Supporting Information

2-Pyridylselenenyl versus 2-Pyridyltellurenyl Halides: Symmetrical Chalcogen Bonding in the Solid State and Reactivity towards Nitriles

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Table S1. Cartesian atomic coordinates for model supramolecular associates.

Atom	X	Y	Z
16			
Te	2.119556	4.845298	10.163529
Te	1.796645	7.659256	12.554535
Br	0.529569	2.655909	10.184077
Br	3.778382	8.498676	14.163216
N	0.260422	7.073247	10.895785
N	3.200416	6.889989	10.016914
C	0.359046	6.030088	10.060947
C	-0.660722	5.743178	9.147176
H	-0.574755	5.014293	8.544083
C	-1.797580	6.534254	9.130541
H	-2.501628	6.350996	8.519620
C	-1.896611	7.596484	10.015283
H	-2.672239	8.143770	10.028167
C	-0.848802	7.845250	10.878172
H	-0.908346	8.579939	11.476372
C	3.121113	7.890858	10.910300
C	3.880923	9.046790	10.748356
H	3.799396	9.763236	11.367104
C	4.757563	9.143809	9.677369
H	5.296478	9.918300	9.565002
C	4.839401	8.092358	8.770936
H	5.436006	8.136307	8.033624
C	4.041970	6.988666	8.959790
H	4.082101	6.276366	8.332071
Te	-2.765259	8.991398	14.299393
Te	-2.442348	11.805356	11.908387
Br	-1.175272	6.802009	14.278844
Br	-4.424084	12.644776	10.299706
N	-0.906125	11.219347	13.567136
N	-3.846119	11.036089	14.446008
C	-1.004749	10.176188	14.401974
C	0.015019	9.889278	15.315746
H	-0.070948	9.160393	15.918839
C	1.151877	10.680354	15.332381
H	1.855925	10.497096	15.943302
C	1.250908	11.742584	14.447639
H	2.026537	12.289870	14.434755
C	0.203099	11.991350	13.584750
H	0.262644	12.726039	12.986550
C	-3.766816	12.036958	13.552622
C	-4.526625	13.192890	13.714566
H	-4.445099	13.909336	13.095817
C	-5.403265	13.289909	14.785553

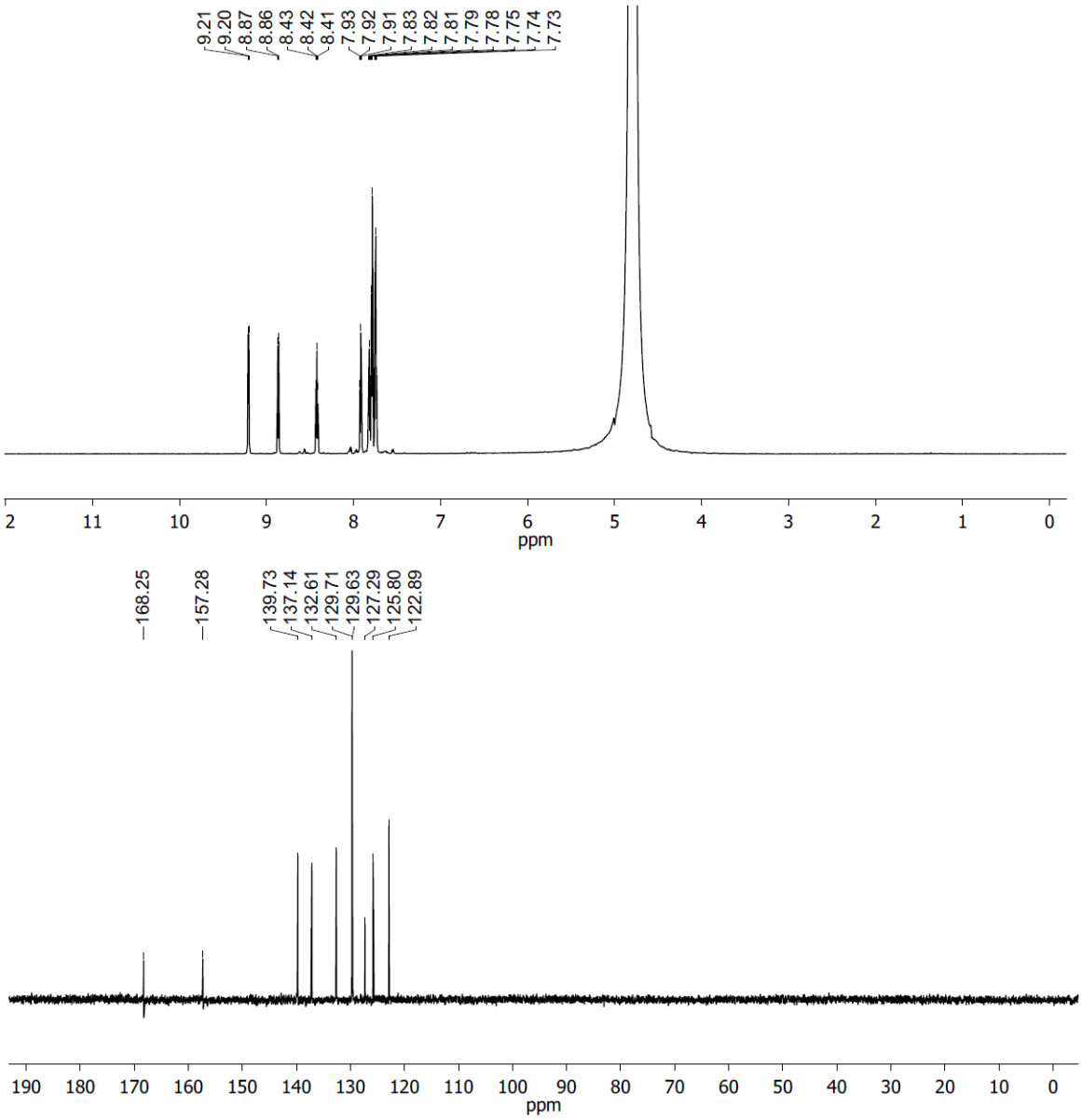
H	-5.942181	14.064400	14.897919
C	-5.485104	12.238458	15.691986
H	-6.081709	12.282407	16.429298
C	-4.687672	11.134766	15.503132
H	-4.727804	10.422466	16.130851
Te	7.347641	8.991398	14.299393
Te	7.670552	11.805356	11.908387
Br	8.937628	6.802009	14.278844
Br	5.688816	12.644776	10.299706
N	9.206775	11.219347	13.567136
N	6.266781	11.036089	14.446008
C	9.108151	10.176188	14.401974
C	10.127919	9.889278	15.315746
H	10.041952	9.160393	15.918839
C	11.264777	10.680354	15.332381
H	11.968825	10.497096	15.943302
C	11.363808	11.742584	14.447639
H	12.139437	12.289870	14.434755
C	10.315999	11.991350	13.584750
H	10.375544	12.726039	12.986550
C	6.346084	12.036958	13.552622
C	5.586275	13.192890	13.714566
H	5.667801	13.909336	13.095817
C	4.709635	13.289909	14.785553
H	4.170719	14.064400	14.897919
C	4.627796	12.238458	15.691986
H	4.031191	12.282407	16.429298
C	5.425228	11.134766	15.503132
H	5.385096	10.422466	16.130851
1			
Se	3.820285	4.758591	9.025811
Cl	3.826054	4.858254	11.427810
N	5.720536	2.922429	8.098761
C	5.543673	3.899422	9.000170
C	6.585222	4.323289	9.814120
H	6.437286	4.983336	10.480984
C	7.839335	3.772078	9.641193
H	8.566471	4.052662	10.184821
C	8.029464	2.794534	8.654315
H	8.891833	2.429128	8.494308
C	6.945101	2.374931	7.923846
H	7.058273	1.685310	7.281829
Se	4.055710	1.919466	7.089820
Cl	2.197232	1.011470	5.941841
N	3.883756	4.705332	6.886283
C	3.880659	3.578145	6.142894

C	3.780453	3.635993	4.763451
H	3.783708	2.836893	4.248645
C	3.675958	4.862809	4.143298
H	3.603362	4.917198	3.197167
C	3.678212	6.023859	4.916502
H	3.601033	6.877980	4.509029
C	3.794200	5.903688	6.280043
H	3.812105	6.691158	6.810751
Se	1.264239	7.408214	10.850889
Cl	1.258469	7.308550	8.448889
N	-0.636012	9.244375	11.777938
C	-0.459149	8.267382	10.876530
C	-1.500698	7.843515	10.062579
H	-1.352762	7.183468	9.395716
C	-2.754811	8.394726	10.235507
H	-3.481948	8.114142	9.691879
C	-2.944940	9.372270	11.222385
H	-3.807309	9.737676	11.382392
C	-1.860577	9.791873	11.952853
H	-1.973750	10.481494	12.594871
Se	1.028814	10.247339	12.786880
Cl	2.887292	11.155334	13.934858
N	1.200768	7.461472	12.990417
C	1.203865	8.588659	13.733806
C	1.304071	8.530811	15.113249
H	1.300816	9.329911	15.628055
C	1.408566	7.303996	15.733402
H	1.481162	7.249606	16.679533
C	1.406312	6.142946	14.960198
H	1.483491	5.288824	15.367670
C	1.290324	6.263116	13.596656
H	1.272419	5.475646	13.065949
15			
Se	15.645786	1.475732	7.258900
N	13.894193	1.575956	7.831312
N	15.036598	2.010098	9.783204
C	16.149623	1.872631	9.007358
C	11.665934	0.884415	9.861586
H	11.943279	0.044852	9.514756
C	10.002792	2.245755	10.924613
H	9.139720	2.339723	11.310048
C	17.415117	1.999577	9.571640
H	18.195087	1.904606	9.038939
C	12.107717	3.219242	10.277398
H	12.686453	3.971640	10.235784
C	15.132562	2.249963	11.129023

H	14.347173	2.320702	11.659041
C	17.513291	2.264691	10.912092
H	18.369245	2.368016	11.311057
C	10.419770	1.009958	10.448145
H	9.851058	0.252882	10.524315
C	13.808565	1.843875	9.075658
C	12.517056	1.984849	9.776537
C	16.356766	2.385325	11.700297
H	16.430970	2.560672	12.631182
C	10.838826	3.334265	10.838426
H	10.546495	4.176423	11.166295
Cl	18.430674	1.377190	6.483867
Cl	14.794062	-1.377190	9.777838
Se	17.578950	-1.475732	9.002805
N	19.330543	-1.575956	8.430393
N	18.188138	-2.010098	6.478501
C	17.075113	-1.872631	7.254347
C	21.558802	-0.884415	6.400119
H	21.281457	-0.044852	6.746949
C	23.221944	-2.245755	5.337092
H	24.085016	-2.339723	4.951657
C	15.809619	-1.999577	6.690065
H	15.029649	-1.904606	7.222766
C	21.117019	-3.219242	5.984307
H	20.538283	-3.971640	6.025921
C	18.092174	-2.249963	5.132682
H	18.877564	-2.320702	4.602664
C	15.711445	-2.264691	5.349613
H	14.855491	-2.368016	4.950648
C	22.804966	-1.009958	5.813560
H	23.373678	-0.252882	5.737390
C	19.416171	-1.843875	7.186047
C	20.707680	-1.984849	6.485168
C	16.867970	-2.385325	4.561408
H	16.793766	-2.560672	3.630523
C	22.385910	-3.334265	5.423279
H	22.678241	-4.176423	5.095410

Table S2. Crystallographic parameters, data collection and structure refinement details for **15** and **16**.

Compound	**15**	**16**
Empirical formula	$C_{12}H_9ClN_2Se$	$C_{10}H_8Br_2N_2Te_2$
Formula weight	295.62	571.18
Temperature/K	120.0	100(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	20.5842(10)	10.1129(2)
b/Å	7.0136(3)	8.2922(2)
c/Å	18.0982(10)	16.7458(3)
α/°	90	90
β/°	116.035(2)	103.1210(10)
γ/°	90	90
Volume/Å^3	2347.7(2)	1367.61(5)
Z	8	4
ρ_{calc}g/cm^3	1.673	2.774
μ/mm^{-1}	3.398	10.085
F(000)	1168.0	1024.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/ °	3.996 to 56.564	4.318 to 65.178
Reflections collected	14484	31297
Independent reflections	5784 [R_{int} = 0.0433, R_{sigma} = 0.0476]	5002 [R_{int} = 0.0407, R_{sigma} = 0.0258]
Data/restraints/parameters	5784/0/278	5002/0/146
Goodness-of-fit on F^2	1.019	1.087
Final R indexes [I>=2σ (I)]	R_1 = 0.0285, wR_2 = 0.0555	R_1 = 0.0214, wR_2 = 0.0356
Final R indexes [all data]	R_1 = 0.0425, wR_2 = 0.0595	R_1 = 0.0280, wR_2 = 0.0375
Largest diff. peak/hole / e Å^{-3}	0.47/-0.40	0.63/-0.60



^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **15** (D_2O).