2)	C9	-H9C	0.9600
C2	-C7	1.50(2)	C12	-H12	0.9300
C3	-C4	1.35(2)	C14	-H14	0.9300
C4	-C5	1.36(2)	C16	-H16A	0.9600
C4	-C8	1.51(2)	C16	-H16B	0.9600
C5	-C6	1.38(2)	C16	-H16C	0.9600

Table S2 - Bond Distances (Angstrom) (continued)
for: **I** P 21/c R = 0.09

C17	-H17A	0.9600	C22	-H22B	0.9600
C17	-H17B	0.9600	C22	-H22C	0.9600
C17	-H17C	0.9600	C23	-H23A	0.9700
C18	-H18A	0.9600	C23	-H23B	0.9700
C18	-H18B	0.9600	C25	-H25	0.9300
C18	-H18C	0.9600	C26	-H26	0.9300
C20	-H20	0.9300	C27	-H27A	0.9600
C21	-H21	0.9300	C27	-H27B	0.9600
C22	-H22A	0.9600	C27	-H27C	0.9600

Table S3 - Bond Angles (Degrees)
for: **I** P 21/c R = 0.09

I1	-Te1	-Se1	174.89(6)	C3	-C4	-C8	123.0(14)
I1	-Te1	-C1	89.0(4)	C5	-C4	-C8	119.7(13)
Se1	-Te1	-C1	87.7(4)	C4	-C5	-C6	123.0(13)
I2	-Te2	-Se2	175.90(5)	C1	-C6	-C5	118.1(13)
I2	-Te2	-C10	87.8(3)	C1	-C6	-C9	121.8(14)
Se2	-Te2	-C10	88.1(3)	C5	-C6	-C9	120.1(15)
Te1	-Se1	-C19	101.4(4)	Te2	-C10	-C11	120.5(7)
Te2	-Se2	-C24	93.7(4)	Te2	-C10	-C15	119.5(7)
C19	-N1	-C20	110.2(13)	C11	-C10	-C15	120.0(8)
C19	-N1	-C22	127.0(15)	C10	-C11	-C12	120.0(9)
C20	-N1	-C22	122.7(14)	C10	-C11	-C16	124.3(11)
C19	-N2	-C21	107.1(12)	C12	-C11	-C16	115.8(12)
C19	-N2	-C23	128.0(12)	C11	-C12	-C13	120.0(9)
C21	-N2	-C23	124.4(12)	C12	-C13	-C14	120.0(9)
C24	-N3	-C25	110.5(12)	C12	-C13	-C17	119.7(13)
C24	-N3	-C27	124.5(14)	C14	-C13	-C17	120.4(14)
C25	-N3	-C27	124.9(14)	C13	-C14	-C15	120.1(9)
C23	-N4	-C24	126.3(11)	C10	-C15	-C14	120.0(9)
C23	-N4	-C26	125.6(12)	C10	-C15	-C18	122.3(11)
C24	-N4	-C26	108.1(12)	C14	-C15	-C18	117.6(11)
Te1	-C1	-C2	119.7(10)	Se1	-C19	-N1	126.4(11)
Te1	-C1	-C6	120.0(9)	Se1	-C19	-N2	125.8(10)
C2	-C1	-C6	120.2(12)	N1	-C19	-N2	107.8(13)
C1	-C2	-C3	117.0(12)	N1	-C20	-C21	105.3(14)
C1	-C2	-C7	123.5(13)	N2	-C21	-C20	109.4(14)
C3	-C2	-C7	119.5(13)	N2	-C23	-N4	114.1(11)
C2	-C3	-C4	124.5(14)	Se2	-C24	-N3	126.7(10)
C3	-C4	-C5	117.1(13)	Se2	-C24	-N4	127.2(10)

Table S3 - Bond Angles (Degrees) (continued)
for: **I** P 21/c R = 0.09

N3	-C24	-N4	106.0(12)	C15	-C14	-H14	120.00
N3	-C25	-C26	106.3(15)	C11	-C16	-H16A	109.00
N4	-C26	-C25	109.1(14)	C11	-C16	-H16B	109.00
C2	-C3	-H3	118.00	C11	-C16	-H16C	110.00
C4	-C3	-H3	118.00	H16A	-C16	-H16B	109.00
C4	-C5	-H5	119.00	H16A	-C16	-H16C	109.00
C6	-C5	-H5	118.00	H16B	-C16	-H16C	109.00
C2	-C7	-H7A	109.00	C13	-C17	-H17A	109.00
C2	-C7	-H7B	109.00	C13	-C17	-H17B	109.00
C2	-C7	-H7C	109.00	C13	-C17	-H17C	109.00
H7A	-C7	-H7B	109.00	H17A	-C17	-H17B	110.00
H7A	-C7	-H7C	110.00	H17A	-C17	-H17C	109.00
H7B	-C7	-H7C	109.00	H17B	-C17	-H17C	109.00
C4	-C8	-H8A	109.00	C15	-C18	-H18A	110.00
C4	-C8	-H8B	109.00	C15	-C18	-H18B	110.00
C4	-C8	-H8C	110.00	C15	-C18	-H18C	109.00
H8A	-C8	-H8B	109.00	H18A	-C18	-H18B	109.00
H8A	-C8	-H8C	109.00	H18A	-C18	-H18C	109.00
H8B	-C8	-H8C	109.00	H18B	-C18	-H18C	109.00
C6	-C9	-H9A	109.00	N1	-C20	-H20	127.00
C6	-C9	-H9B	109.00	C21	-C20	-H20	127.00
C6	-C9	-H9C	110.00	N2	-C21	-H21	125.00
H9A	-C9	-H9B	109.00	C20	-C21	-H21	125.00
H9A	-C9	-H9C	110.00	N1	-C22	-H22A	109.00
H9B	-C9	-H9C	109.00	N1	-C22	-H22B	109.00
C11	-C12	-H12	120.00	N1	-C22	-H22C	110.00
C13	-C12	-H12	120.00	H22A	-C22	-H22B	109.00
C13	-C14	-H14	120.00	H22A	-C22	-H22C	110.00

Table S3 - Bond Angles (Degrees) (continued)
for: **I** P 21/c R = 0.09

H22B	-C22	-H22C	109.00	N4	-C26	-H26	126.00
N2	-C23	-H23A	109.00	C25	-C26	-H26	125.00
N2	-C23	-H23B	109.00	N3	-C27	-H27A	109.00
N4	-C23	-H23A	109.00	N3	-C27	-H27B	109.00
N4	-C23	-H23B	109.00	N3	-C27	-H27C	109.00
H23A	-C23	-H23B	108.00	H27A	-C27	-H27B	110.00
N3	-C25	-H25	127.00	H27A	-C27	-H27C	109.00
C26	-C25	-H25	127.00	H27B	-C27	-H27C	110.00

Table S4 - Torsion Angles (Degrees)
for: **I** P 21/c R = 0.09

C1	-Te1	-Se1	-C19	63.7(5)
I1	-Te1	-C1	-C6	-94.9(11)
I1	-Te1	-C1	-C2	88.2(10)
Se1	-Te1	-C1	-C2	-95.8(10)
Se1	-Te1	-C1	-C6	81.1(11)
C10	-Te2	-Se2	-C24	-60.5(5)
I2	-Te2	-C10	-C15	-79.4(8)
I2	-Te2	-C10	-C11	101.7(8)
Se2	-Te2	-C10	-C11	-78.6(8)
Se2	-Te2	-C10	-C15	100.3(8)
Te1	-Se1	-C19	-N2	-98.4(12)
Te1	-Se1	-C19	-N1	84.9(12)
Te2	-Se2	-C24	-N3	98.2(12)
Te2	-Se2	-C24	-N4	-75.9(12)
C22	-N1	-C19	-Se1	-5(2)
C19	-N1	-C20	-C21	0.8(17)
C20	-N1	-C19	-Se1	178.6(11)
C22	-N1	-C19	-N2	178.1(13)
C20	-N1	-C19	-N2	1.4(16)
C22	-N1	-C20	-C21	-176.1(13)
C21	-N2	-C19	-N1	-2.9(15)
C23	-N2	-C19	-Se1	8(2)
C19	-N2	-C21	-C20	3.5(17)
C23	-N2	-C19	-N1	-175.2(12)
C21	-N2	-C19	-Se1	179.9(10)
C23	-N2	-C21	-C20	176.1(13)
C19	-N2	-C23	-N4	-81.7(17)
C21	-N2	-C23	-N4	107.2(15)

Table S4 - Torsion Angles (Degrees) (continued)
for: **I** P 21/c R = 0.09

C27	-N3	-C25	-C26	-178.9(15)
C25	-N3	-C24	-Se2	-175.1(11)
C27	-N3	-C24	-N4	177.8(13)
C24	-N3	-C25	-C26	-1.1(18)
C27	-N3	-C24	-Se2	3(2)
C25	-N3	-C24	-N4	0.0(16)
C26	-N4	-C24	-N3	1.1(15)
C23	-N4	-C24	-N3	-178.4(12)
C23	-N4	-C24	-Se2	-3(2)
C26	-N4	-C24	-Se2	176.1(11)
C26	-N4	-C23	-N2	98.9(16)
C23	-N4	-C26	-C25	177.7(14)
C24	-N4	-C26	-C25	-1.8(18)
C24	-N4	-C23	-N2	-81.8(17)
Te1	-C1	-C2	-C7	-4.4(18)
Te1	-C1	-C6	-C5	-175.3(10)
C2	-C1	-C6	-C9	-177.5(15)
C2	-C1	-C6	-C5	2(2)
Te1	-C1	-C2	-C3	174.7(10)
C6	-C1	-C2	-C3	-2(2)
C6	-C1	-C2	-C7	178.8(13)
Te1	-C1	-C6	-C9	6(2)
C7	-C2	-C3	-C4	-179.2(14)
C1	-C2	-C3	-C4	2(2)
C2	-C3	-C4	-C5	0(2)
C2	-C3	-C4	-C8	-177.0(14)
C8	-C4	-C5	-C6	176.4(14)
C3	-C4	-C5	-C6	0(2)

Table S4 - Torsion Angles (Degrees) (continued)
for: **I** P 21/c R = 0.09

C4	-C5	-C6	-C1	0(2)
C4	-C5	-C6	-C9	178.8(15)
Te2	-C10	-C15	-C14	-178.9(8)
Te2	-C10	-C11	-C16	-1.3(17)
Te2	-C10	-C11	-C12	178.8(8)
C15	-C10	-C11	-C16	179.8(14)
Te2	-C10	-C15	-C18	5.1(14)
C11	-C10	-C15	-C14	0.1(15)
C11	-C10	-C15	-C18	-176.0(11)
C15	-C10	-C11	-C12	-0.1(15)
C10	-C11	-C12	-C13	0.1(16)
C16	-C11	-C12	-C13	-179.8(14)
C11	-C12	-C13	-C17	179.1(14)
C11	-C12	-C13	-C14	-0.1(18)
C12	-C13	-C14	-C15	0.0(18)
C17	-C13	-C14	-C15	-179.1(14)
C13	-C14	-C15	-C18	176.2(12)
C13	-C14	-C15	-C10	0.0(16)
N1	-C20	-C21	-N2	-2.6(17)
N3	-C25	-C26	-N4	1.8(19)

Table S5 - Contact Distances(Angstrom)
for: **I** P 21/c R = 0.09

I1	.Te2_a	4.1484(16)	Se1	.H22C	3.0100
I2	.I2_d	3.9928(15)	Se1	.H23B	3.0700
I1	.H3_a	3.3000	Se1	.H26	3.0900
I1	.H21_a	3.3500	Se1	.H8C_f	3.1300
Te1	.C7	3.308(17)	Se2	.H23A	3.0000
Te1	.C9	3.34(2)	Se2	.H27C	2.9300
I1	.H20_b	3.1000	N1	.C21	2.14(2)
I2	.H18A	3.2100	N2	.C20	2.20(2)
I2	.H25_c	3.0600	N2	.C24	3.240(17)
Te2	.C18	3.292(19)	N2	.C26	3.39(2)
Te2	.C16	3.37(2)	N3	.C15	3.420(15)
Te2	.I1_e	4.1484(16)	N3	.C26	2.14(2)
Te1	.H7C	3.1300	N4	.C19	3.246(17)
Te1	.H3_a	3.4300	N4	.C21	3.442(19)
Te1	.H9B	3.1500	N4	.C25	2.19(2)
Te1	.H7A	3.1800	C1	.C4	2.798(19)
Te1	.H9C	3.1900	C1	.C23	3.594(19)
Te2	.H16A	3.1600	C2	.C23	3.451(19)
Te2	.H16B	3.2800	C2	.C5	2.770(19)
Te2	.H18B	3.0200	C3	.C22_b	3.55(2)
Te2	.H23A	3.4000	C3	.C6	2.73(2)
Te2	.H18A	3.2500	C3	.C23	3.42(2)
Se1	.C22	3.355(17)	N4	.H18B	2.8300
Se1	.C23	3.342(15)	C4	.C1	2.798(19)
Se1	.C26	3.554(16)	C5	.C2	2.770(19)
Se2	.C27	3.303(18)	C6	.C3	2.73(2)
Se2	.C21	3.755(15)	C7	.Te1	3.308(17)
Se2	.C23	3.339(14)	C9	.Te1	3.34(2)

Table S5 - Contact Distances(Angstrom) (continued)
for: **I** P 21/c R = 0.09

C10	.C27	3.58(2)	C23	.C20	3.57(2)
C10	.C24	3.551(16)	C23	.C25	3.59(2)
C10	.C13	2.780(14)	C24	.C26	2.20(2)
C11	.C14	2.780(13)	C24	.N2	3.240(17)
C12	.C15	2.780(14)	C24	.C10	3.551(16)
C13	.C10	2.780(14)	C25	.C23	3.59(2)
C14	.C11	2.780(13)	C25	.N4	2.19(2)
C15	.C27	3.60(2)	C26	.Se1	3.554(16)
C15	.N3	3.420(15)	C26	.N3	2.14(2)
C15	.C12	2.780(14)	C26	.C27	3.56(2)
C16	.Te2	3.37(2)	C26	.N2	3.39(2)
C18	.Te2	3.292(19)	C27	.Se2	3.303(18)
C19	.C21	2.18(2)	C27	.C15	3.60(2)
C19	.N4	3.246(17)	C27	.C10	3.58(2)
C20	.C23	3.57(2)	C27	.C26	3.56(2)
C20	.N2	2.20(2)	C1	.H7A	2.7700
C21	.C22	3.56(2)	C1	.H9B	2.7700
C21	.Se2	3.755(15)	C1	.H9C	2.8300
C21	.N1	2.14(2)	C1	.H7C	2.7800
C21	.N4	3.442(19)	C1	.H23B	2.7300
C22	.C21	3.56(2)	C2	.H23B	2.7800
C22	.C3_f	3.55(2)	C3	.H8B	2.7000
C22	.Se1	3.355(17)	C3	.H7B	2.5300
C23	.C2	3.451(19)	C3	.H8C	2.8500
C23	.C3	3.42(2)	C3	.H23B	2.8400
C23	.Se2	3.339(14)	C4	.H23B	2.9300
C23	.C1	3.594(19)	C5	.H23B	2.8800
C23	.Se1	3.342(15)	C5	.H9C	3.0900

Table S5 - Contact Distances(Angstrom) (continued)
for: **I** P 21/c R = 0.09

C5	.H8C	3.0400	C16	.H12	2.5600
C5	.H8A	2.5300	C17	.H12	2.6600
C5	.H9A	2.5400	C17	.H14	2.6800
C6	.H23B	2.8000	C18	.H14	2.6000
C7	.H3	2.6200	C19	.H22C	2.6800
C8	.H3	2.6500	C19	.H21	3.0700
C8	.H5	2.6000	C19	.H23B	2.6500
C9	.H5	2.6300	C19	.H22A	2.9000
C10	.H18A	2.8000	C19	.H7C	2.9600
C10	.H27A	2.8800	C19	.H8C_f	3.0700
C10	.H16B	2.8200	C20	.H22B	2.6000
C10	.H16A	2.7800	C20	.H22A	2.9600
C10	.H18B	2.7400	C21	.H23A	2.5500
C11	.H27A	2.8000	C22	.H20	2.7800
C12	.H16A	3.0800	C23	.H26	2.8000
C12	.H16C	2.4500	C23	.H21	2.7600
C12	.H27A	2.7400	C24	.H23A	2.6500
C12	.H16B	3.0400	C24	.H26	3.0900
C12	.H17A	2.6100	C24	.H8A_f	3.1000
C12	.H17B	2.9500	C24	.H18B	3.0700
C13	.H27A	2.7700	C24	.H27A	2.9100
C14	.H18C	2.4900	C24	.H27C	2.6200
C14	.H18A	3.0300	C25	.H27A	2.9400
C14	.H27A	2.8500	C25	.H27B	2.6300
C14	.H17C	2.6200	C26	.H18B	2.9500
C14	.H17B	2.9500	C26	.H23B	2.6100
C15	.H27A	2.9000	C27	.H25	2.8000
C16	.H18C_c	2.9800	H3	.C7	2.6200

Table S5 - Contact Distances(Angstrom) (continued)
for: **I** P 21/c R = 0.09

H3	.C8	2.6500	H9B	.Te1	3.1500
H3	.H7B	2.2900	H9B	.C1	2.7700
H3	.H8B	2.6000	H9B	.H7B_a	2.4900
H3	.I1_e	3.3000	H9C	.Te1	3.1900
H3	.Te1_e	3.4300	H9C	.C1	2.8300
H5	.C8	2.6000	H9C	.C5	3.0900
H5	.C9	2.6300	H12	.C16	2.5600
H5	.H8A	2.3000	H12	.C17	2.6600
H5	.H9A	2.3100	H12	.H16C	2.2000
H7A	.Te1	3.1800	H12	.H17A	2.4400
H7A	.C1	2.7700	H14	.C17	2.6800
H7B	.C3	2.5300	H14	.C18	2.6000
H7B	.H3	2.2900	H14	.H17C	2.4600
H7B	.H9B_e	2.4900	H14	.H18C	2.2600
H7C	.Te1	3.1300	H16A	.Te2	3.1600
H7C	.C1	2.7800	H16A	.C10	2.7800
H7C	.C19	2.9600	H16A	.C12	3.0800
H8A	.C5	2.5300	H16B	.Te2	3.2800
H8A	.H5	2.3000	H16B	.C10	2.8200
H8A	.C24_b	3.1000	H16B	.C12	3.0400
H8B	.C3	2.7000	H16B	.H18C_c	2.2000
H8B	.H3	2.6000	H16C	.C12	2.4500
H8C	.C3	2.8500	H16C	.H12	2.2000
H8C	.C5	3.0400	H17A	.C12	2.6100
H8C	.Se1_b	3.1300	H17A	.H12	2.4400
H8C	.C19_b	3.0700	H17B	.C12	2.9500
H9A	.C5	2.5400	H17B	.C14	2.9500
H9A	.H5	2.3100	H17C	.C14	2.6200

Table S5 - Contact Distances(Angstrom) (continued)
for: **I** P 21/c R = 0.09

H17C	.H14	2.4600	H22C	.C19	2.6800
H18A	.I2	3.2100	H23A	.Te2	3.4000
H18A	.Te2	3.2500	H23A	.Se2	3.0000
H18A	.C10	2.8000	H23A	.C21	2.5500
H18A	.C14	3.0300	H23A	.C24	2.6500
H18B	.Te2	3.0200	H23A	.H21	2.4900
H18B	.N4	2.8300	H23B	.Se1	3.0700
H18B	.C10	2.7400	H23B	.C1	2.7300
H18B	.C24	3.0700	H23B	.C2	2.7800
H18B	.C26	2.9500	H23B	.C3	2.8400
H18C	.C14	2.4900	H23B	.C4	2.9300
H18C	.H14	2.2600	H23B	.C5	2.8800
H18C	.C16_g	2.9800	H23B	.C6	2.8000
H18C	.H16B_g	2.2000	H23B	.C19	2.6500
H20	.C22	2.7800	H23B	.C26	2.6100
H20	.H21	2.4100	H23B	.H26	2.5800
H20	.H22B	2.5600	H25	.C27	2.8000
H20	.I1_f	3.1000	H25	.H26	2.4000
H21	.C19	3.0700	H25	.I2_g	3.0600
H21	.C23	2.7600	H26	.Se1	3.0900
H21	.H20	2.4100	H26	.C23	2.8000
H21	.H23A	2.4900	H26	.C24	3.0900
H21	.I1_e	3.3500	H26	.H23B	2.5800
H22A	.C19	2.9000	H26	.H25	2.4000
H22A	.C20	2.9600	H27A	.C10	2.8800
H22B	.C20	2.6000	H27A	.C11	2.8000
H22B	.H20	2.5600	H27A	.C12	2.7400
H22C	.Se1	3.0100	H27A	.C13	2.7700

Table S5 - Contact Distances(Angstrom) (continued)
for: **I** P 21/c R = 0.09

H27A	.C14	2.8500	H27B	.C25	2.6300
H27A	.C15	2.9000	H27C	.Se2	2.9300
H27A	.C24	2.9100	H27C	.C24	2.6200
H27A	.C25	2.9400			

Table S6 - Hydrogen Bonds (Angstrom, Deg)
for: **I** P 21/c R = 0.09

C25 -- H25 .. I2	0.9300	3.0600	3.940(17)	159.00	2_755
C27 -- H27C .. Se2	0.9600	2.9300	3.303(18)	105.00	.

Translation of Symmetry Code to Equiv.Pos

a =[2655.00] = [2_655] = 1-x,1/2+y,1/2-z
b =[4555.00] = [4_566] = x,1/2-y,1/2+z
c =[2745.00] = [2_745] = 2-x,-1/2+y,1/2-z
d =[3756.00] = [3_756] = 2-x,-y,1-z
e =[2645.00] = [2_645] = 1-x,-1/2+y,1/2-z
f =[4554.00] = [4_565] = x,1/2-y,-1/2+z
g =[2755.00] = [2_755] = 2-x,1/2+y,1/2-z

Table S7 - Crystal Data and Details of the Structure Determination
for: **II** P 1 21/c 1 R = 0.03

Crystal Data			
Formula	C38 H50 N8 Se4 Te2, 2(C9 H11 I2 Te)		
Formula Weight			2191.05
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	8.25477(18)	16.5149(4)	26.0208(5)
alpha, beta, gamma [deg]	90	90.7335(18)	90
V [Ang**3]			3547.04(13)
Z			2
D(calc) [g/cm**3]			2.052
Mu(CuKa) [/mm]			29.166
F(000)			2040
Crystal Size [mm]		0.03 x 0.04 x 0.07	
Data Collection			
Temperature (K)			120
Radiation [Angstrom]		CuKa	1.54184
Theta Min-Max [Deg]			4.3, 73.6
Dataset		-7: 10 ; -20: 20 ; -26: 31	
Tot., Uniq. Data, R(int)		14667, 6935, 0.037	
Observed data [I > 0.0 sigma(I)]			5784
Refinement			
Nref, Npar			6935, 351
R, wR2, S		0.0312, 0.0734, 0.99	
w = ^2^(FO^2^)+(0.0313P)^2^] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-1.15, 0.74

Table S8 - Bond Distances (Angstrom)
for: **II** P 1 21/c 1 R = 0.03

I1	-Te2	2.8947(7)	C14	-C15	1.404(7)
I2	-Te2	3.0258(7)	C14	-C18	1.495(8)
Te1	-Se1	2.9163(7)	C15	-C16	1.402(7)
Te1	-C11	2.139(5)	C16	-C19	1.509(7)
Te1	-Se2	2.7189(7)	C2	-H2	0.9500
Te2	-C20	2.132(4)	C3	-H3	0.9500
Se1	-C1	1.861(5)	C4	-H4A	0.9800
Se2	-C10	1.867(5)	C4	-H4B	0.9800
N1	-C1	1.358(7)	C4	-H4C	0.9800
N1	-C2	1.369(8)	C5	-H5B	0.9900
N1	-C5	1.456(7)	C5	-H5A	0.9900
N2	-C4	1.456(7)	C6	-H6A	0.9900
N2	-C1	1.353(7)	C6	-H6B	0.9900
N2	-C3	1.383(8)	C7	-H7	0.9500
N3	-C7	1.369(7)	C8	-H8	0.9500
N3	-C6	1.461(6)	C9	-H9C	0.9800
N3	-C10	1.351(7)	C9	-H9B	0.9800
N4	-C8	1.376(7)	C9	-H9A	0.9800
N4	-C9	1.461(7)	C13	-H13	0.9500
N4	-C10	1.359(6)	C15	-H15	0.9500
C2	-C3	1.374(8)	C17	-H17A	0.9800
C5	-C6_a	1.526(8)	C17	-H17B	0.9800
C7	-C8	1.350(7)	C17	-H17C	0.9800
C11	-C12	1.395(6)	C18	-H18C	0.9800
C11	-C16	1.399(7)	C18	-H18A	0.9800
C12	-C13	1.399(7)	C18	-H18B	0.9800
C12	-C17	1.506(8)	C19	-H19A	0.9800
C13	-C14	1.385(8)	C19	-H19B	0.9800

Table S8 - Bond Distances (Angstrom) (continued)
for: **II** P 1 21/c 1 R = 0.03

C19	-H19C	0.9800	C24	-H24	0.9500
C20	-C21	1.401(7)	C26	-H26A	0.9800
C20	-C25	1.405(7)	C26	-H26B	0.9800
C21	-C22	1.394(7)	C26	-H26C	0.9800
C21	-C26	1.516(7)	C27	-H27A	0.9800
C22	-C23	1.386(7)	C27	-H27B	0.9800
C23	-C24	1.390(7)	C27	-H27C	0.9800
C23	-C27	1.505(7)	C28	-H28A	0.9800
C24	-C25	1.390(7)	C28	-H28B	0.9800
C25	-C28	1.506(7)	C28	-H28C	0.9800
C22	-H22	0.9500			

Table S9 - Bond Angles (Degrees)
for: **II** P 1 21/c 1 R = 0.03

Se1	-Te1	-Se2	174.58(2)	N4	-C8	-C7	107.3(4)
Se1	-Te1	-C11	85.56(12)	N3	-C10	-N4	106.3(4)
Se2	-Te1	-C11	90.01(12)	Se2	-C10	-N3	126.7(4)
I2	-Te2	-C20	88.02(13)	Se2	-C10	-N4	127.1(4)
I1	-Te2	-C20	90.29(13)	Te1	-C11	-C12	119.4(3)
I1	-Te2	-I2	177.63(2)	Te1	-C11	-C16	119.5(3)
Te1	-Se1	-C1	96.38(15)	C12	-C11	-C16	121.1(4)
Te1	-Se2	-C10	99.87(15)	C13	-C12	-C17	118.5(5)
C1	-N1	-C5	125.7(5)	C11	-C12	-C17	122.8(5)
C1	-N1	-C2	109.9(4)	C11	-C12	-C13	118.7(4)
C2	-N1	-C5	124.3(5)	C12	-C13	-C14	122.0(5)
C1	-N2	-C3	110.2(4)	C15	-C14	-C18	120.3(5)
C1	-N2	-C4	125.5(5)	C13	-C14	-C18	121.6(5)
C3	-N2	-C4	124.2(5)	C13	-C14	-C15	118.0(5)
C7	-N3	-C10	109.8(4)	C14	-C15	-C16	121.4(5)
C6	-N3	-C7	124.4(5)	C11	-C16	-C15	118.5(4)
C6	-N3	-C10	125.9(4)	C11	-C16	-C19	123.4(4)
C8	-N4	-C9	124.4(4)	C15	-C16	-C19	118.1(4)
C8	-N4	-C10	109.3(4)	C3	-C2	-H2	126.00
C9	-N4	-C10	126.2(4)	N1	-C2	-H2	126.00
N1	-C1	-N2	106.3(4)	N2	-C3	-H3	127.00
Se1	-C1	-N1	126.7(4)	C2	-C3	-H3	127.00
Se1	-C1	-N2	127.1(4)	N2	-C4	-H4A	109.00
N1	-C2	-C3	107.5(5)	N2	-C4	-H4B	109.00
N2	-C3	-C2	106.1(5)	H4B	-C4	-H4C	110.00
N1	-C5	-C6_a	111.4(4)	H4A	-C4	-H4C	110.00
N3	-C6	-C5_a	109.3(4)	N2	-C4	-H4C	109.00
N3	-C7	-C8	107.4(4)	H4A	-C4	-H4B	109.00

Table S9 - Bond Angles (Degrees) (continued)
for: **II** P 1 21/c 1 R = 0.03

N1	-C5	-H5A	109.00	H17A	-C17	-H17B	109.00
N1	-C5	-H5B	109.00	H17A	-C17	-H17C	109.00
H5A	-C5	-H5B	108.00	C14	-C18	-H18B	109.00
C6_a	-C5	-H5A	109.00	H18A	-C18	-H18C	110.00
C6_a	-C5	-H5B	109.00	C14	-C18	-H18C	109.00
H6A	-C6	-H6B	108.00	H18A	-C18	-H18B	109.00
C5_a	-C6	-H6B	110.00	C14	-C18	-H18A	109.00
N3	-C6	-H6B	110.00	H18B	-C18	-H18C	109.00
C5_a	-C6	-H6A	110.00	C16	-C19	-H19C	109.00
N3	-C6	-H6A	110.00	H19A	-C19	-H19C	110.00
N3	-C7	-H7	126.00	H19B	-C19	-H19C	109.00
C8	-C7	-H7	126.00	H19A	-C19	-H19B	109.00
N4	-C8	-H8	126.00	C16	-C19	-H19A	109.00
C7	-C8	-H8	126.00	C16	-C19	-H19B	109.00
N4	-C9	-H9C	109.00	Te2	-C20	-C21	119.5(4)
N4	-C9	-H9B	109.00	Te2	-C20	-C25	119.8(3)
H9B	-C9	-H9C	110.00	C21	-C20	-C25	120.8(4)
H9A	-C9	-H9B	110.00	C20	-C21	-C22	118.5(4)
H9A	-C9	-H9C	110.00	C20	-C21	-C26	122.9(4)
N4	-C9	-H9A	109.00	C22	-C21	-C26	118.6(4)
C12	-C13	-H13	119.00	C21	-C22	-C23	121.9(4)
C14	-C13	-H13	119.00	C22	-C23	-C24	118.5(4)
C16	-C15	-H15	119.00	C22	-C23	-C27	121.0(5)
C14	-C15	-H15	119.00	C24	-C23	-C27	120.6(5)
C12	-C17	-H17A	109.00	C23	-C24	-C25	121.9(5)
C12	-C17	-H17B	110.00	C20	-C25	-C24	118.5(4)
C12	-C17	-H17C	110.00	C20	-C25	-C28	123.2(4)
H17B	-C17	-H17C	109.00	C24	-C25	-C28	118.3(5)

Table S9 - Bond Angles (Degrees) (continued)
for: **II** P 1 21/c 1 R = 0.03

C21	-C22	-H22	119.00	C23	-C27	-H27B	109.00
C23	-C22	-H22	119.00	C23	-C27	-H27C	109.00
C23	-C24	-H24	119.00	H27A	-C27	-H27B	109.00
C25	-C24	-H24	119.00	H27A	-C27	-H27C	110.00
C21	-C26	-H26A	109.00	H27B	-C27	-H27C	109.00
C21	-C26	-H26B	109.00	C25	-C28	-H28A	109.00
C21	-C26	-H26C	109.00	C25	-C28	-H28B	109.00
H26A	-C26	-H26B	110.00	C25	-C28	-H28C	109.00
H26A	-C26	-H26C	110.00	H28A	-C28	-H28B	110.00
H26B	-C26	-H26C	110.00	H28A	-C28	-H28C	109.00
C23	-C27	-H27A	109.00	H28B	-C28	-H28C	109.00

Table S10 - Torsion Angles (Degrees)
for: **II** P 1 21/c 1 R = 0.03

C11	-Te1	-Se1	-C1	67.1(2)
C11	-Te1	-Se2	-C10	79.7(2)
Se1	-Te1	-C11	-C12	75.4(4)
Se1	-Te1	-C11	-C16	-101.4(4)
Se2	-Te1	-C11	-C12	-107.7(4)
Se2	-Te1	-C11	-C16	75.5(4)
I2	-Te2	-C20	-C21	75.7(4)
I2	-Te2	-C20	-C25	-103.7(4)
I1	-Te2	-C20	-C21	-102.6(4)
I1	-Te2	-C20	-C25	78.0(4)
Te1	-Se1	-C1	-N1	83.6(4)
Te1	-Se1	-C1	-N2	-95.3(4)
Te1	-Se2	-C10	-N4	-89.3(4)
Te1	-Se2	-C10	-N3	92.6(4)
C2	-N1	-C1	-Se1	-179.4(4)
C5	-N1	-C2	-C3	178.0(5)
C1	-N1	-C5	-C6_a	-97.9(6)
C2	-N1	-C5	-C6_a	84.4(6)
C5	-N1	-C1	-N2	-178.3(5)
C2	-N1	-C1	-N2	-0.4(6)
C5	-N1	-C1	-Se1	2.6(8)
C1	-N1	-C2	-C3	0.0(6)
C3	-N2	-C1	-Se1	179.6(4)
C4	-N2	-C3	-C2	-177.2(5)
C4	-N2	-C1	-Se1	-3.8(7)
C4	-N2	-C1	-N1	177.2(5)
C3	-N2	-C1	-N1	0.6(6)
C1	-N2	-C3	-C2	-0.6(6)

Table S10 - Torsion Angles (Degrees) (continued)
for: **II** P 1 21/c 1 R = 0.03

C7	-N3	-C6	-C5_a	-84.4(6)
C10	-N3	-C6	-C5_a	93.9(6)
C7	-N3	-C10	-Se2	178.6(4)
C7	-N3	-C10	-N4	0.2(5)
C6	-N3	-C7	-C8	178.3(4)
C10	-N3	-C7	-C8	-0.3(6)
C6	-N3	-C10	-Se2	0.1(7)
C6	-N3	-C10	-N4	-178.3(4)
C10	-N4	-C8	-C7	-0.1(6)
C8	-N4	-C10	-Se2	-178.5(4)
C9	-N4	-C8	-C7	-175.6(5)
C8	-N4	-C10	-N3	-0.1(5)
C9	-N4	-C10	-Se2	-3.1(7)
C9	-N4	-C10	-N3	175.3(4)
N1	-C2	-C3	-N2	0.3(6)
N1	-C5	-C6_a	-N3_a	-178.0(4)
N3	-C7	-C8	-N4	0.2(6)
Te1	-C11	-C12	-C13	-173.2(4)
Te1	-C11	-C16	-C19	-5.1(6)
C12	-C11	-C16	-C15	-1.6(7)
C12	-C11	-C16	-C19	178.1(5)
C16	-C11	-C12	-C17	-177.2(5)
Te1	-C11	-C12	-C17	6.1(7)
C16	-C11	-C12	-C13	3.5(7)
Te1	-C11	-C16	-C15	175.2(4)
C11	-C12	-C13	-C14	-0.9(8)
C17	-C12	-C13	-C14	179.8(5)
C12	-C13	-C14	-C15	-3.6(8)

Table S10 - Torsion Angles (Degrees) (continued)
for: **II** P 1 21/c 1 R = 0.03

C12	-C13	-C14	-C18	174.0(5)
C18	-C14	-C15	-C16	-172.0(5)
C13	-C14	-C15	-C16	5.6(8)
C14	-C15	-C16	-C11	-3.1(7)
C14	-C15	-C16	-C19	177.2(5)
Te2	-C20	-C21	-C22	-177.8(4)
Te2	-C20	-C21	-C26	4.0(6)
C25	-C20	-C21	-C22	1.6(7)
C25	-C20	-C21	-C26	-176.5(5)
Te2	-C20	-C25	-C24	177.7(4)
Te2	-C20	-C25	-C28	-3.4(7)
C21	-C20	-C25	-C24	-1.8(7)
C21	-C20	-C25	-C28	177.2(5)
C20	-C21	-C22	-C23	-0.2(7)
C26	-C21	-C22	-C23	178.1(5)
C21	-C22	-C23	-C24	-1.1(8)
C21	-C22	-C23	-C27	178.2(5)
C22	-C23	-C24	-C25	1.0(8)
C27	-C23	-C24	-C25	-178.3(5)
C23	-C24	-C25	-C20	0.4(7)
C23	-C24	-C25	-C28	-178.6(5)

Table S11 - Contact Distances(Angstrom)
for: **II** P 1 21/c 1 R = 0.03

I1	.C10_a	3.685(5)	Te2	.H26C	3.0900
I1	.Se2_a	3.7940(7)	Te2	.H27C_o	3.3600
I2	.C4_p	3.752(6)	Se1	.C17_b	3.645(7)
I1	.H24_e	3.3800	Se1	.C7_b	3.677(5)
I1	.H18A_n	3.1800	Se2	.Te1_a	3.9091(7)
I1	.H5B	3.3700	Se2	.I1_d	3.7940(7)
I1	.H28A	3.2900	Se1	.H17C_b	3.0400
I2	.H2_q	3.0900	Se1	.H5B	2.8900
I2	.H22_o	3.2700	Se1	.H17A	3.2300
I2	.H4A_p	2.9000	Se1	.H4C	2.9500
I2	.H3_n	3.0700	Se2	.H17B_c	2.9700
I2	.H7_r	3.2100	Se2	.H19B	3.0200
I2	.H26C	3.2700	Se2	.H9B	2.9100
I2	.H27C_o	3.1900	Se2	.H6A	2.9100
Te1	.Se2_a	3.9091(7)	N3	.N4	2.168(6)
Te1	.Te1_a	4.1860(5)	N4	.N3	2.168(6)
Te2	.C18_n	3.889(6)	C2	.C22_e	3.506(7)
Te1	.H17A_b	3.3900	C4	.C14	3.492(7)
Te1	.H6A_a	3.1200	C4	.C15	3.464(7)
Te1	.H17C	3.0900	C4	.C16	3.504(8)
Te1	.H19A	3.1800	C4	.I2_f	3.752(6)
Te1	.H19B	3.1800	C5	.C23_e	3.584(8)
Te1	.H17A	3.2400	C7	.Se1_b	3.677(5)
Te2	.H26B	3.2500	C7	.C27_g	3.502(8)
Te2	.H28C	3.0500	C8	.C27_g	3.599(8)
Te2	.H28A	3.3200	C9	.C24_d	3.452(7)
Te2	.H15_n	3.2300	C9	.C12	3.559(7)
Te2	.H18A_n	3.3600	C9	.C23_d	3.583(7)

Table S11 - Contact Distances(Angstrom) (continued)
for: **II** P 1 21/c 1 R = 0.03

C10	.I1_d	3.685(5)	C18	.H27B_d	2.8600
C12	.C9	3.559(7)	C20	.H9C_a	3.0100
C14	.C4	3.492(7)	C21	.H9C_a	3.0800
C15	.C4	3.464(7)	C23	.H9C_a	3.1000
C16	.C4	3.504(8)	C23	.H5A_q	2.9800
C17	.Se1_b	3.645(7)	C24	.H9C_a	3.0000
C18	.Te2_i	3.889(6)	C24	.H5A_q	2.9700
C22	.C2_q	3.506(7)	C25	.H9C_a	2.9600
C23	.C5_q	3.584(8)	C27	.H7_t	2.8900
C23	.C9_a	3.583(7)	C27	.H8_t	3.1000
C24	.C9_a	3.452(7)	C27	.H28C_s	3.0600
C27	.C8_t	3.599(8)	C28	.H13_b	3.0500
C27	.C7_t	3.502(8)	C28	.H18B_b	2.9500
C2	.H6B_a	3.0600	H2	.I2_e	3.0900
C7	.H27A_g	3.0100	H3	.I2_i	3.0700
C7	.H5A_a	3.0000	H4A	.I2_f	2.9000
C8	.H27A_g	3.0200	H4B	.C15	3.0200
C11	.H4C	2.8800	H4B	.C14	3.0700
C11	.H9B	2.8700	H4C	.C11	2.8800
C12	.H4C	2.8100	H4C	.C12	2.8100
C12	.H9B	3.0400	H4C	.C13	2.8500
C13	.H4C	2.8500	H4C	.C14	3.0100
C14	.H4B	3.0700	H4C	.C16	3.0800
C14	.H4C	3.0100	H4C	.Se1	2.9500
C14	.H27B_d	3.0500	H5A	.C24_e	2.9700
C15	.H4B	3.0200	H5A	.C7_a	3.0000
C16	.H4C	3.0800	H5A	.C23_e	2.9800
C18	.H8_h	3.0400	H5B	.I1	3.3700

Table S11 - Contact Distances(Angstrom) (continued)
for: **II** P 1 21/c 1 R = 0.03

H5B	.Se1	2.8900	H17A	.Te1_b	3.3900
H6A	.Se2	2.9100	H17B	.H13	2.2900
H6A	.Te1_a	3.1200	H17B	.Se2_m	2.9700
H6B	.C2_a	3.0600	H17C	.Se1_b	3.0400
H7	.I2_j	3.2100	H17C	.Te1	3.0900
H7	.C27_g	2.8900	H18A	.H15	2.4700
H7	.H27C_g	2.4700	H18A	.H8_h	2.4400
H7	.H27A_g	2.5300	H18A	.I1_i	3.1800
H8	.H18A_k	2.4400	H18A	.Te2_i	3.3600
H8	.C27_g	3.1000	H18A	.H27B_d	2.5000
H8	.C18_k	3.0400	H18B	.H28B_l	2.4500
H8	.H27A_g	2.5500	H18B	.C28_l	2.9500
H9B	.Se2	2.9100	H18B	.H13	2.4100
H9B	.C11	2.8700	H19A	.Te1	3.1800
H9B	.C12	3.0400	H19B	.Te1	3.1800
H9C	.C21_d	3.0800	H19B	.Se2	3.0200
H9C	.C20_d	3.0100	H19C	.H26B_i	2.4400
H9C	.C25_d	2.9600	H19C	.H15	2.2800
H9C	.C23_d	3.1000	H22	.I2_s	3.2700
H9C	.C24_d	3.0000	H22	.H26A	2.2900
H13	.C28_l	3.0500	H22	.H27C	2.3800
H13	.H17B	2.2900	H24	.H27B	2.5100
H13	.H18B	2.4100	H24	.H28B	2.2700
H15	.Te2_i	3.2300	H24	.I1_u	3.3800
H15	.H18A	2.4700	H26A	.H22	2.2900
H15	.H19C	2.2800	H26B	.Te2	3.2500
H17A	.Se1	3.2300	H26B	.H19C_n	2.4400
H17A	.Te1	3.2400	H26C	.I2	3.2700

Table S11 - Contact Distances(Angstrom) (continued)
for: **II** P 1 21/c 1 R = 0.03

H26C	.Te2	3.0900	H27C	.H22	2.3800
H27A	.C7_t	3.0100	H27C	.H28C_s	2.5500
H27A	.C8_t	3.0200	H27C	.H7_t	2.4700
H27A	.H7_t	2.5300	H28A	.I1	3.2900
H27A	.H8_t	2.5500	H28A	.Te2	3.3200
H27B	.H24	2.5100	H28B	.H24	2.2700
H27B	.C14_a	3.0500	H28B	.H18B_b	2.4500
H27B	.C18_a	2.8600	H28C	.Te2	3.0500
H27B	.H18A_a	2.5000	H28C	.C27_o	3.0600
H27C	.I2_s	3.1900	H28C	.H27C_o	2.5500
H27C	.Te2_s	3.3600			

Table S12 - Hydrogen Bonds (Angstrom, Deg)
for: **II** P 1 21/c 1 R = 0.03

C4 -- H4A .. I2	0.9800	2.9000	3.752(6)	146.00	2_656
C4 -- H4C .. Se1	0.9800	2.9500	3.333(6)	105.00	.
C5 -- H5B .. Se1	0.9900	2.8900	3.335(6)	109.00	.
C6 -- H6A .. Se2	0.9900	2.9100	3.336(5)	107.00	.
C9 -- H9B .. Se2	0.9800	2.9100	3.361(5)	109.00	.
C17 -- H17B .. Se2	0.9800	2.9700	3.842(6)	149.00	1_655

Translation of Symmetry Code to Equiv.Pos for **II**

a =[2655.00] = [2_655] =1-x,1/2+y,1/2-z
b =[2645.00] = [2_645] =1-x,-1/2+y,1/2-z
c =[4555.00] = [4_566] =x,1/2-y,1/2+z
d =[2646.00] = [2_646] =1-x,-1/2+y,3/2-z
e =[2745.00] = [2_745] =2-x,-1/2+y,1/2-z
f =[3756.00] = [3_756] =2-x,-y,1-z
g =[1554.00] = [1_554] =x,y,-1+z
h =[2645.00] = [2_645] =1-x,-1/2+y,1/2-z
i =[4554.00] = [4_565] =x,1/2-y,-1/2+z
j =[3765.00] = [3_765] =2-x,1-y,-z
k =[4654.00] = [4_665] =1+x,1/2-y,-1/2+z
l =[3666.00] = [3_666] =1-x,1-y,1-z
m =[1545.00] = [1_545] =x,-1+y,z
n =[2755.00] = [2_755] =2-x,1/2+y,1/2-z
o =[3665.00] = [3_665] =1-x,1-y,-z
p =[1565.00] = [1_565] =x,1+y,z
q =[3765.00] = [3_765] =2-x,1-y,-z
r =[3665.00] = [3_665] =1-x,1-y,-z
s =[1556.00] = [1_556] =x,y,1+z
t =[3666.00] = [3_666] =1-x,1-y,1-z
u =[3666.00] = [3_666] =1-x,1-y,1-z
v =[4455.00] = [4_466] =-1+x,1/2-y,1/2+z
w =[2656.00] = [2_656] =1-x,1/2+y,3/2-z

Table S13. DFT-optimized geometry of the donor **L**[1] in orthogonal Cartesian coordinate format.

C	0.00000	0.00000	1.12610
H	-0.76965	-0.47853	1.74565
H	0.76965	0.47853	1.74565
C	-1.86644	0.97619	-0.23571
C	0.00000	2.22650	0.02463
H	-2.49053	0.09316	-0.12581
C	0.00000	-2.22650	0.02463
C	1.86644	-0.97619	-0.23571
C	2.05184	-2.14393	-0.89587
H	2.49053	-0.09316	-0.12581
H	2.89941	-2.50034	-1.47168
C	-2.05184	2.14393	-0.89587
H	-2.89941	2.50034	-1.47168
N	-0.60670	1.03797	0.33181
N	0.60670	-1.03797	0.33181
N	-0.90677	2.90202	-0.72862
N	0.90677	-2.90202	-0.72862
Se	1.67612	2.80536	0.51972
Se	-1.67612	-2.80536	0.51972
C	-0.67997	4.22365	-1.26315
H	-0.53036	4.94450	-0.44806
H	0.22303	4.22716	-1.88818
H	-1.54949	4.51591	-1.86239
C	0.67997	-4.22365	-1.26315
H	0.53036	-4.94450	-0.44806
H	-0.22303	-4.22716	-1.88818
H	1.54949	-4.51591	-1.86239

Table S14. DFT-optimized geometry of the donor **L²** in orthogonal Cartesian coordinate format.

C	1.80875	-2.21985	-0.30912
C	2.77584	-0.19301	-0.12939
H	1.00209	-2.92800	-0.46953
C	-2.77584	0.19299	0.12939
C	-1.80870	2.21976	0.30999
C	-3.11931	2.41306	0.02081
H	-1.00202	2.92786	0.47060
H	-3.68348	3.32961	-0.11541
C	3.11941	-2.41301	-0.02007
H	3.68365	-3.32949	0.11643
N	1.60906	-0.85628	-0.38174
N	3.70301	-1.16646	0.08795
N	-3.70293	1.16656	-0.08776
Se	3.04842	1.62661	-0.08872
Se	-3.04848	-1.62661	0.08822
C	5.09029	-0.89947	0.38199
H	5.56318	-0.37062	-0.45661
H	5.16973	-0.26059	1.27175
H	5.60395	-1.85118	0.55849
C	-5.09017	0.89975	-0.38213
H	-5.16941	0.26051	-1.27165
H	-5.56348	0.37135	0.45653
H	-5.60355	1.85150	-0.55922
C	0.34820	-0.20536	-0.64784
H	0.55439	0.68289	-1.26193
H	-0.29351	-0.89817	-1.20826
N	-1.60907	0.85617	0.38210
C	-0.34833	0.20507	0.64820
H	-0.55466	-0.68312	1.26231
H	0.29351	0.89781	1.20856

Table S15. DFT-optimized geometry of $[MesTe]^+$ (singlet GS) in orthogonal Cartesian coordinate format.

C	0.80120	1.26575	-0.01426
C	2.17840	1.22036	-0.01171
C	2.89163	0.00010	-0.00866
C	2.17844	-1.22016	-0.01212
C	0.80124	-1.26560	-0.01435
C	0.06832	0.00004	-0.01135
H	2.74217	2.15438	-0.01575
H	2.74217	-2.15422	-0.01651
C	0.12018	2.59709	-0.02272
H	0.86032	3.40522	-0.02460
H	-0.51939	2.71852	-0.90846
H	-0.52525	2.72795	0.85733
C	0.12029	-2.59697	-0.02252
H	-0.52497	-2.72767	0.85767
H	-0.51953	-2.71853	-0.90808
H	0.86042	-3.40508	-0.02452
C	4.37265	-0.00003	0.02825
H	4.69619	-0.00543	1.08631
H	4.79890	-0.89790	-0.43687
H	4.79932	0.90177	-0.42858
Te	-1.93470	-0.00005	0.00959

Table S16. DFT-optimized geometry of $[MesTe]^+$ (triplet GS) in orthogonal Cartesian coordinate format.

C	0.80635	1.24996	-0.00577
C	2.19009	1.21280	-0.01128
C	2.90801	0.00012	-0.01221
C	2.19013	-1.21264	-0.01130
C	0.80643	-1.24988	-0.00577
C	0.11424	0.00003	-0.00303
H	2.74241	2.15440	-0.01695
H	2.74251	-2.15421	-0.01697
C	0.07391	2.55850	-0.00565
H	0.77277	3.40358	-0.00657
H	-0.56210	2.66863	-0.89903
H	-0.56039	2.66932	0.88886
C	0.07402	-2.55845	-0.00564
H	-0.56022	-2.66931	0.88890
H	-0.56204	-2.66858	-0.89899
H	0.77291	-3.40351	-0.00662
C	4.39719	-0.00002	0.01617
H	4.74481	-0.00491	1.06402
H	4.81544	-0.89313	-0.46507
H	4.81575	0.89705	-0.45725
Te	-1.93316	-0.00003	0.00370

Table S17. DFT-optimized geometry of MesTeI in orthogonal Cartesian coordinate format.

C	1.71852	-0.93304	-0.81382
C	3.01904	-1.25178	-0.41468
C	3.75136	-0.44089	0.45432
C	3.14305	0.71660	0.94333
C	1.84428	1.08609	0.58345
C	1.13595	0.25368	-0.31285
H	3.47229	-2.17042	-0.79470
H	3.69482	1.35480	1.63761
C	0.99369	-1.87625	-1.73201
H	1.63306	-2.72881	-1.99427
H	0.07961	-2.26823	-1.26139
H	0.68149	-1.38089	-2.66236
C	1.26165	2.33783	1.17932
H	1.04737	3.09625	0.41239
H	0.31220	2.13282	1.69444
H	1.95761	2.77898	1.90431
C	5.16016	-0.79220	0.83481
H	5.87606	-0.35418	0.12079
H	5.41744	-0.40814	1.83101
H	5.32062	-1.87866	0.83147
Te	-0.80128	0.82016	-0.95244
I	-2.26401	-0.66834	0.82030

Table S18. DFT-optimized geometry of $(MesTeI_2)^-$ in orthogonal Cartesian coordinate format.

C	-0.18352	1.77131	1.20564
C	-0.16668	3.17022	1.17707
C	0.03869	3.88665	-0.00152
C	0.22437	3.16478	-1.18072
C	0.21444	1.76636	-1.20744
C	0.00995	1.06800	-0.00003
H	-0.32099	3.71447	2.11306
H	0.38101	3.70481	-2.11883
C	-0.41601	1.07584	2.51618
H	-0.51505	1.80549	3.33210
H	-1.33127	0.46571	2.48001
H	0.41206	0.39189	2.75274
C	0.42429	1.06444	-2.51837
H	1.32485	0.43267	-2.48532
H	-0.42085	0.40027	-2.75098
H	0.53754	1.79087	-3.33532
C	0.08992	5.38939	0.00192
H	1.12591	5.75174	0.10794
H	-0.30541	5.80897	-0.93439
H	-0.48952	5.81115	0.83533
Te	-0.01183	-1.06918	0.00079
I	-3.01961	-0.99574	-0.08661
I	2.99705	-1.05375	0.08673

Table S19. DFT-optimized geometry of compound **1** in **I** in orthogonal Cartesian coordinate format.

C	3.37234	1.00906	0.32430
C	2.93952	1.37155	-0.96858
C	1.81579	2.19947	-1.09069
H	1.49152	2.49645	-2.09134
C	1.11715	2.67931	0.01770
C	1.57306	2.30500	1.28524
H	1.05327	2.68423	2.16880
C	2.69215	1.48693	1.46756
C	3.65782	0.94902	-2.21881
H	4.66990	1.38126	-2.25305
H	3.11447	1.28153	-3.11290
H	3.78426	-0.14171	-2.27015
C	-0.08094	3.56990	-0.13731
H	-0.04782	4.41017	0.57020
H	-1.01616	3.02272	0.06073
H	-0.15014	3.98253	-1.15212
C	3.13410	1.17139	2.86852
H	2.50520	1.69407	3.60095
H	4.17943	1.47132	3.03140
H	3.07999	0.09224	3.07638
C	-4.94829	-0.10566	0.32840
C	-6.10663	-0.68688	-0.23172
C	-6.97689	-1.38645	0.61116
H	-7.87493	-1.83478	0.17869
C	-6.74446	-1.51600	1.98217
C	-5.59380	-0.92541	2.50802
H	-5.39663	-1.00501	3.58022
C	-4.68755	-0.21499	1.71125
C	-6.44567	-0.58096	-1.69095
H	-5.68626	-1.07506	-2.31542
H	-6.48627	0.46965	-2.01289
H	-7.41777	-1.04631	-1.89965
C	-7.72578	-2.22817	2.86876
H	-8.21943	-3.05771	2.34410
H	-8.51790	-1.53898	3.20235
H	-7.24296	-2.62833	3.77059
C	-3.49979	0.42507	2.37172
H	-3.56634	1.52255	2.31251
H	-2.55729	0.14412	1.88099
H	-3.44251	0.14417	3.43145
C	2.43048	-2.48795	-0.60837
C	2.24079	-2.86199	-2.80682
H	2.53223	-3.23538	-3.78283
C	1.14483	-2.16193	-2.42377
H	0.27460	-1.82036	-2.97641
C	4.30518	-3.72245	-1.65591
H	5.10636	-2.98372	-1.51308
H	4.44905	-4.25044	-2.60456
H	4.33239	-4.43462	-0.82213
C	0.33532	-1.18690	-0.25934
H	-0.15422	-0.43651	-0.88989
H	0.89758	-0.68845	0.53964
C	-1.89556	-2.30242	-0.24450
C	-1.75426	-3.31997	1.74268
H	-2.08627	-3.93597	2.57161
C	-0.59526	-2.64171	1.55822
H	0.30158	-2.56018	2.16545
C	-3.87440	-3.64507	0.44958
H	-4.61258	-3.01890	0.96882

H	-3.90299	-4.66784	0.84359
H	-4.10399	-3.65065	-0.62154
I	6.89235	1.90948	0.08364
I	-4.66043	3.48669	-0.07738
N	3.01872	-3.05830	-1.68445
N	1.27302	-1.93369	-1.06781
N	-2.54020	-3.10792	0.62936
N	-0.69184	-2.01831	0.33021
Se	3.08578	-2.47225	1.13074
Se	-2.53356	-1.70244	-1.88847
Te	5.08990	-0.23420	0.56665
Te	-3.60432	0.98098	-0.92342

Table S20. DFT-optimized geometry of the dication [**2**]$^{2+}$ in orthogonal Cartesian coordinate format.

Te	0.32806	2.22789	-0.06182
Se	-1.19746	1.07184	-2.22606
Se	1.76504	3.30630	2.09271
N	-0.03999	2.47588	-4.48237
N	0.84636	0.51607	-4.19841
C	-0.87711	3.65525	-4.33647
H	-1.17157	4.00576	-5.33207
H	-0.33746	4.44754	-3.80178
H	-1.76799	3.38045	-3.76214
C	1.45981	1.08354	-5.29410
H	2.23975	0.57775	-5.85458
C	0.90643	2.31169	-5.46652
H	1.10981	3.07834	-6.20773
C	-0.07556	1.37794	-3.69402
C	1.03371	4.91190	-1.41531
C	-1.51705	6.05130	-1.23785
H	-2.51546	6.49068	-1.17342
C	-0.02968	4.19157	-0.82283
C	-0.48738	6.79195	-1.82305
C	0.77700	6.20010	-1.89927
H	1.59820	6.76011	-2.35337
N	-0.18215	5.15726	3.15674
N	-0.36103	3.19488	4.06491
C	-2.49512	4.04802	-0.12377
H	-2.25269	3.62226	0.86017
H	-2.81974	3.20808	-0.75737
H	-3.34882	4.72787	-0.00969
C	0.32975	3.90807	3.13812
C	-1.31883	4.76257	-0.72770
C	0.30630	6.27361	2.36132
H	1.27641	6.61381	2.74579
H	-0.42090	7.08900	2.42670
H	0.41656	5.96256	1.31661
C	-1.30798	4.00282	4.65482
H	-1.97232	3.65130	5.43797
C	-0.11058	1.81064	4.41943
H	-0.18877	1.72254	5.51192
H	0.92232	1.57763	4.12460
C	-1.19217	5.23152	4.08573
H	-1.74008	6.14930	4.27535
C	1.07258	-0.83828	-3.72950
H	0.92003	-0.86019	-2.64161
H	2.11960	-1.09648	-3.93759
C	-0.72087	8.18584	-2.32762
H	-1.77260	8.35085	-2.59472
H	-0.10140	8.40762	-3.20676
H	-0.45935	8.92766	-1.55649
C	2.43096	4.37168	-1.53769
H	2.92539	4.32185	-0.55510
H	3.04353	5.01622	-2.18056
H	2.44417	3.35203	-1.94762
Te	-0.32806	-2.22789	0.06182
Se	1.19746	-1.07184	2.22606
Se	-1.76504	-3.30630	-2.09271
N	0.03999	-2.47588	4.48237
N	-0.84636	-0.51607	4.19841
C	0.87711	-3.65525	4.33647
H	1.17157	-4.00576	5.33207
H	0.33746	-4.44754	3.80178

H	1.76799	-3.38045	3.76214
C	-1.45981	-1.08354	5.29410
H	-2.23975	-0.57775	5.85458
C	-0.90643	-2.31169	5.46652
H	-1.10981	-3.07834	6.20773
C	0.07556	-1.37794	3.69402
C	-1.03371	-4.91190	1.41531
C	1.51705	-6.05130	1.23785
H	2.51546	-6.49068	1.17342
C	0.02968	-4.19157	0.82283
C	0.48738	-6.79195	1.82305
C	-0.77700	-6.20010	1.89927
H	-1.59820	-6.76011	2.35337
N	0.18215	-5.15726	-3.15674
N	0.36103	-3.19488	-4.06491
C	2.49512	-4.04802	0.12377
H	2.25269	-3.62226	-0.86017
H	2.81974	-3.20808	0.75737
H	3.34882	-4.72787	0.00969
C	-0.32975	-3.90807	-3.13812
C	1.31883	-4.76257	0.72770
C	-0.30630	-6.27361	-2.36132
H	-1.27641	-6.61381	-2.74579
H	0.42090	-7.08900	-2.42670
H	-0.41656	-5.96256	-1.31661
C	1.30798	-4.00282	-4.65482
H	1.97232	-3.65130	-5.43797
C	0.11058	-1.81064	-4.41943
H	0.18877	-1.72254	-5.51192
H	-0.92232	-1.57763	-4.12460
C	1.19217	-5.23152	-4.08573
H	1.74008	-6.14930	-4.27535
C	-1.07258	0.83828	3.72950
H	-0.92003	0.86019	2.64161
H	-2.11960	1.09648	3.93759
C	0.72087	-8.18584	2.32762
H	1.77260	-8.35085	2.59472
H	0.10140	-8.40762	3.20676
H	0.45935	-8.92766	1.55649
C	-2.43096	-4.37168	1.53769
H	-2.92539	-4.32185	0.55510
H	-3.04353	-5.01622	2.18056
H	-2.44417	-3.35203	1.94762

Table S21. DFT-optimized geometry of N,N’-dibutylbenzimidazole-2-selone in orthogonal Cartesian coordinate format.

Se	0.00048	-2.19961	-0.58724
N	1.09879	0.43990	-0.37270
N	-1.09881	0.43950	-0.37264
C	0.00014	-0.37579	-0.43745
C	0.70244	1.75873	-0.25193
C	3.04903	-0.21173	1.00908
C	1.42537	2.94488	-0.15618
C	-2.47126	-0.02405	-0.38965
C	-1.42630	2.94436	-0.15616
C	4.51378	-0.64368	1.01308
C	4.77543	-2.02292	0.42108
C	2.47142	-0.02317	-0.38966
C	-0.70293	1.75848	-0.25191
C	-0.70069	4.13202	-0.06030
C	0.69932	4.13227	-0.06031
C	-3.04902	-0.21244	1.00907
C	-4.51377	-0.64437	1.01293
C	-4.77535	-2.02365	0.42101
H	2.43445	-0.95977	1.53556
H	2.94456	0.73169	1.56886
H	2.51508	2.95004	-0.15376
H	-2.46778	-0.97259	-0.94362
H	-3.06286	0.70321	-0.96704
H	-2.51601	2.94910	-0.15371
H	5.11882	0.11035	0.47972
H	4.87198	-0.62479	2.05449
H	4.52017	-2.07457	-0.64733
H	4.18344	-2.79490	0.93484
H	5.83591	-2.29722	0.51463
H	3.06282	0.70450	-0.96674
H	2.46838	-0.97153	-0.94393
H	-1.23683	5.07877	0.01760
H	1.23513	5.07922	0.01758
H	-2.94458	0.73104	1.56877
H	-2.43450	-0.96042	1.53571
H	-4.87213	-0.62539	2.05429
H	-5.11873	0.10962	0.47944
H	-4.18351	-2.79561	0.93497
H	-4.51983	-2.07540	-0.64734
H	-5.83586	-2.29790	0.51434

Table S22. DFT-optimized geometry of 2,6-dimethylphenyltellurenium $[Me_2C_6H_3Te]^+$ in orthogonal Cartesian coordinate format.

Te	1.59631	-0.00000	0.00008
C	-0.40948	-0.00000	-0.00013
C	-1.13465	1.27073	-0.00010
C	-2.51734	1.22489	0.00013
C	-3.19705	0.00001	0.00024
C	-2.51735	-1.22487	0.00010
C	-1.13467	-1.27073	-0.00010
C	-0.45343	-2.60115	-0.00029
C	-0.45340	2.60115	-0.00030
H	-3.08848	2.15365	0.00019
H	-4.28963	0.00002	0.00040
H	-3.08850	-2.15363	0.00014
H	-1.19493	-3.40793	-0.00033
H	0.18824	-2.73000	0.88300
H	0.18812	-2.72981	-0.88370
H	0.18826	2.72974	-0.88364
H	0.18815	2.73006	0.88306
H	-1.19490	3.40793	-0.00048

Table S23. DFT-optimized geometry of 2,6-dimethylphenyltellurenium iodide ($Me_2C_6H_3TeI$) in orthogonal Cartesian coordinate format.

C	-1.43156	-0.05592	0.16328
C	-2.15300	-0.98580	-0.62045
C	-3.38152	-0.58238	-1.15549
C	-3.87788	0.69652	-0.93301
C	-3.15072	1.60345	-0.17135
C	-1.91886	1.25188	0.39132
C	-1.16657	2.28011	1.18755
C	-1.66042	-2.37582	-0.91468
H	-3.95190	-1.28820	-1.76228
H	-4.83774	0.99069	-1.36152
H	-3.53993	2.60992	-0.00646
H	-1.73399	3.21798	1.24098
H	-0.18840	2.50020	0.73425
H	-0.96910	1.93773	2.21335
H	-1.59177	-2.98910	-0.00437
H	-0.65638	-2.36066	-1.36215
H	-2.33966	-2.88384	-1.61123
Te	0.39247	-0.65897	1.06522
I	2.11026	0.40641	-0.77651

Table S24. DFT-optimized geometry of the 1:1 adduct between 2,6-dimethylphenyltellurenium $[Me_2C_6H_3Te]^+$ and N,N'-dibutylbenzimidazole-2-selone in orthogonal Cartesian coordinate format.

Te	1.05078	-1.93828	0.12507
Se	-0.07973	-0.63869	-1.78180
N	-1.27636	1.75974	-0.68735
N	-2.56512	0.00087	-0.40650
C	-1.37154	0.42710	-0.86848
C	-2.43670	2.20956	-0.07958
C	0.75271	2.97029	0.10726
C	-2.85096	3.48952	0.29964
C	-3.08539	-1.36414	-0.43900
C	-4.53256	1.19704	0.66442
C	1.79662	4.02947	-0.24430
C	2.78755	3.62128	-1.32618
C	2.61250	-0.61801	0.67949
C	2.55055	0.00953	1.94704
C	3.63725	0.79838	2.33995
C	4.74324	0.96322	1.51381
C	4.78759	0.33856	0.27260
C	3.73321	-0.46681	-0.17169
C	3.83883	-1.11634	-1.52175
C	1.39552	-0.14639	2.89864
C	-0.15964	2.62546	-1.06391
C	-3.25800	1.08753	0.10080
C	-4.93996	2.46749	1.04231
C	-4.11298	3.59397	0.86456
C	-3.05348	-2.05402	0.92082
C	-3.65668	-3.45797	0.88928
C	-2.88673	-4.47092	0.05205
H	1.25270	2.05069	0.45152
H	0.13919	3.32938	0.94843
H	-2.21978	4.36622	0.16052
H	-2.49131	-1.90965	-1.18240
H	-4.11365	-1.30431	-0.82568
H	-5.18105	0.33261	0.79986
H	1.28538	4.96206	-0.53781
H	2.34645	4.27222	0.67747
H	2.30563	3.46447	-2.30299
H	3.31206	2.69279	-1.05547
H	3.54797	4.40072	-1.47086
H	3.61351	1.28384	3.31720
H	5.58171	1.57896	1.84340
H	5.66223	0.46581	-0.36763
H	4.84002	-0.96953	-1.94476
H	3.11516	-0.68985	-2.23371
H	3.64402	-2.19718	-1.47170
H	1.33660	-1.16763	3.30499
H	0.43043	0.06141	2.41523
H	1.50537	0.53587	3.75066
H	-0.60043	3.53197	-1.50378
H	0.39100	2.11306	-1.86139
H	-5.92736	2.59944	1.48589
H	-4.47717	4.57346	1.17619
H	-3.59987	-1.43870	1.65207
H	-2.01018	-2.09822	1.27334
H	-3.71674	-3.81830	1.92725
H	-4.70053	-3.39939	0.53750
H	-1.84464	-4.56484	0.39427
H	-2.86736	-4.21167	-1.01715
H	-3.34446	-5.46651	0.12721

Table S25. DFT-optimized geometry of N,N'-dimethylimidazole-2-thione in orthogonal Cartesian coordinate format.

N	-1.08670	-0.50741	0.00001
N	1.08678	-0.50724	0.00031
C	-2.44559	-0.02815	-0.00005
H	-3.12575	-0.88747	0.00001
H	-2.63033	0.59247	0.88748
H	-2.63038	0.59235	-0.88767
C	0.67824	-1.82521	0.00001
H	1.38226	-2.65064	0.00006
C	-0.67792	-1.82530	-0.00011
H	-1.38178	-2.65086	-0.00022
C	-0.00002	0.32419	0.00014
C	2.44560	-0.02777	-0.00016
H	2.63197	0.58811	-0.89069
H	2.62858	0.59750	0.88443
H	3.12587	-0.88699	0.00561
S	-0.00018	2.00634	-0.00001

Table S26. DFT-optimized geometry of N,N'-dimethylimidazole-2-selone in orthogonal Cartesian coordinate format.

N	0.98424	-1.08515	-0.00024
N	0.98432	1.08509	-0.00023
C	0.51159	-2.44762	0.00020
H	1.37507	-3.12252	0.00051
H	-0.10851	-2.63314	0.88777
H	-0.10837	-2.63388	-0.88731
C	2.30192	0.67825	0.00003
H	3.12676	1.38293	0.00021
C	2.30185	-0.67845	0.00010
H	3.12665	-1.38320	-0.00008
C	0.15689	0.00001	-0.00023
C	0.51181	2.44763	0.00018
H	-0.11664	2.63031	-0.88201
H	-0.09964	2.63692	0.89297
H	1.37533	3.12239	-0.01043
Se	-1.67809	0.00005	0.00000

Table S27. DFT-optimized geometry of N,N'-dimethylimidazole-2-tellone in orthogonal Cartesian coordinate format.

N	1.38256	-1.08306	-0.00045
N	1.38270	1.08301	0.00062
C	0.92245	-2.45159	0.00037
H	1.79324	-3.11706	0.00141
H	0.30433	-2.64231	0.88818
H	0.30513	-2.64408	-0.88762
C	2.69965	0.67852	0.00021
H	3.52390	1.38393	0.00046
C	2.69953	-0.67868	-0.00051
H	3.52372	-1.38416	-0.00125
C	0.55696	0.00008	0.00009
C	0.92260	2.45159	-0.00012
H	0.30962	2.64453	-0.89103
H	0.30010	2.64172	0.88472
H	1.79319	3.11733	0.00556
Te	-1.50033	0.00002	-0.00003

Table S28. DFT-optimized geometry of the 1:1 adduct between N,N'-dimethylimidazole-2-thione and $[MesTe]^+$ in orthogonal Cartesian coordinate format.

Te	-0.25921	-1.70293	0.46335
N	-1.71626	1.96899	-0.76547
N	-3.32123	0.80770	0.13200
C	-0.54924	2.34166	-1.55239
H	-0.84178	2.55064	-2.58965
H	-0.09924	3.23562	-1.10867
H	0.17757	1.52309	-1.53156
C	-3.51520	2.11481	0.49472
H	-4.34548	2.42687	1.12083
C	-2.51288	2.84371	-0.07344
H	-2.31235	3.91016	-0.04079
C	-2.21345	0.72100	-0.63443
C	1.70912	0.50091	1.27684
C	3.45815	0.15777	-0.88789
H	4.14302	0.02180	-1.72778
C	1.44619	-0.47273	0.28326
C	3.74717	1.12983	0.07414
C	2.86002	1.28134	1.14339
H	3.07566	2.03023	1.90880
C	2.10544	-1.68810	-1.88142
H	1.93547	-2.68837	-1.45826
H	1.22666	-1.44760	-2.49963
H	2.97249	-1.74476	-2.55053
C	2.33019	-0.66158	-0.80753
C	4.99420	1.95636	-0.01817
H	5.27241	2.15573	-1.06139
H	4.88723	2.91531	0.50500
H	5.83932	1.42354	0.44610
C	0.83262	0.72018	2.48043
H	0.86342	-0.13898	3.16753
H	1.16669	1.59909	3.04552
H	-0.22169	0.86818	2.20646
C	-4.14514	-0.31444	0.55029
H	-4.21674	-1.03797	-0.26927
H	-3.70225	-0.80259	1.42898
H	-5.14448	0.05645	0.79969
S	-1.57612	-0.72034	-1.38364

Table S29. DFT-optimized geometry of the 1:1 adduct between N,N'-dimethylimidazole-2-selone and $[MesTe]^+$ in orthogonal Cartesian coordinate format.

Te	-0.06946	-1.59305	0.76442
N	-1.65016	2.04468	-0.75768
N	-3.20638	0.99563	0.33596
C	-0.52663	2.33045	-1.63975
H	-0.86243	2.37099	-2.68399
H	-0.09852	3.29673	-1.35469
H	0.23368	1.55027	-1.52638
C	-3.35137	2.33118	0.60803
H	-4.12933	2.70958	1.26409
C	-2.37852	2.98997	-0.08307
H	-2.15544	4.05051	-0.14747
C	-2.15913	0.82318	-0.49652
C	1.91537	0.69549	1.23375
C	3.62036	0.07225	-0.90179
H	4.28818	-0.17352	-1.73042
C	1.63176	-0.39641	0.37947
C	3.92906	1.15944	-0.07974
C	3.06327	1.44980	0.97797
H	3.29426	2.29014	1.63657
C	2.24690	-1.88064	-1.62390
H	2.07096	-2.81594	-1.07385
H	1.36419	-1.71058	-2.25991
H	3.10568	-2.03290	-2.28880
C	2.49304	-0.72598	-0.69480
C	5.17458	1.96337	-0.30299
H	5.42355	2.03708	-1.36987
H	5.08348	2.97800	0.10558
H	6.03191	1.48532	0.19703
C	1.06442	1.06877	2.41763
H	1.11295	0.30549	3.20908
H	1.40765	2.01375	2.85669
H	0.00375	1.17846	2.15015
C	-4.01914	-0.06540	0.90926
H	-4.14809	-0.86442	0.17121
H	-3.53124	-0.47349	1.80463
H	-4.99734	0.34654	1.17769
Se	-1.53276	-0.81995	-1.21048

Table S30. DFT-optimized geometry of the 1:1 adduct between N,N'-dimethylimidazole-2-tellone and $[MesTe]^+$ in orthogonal Cartesian coordinate format.

Te	0.23103	-1.45655	0.99971
N	-1.91960	2.13358	-0.79646
N	-3.15570	1.05494	0.62058
C	-0.99133	2.45603	-1.87046
H	-1.52520	2.53602	-2.82642
H	-0.50440	3.40997	-1.64161
H	-0.23177	1.66994	-1.93991
C	-3.40104	2.39084	0.80753
H	-4.09956	2.75500	1.55473
C	-2.62961	3.06849	-0.08737
H	-2.53587	4.13401	-0.27357
C	-2.24275	0.89713	-0.36100
C	2.10302	0.97129	1.10728
C	3.87547	0.09099	-0.87523
H	4.56840	-0.25394	-1.64589
C	1.87967	-0.25050	0.43201
C	4.12728	1.30340	-0.22872
C	3.22741	1.72177	0.75486
H	3.41155	2.66420	1.27573
C	2.58274	-1.99625	-1.31438
H	2.43505	-2.84783	-0.63529
H	1.70230	-1.95567	-1.97494
H	3.45501	-2.21019	-1.94385
C	2.77169	-0.70745	-0.56574
C	5.34777	2.11096	-0.55506
H	5.61878	2.02455	-1.61560
H	5.20900	3.17326	-0.31617
H	6.21038	1.75413	0.02985
C	1.20588	1.49334	2.19690
H	1.22384	0.84492	3.08581
H	1.52681	2.49319	2.51477
H	0.15646	1.55709	1.87359
C	-3.75299	-0.00911	1.41252
H	-3.94782	-0.87709	0.77281
H	-3.07558	-0.30288	2.22546
H	-4.69714	0.35310	1.83225
Te	-1.46165	-0.93743	-1.08124

Table S31. DFT-optimized geometry of the 2:1 adduct between N,N'-dimethylimidazole-2-thione and $[MesTe]^+$ in orthogonal Cartesian coordinate format.

Te	0.02072	-1.28071	0.00550
N	-3.88509	0.51339	-0.44914
N	-4.04788	-1.49014	0.37416
C	-3.45667	1.65040	-1.24254
H	-4.33214	2.25706	-1.50055
H	-2.73008	2.25557	-0.68370
H	-2.98348	1.27933	-2.15742
C	-4.95990	-0.70437	1.03650
H	-5.61094	-1.09803	1.81038
C	-4.85940	0.54929	0.51940
H	-5.40746	1.45545	0.75616
C	-3.37903	-0.74051	-0.53485
C	-0.46843	1.54479	1.14912
C	0.33039	2.95761	-1.13125
H	0.63808	3.50582	-2.02507
C	-0.02675	0.85175	-0.00081
C	-0.09865	3.67262	-0.01059
C	-0.49332	2.94427	1.11494
H	-0.83417	3.48216	2.00306
N	3.93157	0.57220	0.42363
N	4.08016	-1.44424	-0.36925
C	0.83940	0.88097	-2.41464
H	1.63491	0.14870	-2.21705
H	0.01646	0.32725	-2.89189
H	1.21485	1.61520	-3.13855
C	3.41668	-0.67559	0.52762
C	0.37923	1.55886	-1.15486
C	3.52048	1.70413	1.23411
H	3.78888	1.53570	2.28476
H	4.03236	2.59830	0.86449
H	2.43550	1.84268	1.15663
C	5.00188	-0.67591	-1.03925
H	5.64795	-1.08473	-1.80939
C	4.91238	0.58561	-0.53858
H	5.46963	1.48305	-0.78677
C	-0.10732	5.17391	-0.00458
H	-0.27144	5.58253	-1.01039
H	-0.88411	5.57228	0.66142
H	0.85730	5.56832	0.35249
C	-0.89467	0.85368	2.41370
H	-0.04192	0.35621	2.90050
H	-1.31579	1.57201	3.12839
H	-1.64381	0.07294	2.22114
C	-3.81506	-2.90150	0.61275
H	-3.69788	-3.41830	-0.34673
H	-2.90282	-3.04359	1.20780
H	-4.67438	-3.31357	1.15183
C	3.83245	-2.85480	-0.59447
H	3.60486	-3.33582	0.36378
H	2.98015	-2.99178	-1.27382
H	4.72919	-3.30679	-1.03130
S	-2.15909	-1.29331	-1.61938
S	2.19718	-1.18362	1.63298

Table S32. DFT-optimized geometry of the 2:1 adduct between N,N'-dimethylimidazole-2-selone and $[MesTe]^+$ in orthogonal Cartesian coordinate format.

Te	0.00312	-1.16558	0.00147
Se	-2.35831	-1.13544	-1.57404
Se	2.36469	-1.12428	1.57658
N	-4.00225	0.75105	-0.13377
N	-4.12471	-1.23963	0.71989
C	-3.64033	1.85968	-0.99952
H	-4.12744	2.76474	-0.62297
H	-2.55229	1.99828	-0.99400
H	-3.97496	1.66294	-2.02560
C	-4.94485	-0.42841	1.46646
H	-5.51621	-0.79980	2.31105
C	-4.87112	0.81880	0.92821
H	-5.36959	1.73977	1.21264
C	-3.54071	-0.51357	-0.26111
C	-0.39780	1.67189	1.16279
C	0.36245	3.07313	-1.13642
H	0.65348	3.61661	-2.03873
C	-0.00188	0.97110	0.00080
C	-0.01989	3.79435	-0.00329
C	-0.39542	3.07136	1.13166
H	-0.70125	3.61369	2.02982
N	4.00375	0.75850	0.12610
N	4.12910	-1.23573	-0.71866
C	0.79318	0.99050	-2.43750
H	1.55665	0.21973	-2.26224
H	-0.06353	0.48163	-2.90580
H	1.18748	1.71573	-3.16055
C	3.54472	-0.50642	0.25966
C	0.38461	1.67318	-1.16293
C	3.64165	1.86970	0.98831
H	3.99378	1.68579	2.01099
H	4.11189	2.77746	0.59703
H	2.55199	1.99434	0.99790
C	4.94710	-0.42636	-1.46962
H	5.51814	-0.80045	-2.31324
C	4.87167	0.82310	-0.93691
H	5.36816	1.74368	-1.22601
C	-0.00304	5.29568	0.00505
H	-0.13501	5.70852	-1.00365
H	-0.79056	5.70568	0.65147
H	0.95742	5.67449	0.38921
C	-0.80343	0.98708	2.43719
H	0.05525	0.48079	2.90455
H	-1.19955	1.71062	3.16093
H	-1.56453	0.21385	2.26223
C	-3.89595	-2.65209	0.95910
H	-3.86457	-3.18190	0.00005
H	-2.94028	-2.80172	1.47933
H	-4.71528	-3.04278	1.57147
C	3.90231	-2.64952	-0.95181
H	3.86911	-3.17470	0.00973
H	2.94804	-2.80253	-1.47363
H	4.72351	-3.04236	-1.56030

Table S33. DFT-optimized geometry of the 2:1 adduct between N,N'-dimethylimidazole-2-tellone and $[MesTe]^+$ in orthogonal Cartesian coordinate format.

Te	-0.00385	-1.09951	-0.00434
N	4.09731	1.00372	-0.19549
N	4.26779	-0.95822	-1.09688
C	3.74353	2.08225	0.71180
H	4.19027	3.00874	0.33685
H	2.65276	2.19305	0.75764
H	4.12888	1.87123	1.71671
C	4.94742	-0.08241	-1.90787
H	5.45275	-0.40123	-2.81383
C	4.84227	1.14942	-1.33997
H	5.24100	2.10790	-1.65607
C	3.74069	-0.29172	-0.04449
C	0.36312	1.74417	-1.17320
C	-0.32301	3.14329	1.14956
H	-0.58361	3.68551	2.06197
C	0.00345	1.04134	-0.00081
C	0.02277	3.86609	0.00578
C	0.36129	3.14377	-1.14105
H	0.63722	3.68663	-2.04862
N	-4.09775	1.00881	0.21528
N	-4.26957	-0.96257	1.09542
C	-0.71637	1.05940	2.45968
H	-1.47894	0.28340	2.30481
H	0.15623	0.55524	2.90389
H	-1.09384	1.78267	3.19372
C	-3.74390	-0.28554	0.04910
C	-0.34591	1.74320	1.17467
C	-3.74515	2.09594	-0.68199
H	-4.14960	1.90518	-1.68354
H	-4.17327	3.02245	-0.28594
H	-2.65387	2.19254	-0.74428
C	-4.94576	-0.09455	1.91760
H	-5.44918	-0.42237	2.82141
C	-4.83990	1.14327	1.36302
H	-5.23617	2.09889	1.69068
C	0.00577	5.36763	-0.00030
H	0.17550	5.77935	1.00327
H	0.76881	5.77849	-0.67497
H	-0.96798	5.74775	-0.34808
C	0.72990	1.06089	-2.45957
H	-0.14592	0.56402	-2.90552
H	1.11277	1.78337	-3.19159
H	1.48691	0.27909	-2.30640
C	4.11803	-2.38045	-1.34738
H	4.35797	-2.94449	-0.43832
H	3.08563	-2.60777	-1.64397
H	4.80404	-2.66803	-2.15082
C	-4.12119	-2.38765	1.33010
H	-4.36561	-2.94155	0.41600
H	-3.08799	-2.61966	1.62016
H	-4.80450	-2.68270	2.13313
Te	2.61468	-1.09949	1.51969
Te	-2.62290	-1.07773	-1.52660

Table S34. DFT-optimized geometry of the 1:2 adduct between **L²** and MesTeI in orthogonal Cartesian coordinate format.

C	0.59641805	0.99944804	-0.3798411
C	0.33811217	0.7570833	0.93101248
N	1.45796011	0.16372885	1.46373721
C	2.40730652	0.02898204	0.5058703
N	1.87198544	0.54376932	-0.6341688
Se	4.11357788	-0.677985	0.7525626
Te	3.44423415	-3.4812986	0.10945223
I	2.83574613	-6.2361274	-0.5823274
C	1.63397319	-0.2000126	2.85786742
C	2.58365928	0.72866722	-1.8916502
C	1.87707602	0.17093288	-3.1177635
N	1.91933774	-1.2721363	-3.2372338
C	2.96384623	-1.9612401	-3.767282
N	2.60693623	-3.2662486	-3.7403918
C	1.34592245	-3.3953854	-3.2074364
C	0.9135961	-2.1478178	-2.8910901
Se	4.54706393	-1.2301733	-4.4247203
Te	3.67577502	-1.2474722	-7.2808933
I	2.82413225	-1.119994	-10.024603
C	3.41123141	-4.3605912	-4.2476627
C	2.27358511	0.27091778	-6.7322548
C	0.90996316	-0.0550028	-6.5698144
C	0.01705922	0.95915686	-6.1998178
C	0.42891135	2.27652819	-5.9951385
C	1.78286866	2.57137303	-6.1702229
C	2.71703764	1.59928549	-6.5461507
C	0.3686615	-1.435016	-6.8112565
C	-0.5586561	3.35635556	-5.652876
C	4.14709772	2.01295033	-6.744486
C	2.46125877	-3.6779629	1.99484578
C	3.23351386	-3.7817714	3.17342232
C	2.56879746	-3.8849778	4.39992834
C	1.17595773	-3.9108724	4.49565577
C	0.43990767	-3.8220441	3.31377156
C	1.05125847	-3.7060944	2.05993708
C	4.73536992	-3.7852156	3.16737146
C	0.49666538	-4.0730223	5.82535248
C	0.17689158	-3.6407398	0.84079908
H	-1.0410051	0.70756755	-6.086874
H	2.12685977	3.59974027	-6.0314556
H	0.49459523	-1.7215541	-7.86693
H	-0.7009269	-1.4851251	-6.5681691
H	0.90092895	-2.1925839	-6.218855
H	-0.8944167	3.87903638	-6.5627188
H	-0.1189159	4.11589256	-4.9911318
H	-1.4553228	2.94920348	-5.1655205
H	4.25760115	3.09973616	-6.6343553
H	4.50587096	1.72458744	-7.7429295
H	4.81182105	1.52400642	-6.0165468
H	3.16642811	-3.961624	5.31173239
H	-0.6517435	-3.8502609	3.36289946

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H           5.13759407   -2.815901  2.83610022
H           5.12836144  -4.5447268  2.47670681
H           5.12753878  -3.9894903   4.1720231
H           1.03972525  -3.5493912  6.62429679
H           0.44873912  -5.1361327   6.1102463
H            -0.534285  -3.6948857  5.80380058
H           0.29558904  -4.5498935  0.23053345
H           0.44765428  -2.7943758  0.19358504
H           -0.8810944  -3.5531133  1.12157944
H           0.87787413  -4.3644459   -3.069456
H           -0.0172739  -1.8158531  -2.4449303
H            3.1791054   -4.542756  -5.3060183
H           3.21022471  -5.2555774  -3.6473451
H           4.46844583   -4.086069  -4.1606462
H           -0.5472931  0.95936482  1.52461122
H           1.97196113  -1.2396063   2.9356259
H           0.67157391  -0.0902292  3.36814985
H           2.38008723  0.45639559   3.3245662
H           0.82527556  0.48063307  -3.1694018
H           2.37114892  0.58645749  -4.0066773
H           2.73573567  1.80761996  -2.0432611
H           3.57455985  0.26907076  -1.7738267
H           -0.0191671  1.46893326  -1.1399867
```

Table S35. DFT-optimized geometry of the dimeric 1:1 adduct between **L^1** and [MesTe]$^{2+}$ in orthogonal Cartesian coordinate format.

Te	1.95984	1.29676	-0.80705
Se	0.14162	-0.51821	-2.52203
Se	3.20602	2.85319	1.01617
N	1.95673	-1.79792	-4.39016
N	0.15123	-2.95023	-4.04950
C	2.95663	-0.74988	-4.32958
H	3.67476	-0.90237	-5.14149
H	3.48118	-0.77868	-3.36638
H	2.47712	0.23043	-4.44155
C	0.89026	-3.62549	-5.01000
H	0.53996	-4.53643	-5.48577
C	2.01892	-2.90667	-5.21028
H	2.85543	-3.08357	-5.87910
C	0.80944	-1.80789	-3.67634
C	4.21569	2.17254	-2.72676
C	2.59793	3.64848	-4.46897
H	1.96443	4.22072	-5.15098
C	2.82510	2.28783	-2.48409
C	3.96578	3.55388	-4.73499
C	4.75105	2.81176	-3.84925
H	5.82409	2.72573	-4.03638
N	1.57406	5.21506	0.54004
N	1.06253	4.23108	2.40349
C	0.51896	3.19242	-3.18057
H	0.24286	3.37073	-2.13175
H	-0.01462	2.27927	-3.48816
H	0.13681	4.01883	-3.79354
C	1.87259	4.15381	1.31675
C	2.00341	3.03713	-3.35951
C	2.22731	5.58101	-0.70708
H	2.69311	6.56820	-0.59707
H	1.49080	5.60582	-1.51825
H	2.99412	4.83477	-0.93758
C	0.25330	5.34010	2.29684
H	-0.48598	5.60504	3.04542
C	1.13862	3.35091	3.56732
H	1.67071	3.87036	4.37549
H	1.71351	2.46400	3.26617
C	0.57013	5.94893	1.12513
H	0.16504	6.84537	0.66550
C	4.57836	4.25025	-5.91380
H	3.84636	4.41442	-6.71494
H	5.42246	3.68159	-6.32593
H	4.96881	5.23743	-5.61980
C	5.15751	1.42334	-1.82575
H	5.39742	2.01204	-0.92557
H	6.10760	1.22033	-2.33583
H	4.73531	0.47066	-1.47617
Te	-1.95984	-1.29676	0.80705
Se	-0.14162	0.51821	2.52203
Se	-3.20602	-2.85319	-1.01617
N	-1.95673	1.79792	4.39016
N	-0.15123	2.95023	4.04950
C	-2.95663	0.74988	4.32958
H	-3.67476	0.90237	5.14149
H	-3.48118	0.77868	3.36638
H	-2.47712	-0.23043	4.44155
C	-0.89026	3.62549	5.01000
H	-0.53996	4.53643	5.48577
C	-2.01892	2.90667	5.21028
H	-2.85543	3.08357	5.87910
C	-0.80944	1.80789	3.67634
C	-4.21569	-2.17254	2.72676
C	-2.59793	-3.64848	4.46897
H	-1.96443	-4.22072	5.15098
C	-2.82510	-2.28783	2.48409

C	-3.96578	-3.55388	4.73499
C	-4.75105	-2.81176	3.84925
H	-5.82409	-2.72573	4.03638
N	-1.57406	-5.21506	-0.54004
N	-1.06253	-4.23108	-2.40349
C	-0.51896	-3.19242	3.18057
H	-0.24286	-3.37073	2.13175
H	0.01462	-2.27927	3.48816
H	-0.13681	-4.01883	3.79354
C	-1.87259	-4.15381	-1.31675
C	-2.00341	-3.03713	3.35951
C	-2.22731	-5.58101	0.70708
H	-2.69311	-6.56820	0.59707
H	-1.49080	-5.60582	1.51825
H	-2.99412	-4.83477	0.93758
C	-0.25330	-5.34010	-2.29684
H	0.48598	-5.60504	-3.04542
C	-1.13862	-3.35091	-3.56732
H	-1.67071	-3.87036	-4.37549
H	-1.71351	-2.46400	-3.26617
C	-0.57013	-5.94893	-1.12513
H	-0.16504	-6.84537	-0.66550
C	-4.57836	-4.25025	5.91380
H	-3.84636	-4.41442	6.71494
H	-5.42246	-3.68159	6.32593
H	-4.96881	-5.23743	5.61980
C	-5.15751	-1.42334	1.82575
H	-5.39742	-2.01204	0.92557
H	-6.10760	-1.22033	2.33583
H	-4.73531	-0.47066	1.47617

Table S36. DFT-optimized geometry of the 1:1 adduct between 2,6-dimethylphenyltellurenium iodide $Me_2C_6H_3TeI$ and N,N'-dibutylbenzimidazole-2-selone in orthogonal Cartesian coordinate format.

Se	0.90178	-0.03506	2.10919
N	3.15680	0.46873	0.40653
N	2.57667	-1.64994	0.39766
C	2.25855	-0.42550	0.90159
C	4.05096	-0.18292	-0.42349
C	2.52061	2.75038	-0.34881
C	5.15140	0.27322	-1.14778
C	1.90229	-2.90177	0.70296
C	4.40877	-2.48427	-1.14707
C	2.71193	4.24808	-0.11959
C	2.11061	4.78073	1.17462
C	-1.41709	1.50225	-0.37906
C	-0.99451	1.56420	-1.72506
C	-0.86591	2.82342	-2.32464
C	-1.14594	3.98773	-1.61946
C	-1.56316	3.91094	-0.29564
C	-1.71071	2.67612	0.34867
C	-2.18439	2.65720	1.77415
C	-0.70481	0.34114	-2.54767
C	3.19743	1.88999	0.71107
C	3.68268	-1.53666	-0.42663
C	5.50746	-2.02788	-1.86964
C	5.87104	-0.67288	-1.87188
C	1.03130	-3.41418	-0.43907
C	0.41547	-4.78356	-0.15718
C	-0.58903	-4.81216	0.98788
H	1.44689	2.50594	-0.37152
H	2.92170	2.48162	-1.33916
H	5.43878	1.32409	-1.15053
H	1.30720	-2.71430	1.60638
H	2.68063	-3.63695	0.96290
H	4.13245	-3.53795	-1.14732
H	3.78873	4.49026	-0.15637
H	2.25841	4.77748	-0.97160
H	2.59454	4.35752	2.06741
H	1.03780	4.54632	1.23534
H	2.21898	5.87286	1.23780
H	-0.54782	2.88232	-3.36763
H	-1.04753	4.95983	-2.10653
H	-1.79587	4.82512	0.25447
H	-2.42043	3.67298	2.11741
H	-1.42027	2.23910	2.44637
H	-3.08307	2.03397	1.88754
H	-1.60751	-0.27793	-2.66506
H	0.05627	-0.29573	-2.07461
H	-0.35048	0.62118	-3.54838
H	4.25727	2.16466	0.82681
H	2.71287	2.01210	1.68827
H	6.09799	-2.74037	-2.44686
H	6.73711	-0.35313	-2.45263
H	1.63513	-3.47139	-1.35850
H	0.23589	-2.67613	-0.63084
H	-0.08132	-5.12557	-1.07825
H	1.22029	-5.51489	0.03466
H	-1.41398	-4.10638	0.81005
H	-0.13233	-4.55244	1.95441
H	-1.02907	-5.81320	1.09851
Te	-1.68307	-0.40198	0.55470
I	-4.20744	-0.78432	-0.71884

Table S37. Selected average natural charges *Q* (|e|) calculated on the (R)N-C(E)-N(R) fragment of dimethylimidazole-2-chalcogenone [Me_2imidE: E = S (a), Se (b), and Te(c)], dibutylbenzoimidazole-2-selone(Bu_2benzImSe, d), **L¹** (e), and **L²** (f).

		R	E	Q_N	Q_C	Q_E
a	Me_2imidS	Me	S	-0.438	+0.238	-0.289
b	Me_2imidSe	Me	Se	-0.424	+0.181	-0.254
c	Me_2imidTe	Me	Te	-0.429	+0.108	-0.205
d	Bu_2benzImSe	Bu	Se	-0.436	+0.207	-0.208
e	**L¹**	Me, $-CH_2-$imidSe	Se	-0.453, -0.431	+0.193	-0.266
f	**L²**	Me, $-(CH_2)_2-$imidSe	Se	-0.439, -0.432	+0.188	-0.271

Table S38. Selected average natural charges *Q* (|e|) calculated on the C–E' groups of 2,6-R_1-4-R_2-phenylchalcogenyl cations [MesE'$^+$: E = S (a), Se (b), and Te (d)], and the C–Te–I groups of mesityltellurenyl iodide (MesTeI, e) and mesityltellurenyldiiodide ($MesTeI_2^-$, f).

		R_1	R_2	E'	Ground State	Q_C	Q_E	Q_I
a	$MesS^+$	Me	Me	S	Singlet	-0.263	+0.400	–
					Triplet	-0.261	+0.642	–
b	$MesSe^+$	Me	Me	Se	Singlet	-0.355	+0.553	–
					Triplet	-0.348	+0.770	–
c	$MesTe^+$	Me	Me	Te	Singlet	-0.470	+0.770	–
					Triplet	-0.452	+0.973	–
d	Me_2PhTe^+	Me	H	Te	Singlet	-0.477	+0.821	–
					Triplet	-0.457	+1.022	–
e	MesTeI	Me	Me	Te	Singlet	-0.385	+0.434	-0.188
f	$MesTeI_2^-$	Me	Me	Te	Singlet	-0.339	+0.385	-0.530

Table S39. Selected average natural charges *Q* (|e|) calculated on the (R)N-C(E)-N(R) fragment of the donors dimethylimidazole-2-chalcogenone [Me_2imidE: E = S (a, f), Se (b, g), and Te(c, h)], dibutylbenzoimidazole-2-selone(Bu_2benzImSe, d), **L**^{1} (i, k), **L**^{2} (j, l), and the C–Te groups of the acceptors 2,6-R_1-4-R_2-phenylchalcogenyl cations [MesTe$^+$ (a–c, f–h, k, l), Me_2PhTe$^+$ (d)], and the C–Te–I groups of mesityltellurenyl iodide [MesTeI (e, i–h)] in the corresponding adducts.

		Donor			Acceptor		
		Q_N	Q_C	Q_E	Q_C	Q_{Te}	Q_I
a	Me_2imidS·MesTe$^+$	−0.391	+0.288	−0.044	−0.380	+0.589	–
b	Me_2imidSe·MesTe$^+$	−0.395	+0.227	+0.109	−0.404	+0.509	–
c	Me_2imidTe·MesTe$^+$	−0.400	+0.135	+0.341	−0.387	+0.384	–
d	Bu_2benzImSe·Me_2PhTe$^+$	−0.394	+0.272	+0.104	−0.385	+0.504	–
e	Bu_2benzImSe·Me_2PhTeI	−0.420	+0.252	−0.124	−0.348	+0.389	−0.338
f	(Me_2imidS)$_2$·MesTe$^+$	−0.406	+0.289	−0.189	−0.380	+0.499	–
g	(Me_2imidSe)$_2$·MesTe$^+$	−0.406	+0.228	−0.055	−0.375	+0.404	–
h	(Me_2imidTe)$_2$·MesTe$^+$	−0.407	+0.140	+0.103	−0.367	+0.279	–
i	**L**^{1}·(MesTeI)$_2$ (**1**)	−0.439, −0.412	+0.224	−0.159	−0.366	+0.390	−0.327
j	**L**^{2}·(MesTeI)$_2$	−0.426, −0.411	+0.225	−0.113	−0.365	+0.397	−0.381
k	(**L**^{1}·MesTe)$_2^{2+}$	−0.440, −0.405	+0.235	−0.082	−0.401	+0.468	–
l	(**L**^{2}·MesTe)$_2^{2+}$ (**2**$^{2+}$)	−0.420, −0.402	+0.231	−0.045	−0.383	+0.403	–

Table S40. Selected thermochemical data (a.u.) calculated at 298.15 K for $MesTe^+$ (a), the donors dimethylimidazole-2-chalcogenone [Me_2imidE: E = S (b), Se (c), and Te(d)], the 1:1 (e–g) and 1:2 (h–g) adducts between Me_2imidE and $MesTe^+$, **L¹** (k), **L²** (l), MesTeI (m), $MesTeI_2^-$ (o), the compounds **1**, and the cation [**2**]$^{2+}$.

		$E_0+\Delta H^a$	$E_0+\Delta G^b$	ΔS (x 10^3)^c
a	$MesTe^+$	-356.847	-356.899	0.177
b	Me_2imidS	-314.570	-314.614	0.145
c	$Me_2imidSe$	-313.680	-313.724	0.149
d	$Me_2imidTe$	-312.494	-312.539	0.152
e	$Me_2imidS \cdot MesTe^+$	-671.515	-671.592	0.257
f	$Me_2imidSe \cdot MesTe^+$	-670.633	-670.711	0.263
g	$Me_2imidTe \cdot MesTe^+$	-669.456	-669.536	0.268
h	$MesTe^+ \cdot 2Me_2imidS$	-986.122	-986.223	0.338
i	$MesTe^+ \cdot 2Me_2imidSe$	-984.349	-984.454	0.351
g	$MesTe^+ \cdot 2Me_2imidTe$	-981.984	-982.093	0.365
k	**L¹**	-586.944	-587.005	0.206
l	**L²**	-626.191	-626.257	0.222
m	MesTeI	-368.579	-368.639	0.201
n	$MesTeI_2^-$	-380.122	-380.189	0.224
o	**1**	-1324.132	-1324.272	0.471
g	[**2**]$^{2+}$	-1966.283	-1966.454	0.573

[a] Sum of electronic (E_0) and thermal enthalpy. [b] Sum of electronic (E_0) and thermal free energy. [c] Thermal enthalpy, calculated from $E_0+\Delta H$ and $E_0+\Delta G$.