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IMIDAZOLE-FUNCTIONALIZED PYRIDINIUM-FUSED SELENADIAZOLIUM SALTS AS VERSATILE CHALCOGEN BOND DONORS

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Table S1

Cartesian atomic coordinates for model supramolecular associate 3.

Atom	*X*	*Y*	*Z*
Se1	-0.081914	1.823521	9.197029
N2	0.595664	4.316855	8.727499
N3	0.499746	2.895114	10.549385
N4	1.080668	6.447943	10.929690
N5	2.232167	6.021568	12.784080
H6	2.654245	6.168551	13.542820
N7	3.132719	2.602525	12.875093
C8	0.124216	3.257802	8.028649
C9	-0.093077	3.347804	6.652077
H10	-0.415737	2.598829	6.164117
C11	0.161214	4.511918	6.024737
H12	0.011867	4.595981	5.090749
C13	0.652238	5.608834	6.769094
H14	0.830755	6.428829	6.324138
C15	0.869933	5.518243	8.069280
H16	1.208724	6.264001	8.550739
C17	0.777652	4.076395	10.131700

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Continuation of Table S1

Atom	*X*	*Y*	*Z*
C18	2.056385	4.814655	12.148614
C19	1.619808	6.930840	11.997467
H20	1.587427	7.855424	12.213445
C21	2.630266	3.603046	12.566299
Se22	2.986042	0.147624	15.175285
N23	0.678050	0.721536	14.012756
N24	2.347293	-0.836938	13.773847
N25	-0.132053	-0.451327	11.238484
N26	-0.105902	-2.626842	10.822424
H27	-0.259291	-3.399739	10.430044
N28	1.303282	-4.353733	13.547939
C29	1.468568	1.166780	15.059406
C30	1.048930	2.230427	15.837892
H31	1.548434	2.504654	16.597510
C32	-0.099850	2.877151	15.485217
H33	-0.361909	3.657778	15.958224
C34	-0.905934	2.396197	14.423940
H35	-1.724139	2.828138	14.206727
C36	-0.516441	1.375085	13.764095
H37	-1.074159	1.047289	13.068138
C38	1.219252	-0.409097	13.297654
C39	0.491647	-1.084528	12.184369
C40	0.547226	-2.433151	12.021846
C41	-0.470808	-1.384313	10.355982
H42	-0.901555	-1.219172	9.524757
C43	0.927039	-3.488510	12.850715
Cl44	-0.933637	0.038120	6.961522
Cl45	3.807687	1.503257	17.612646
Cl46	5.512971	-1.897830	14.892007
Se47	6.334616	-0.542197	17.329368
N48	8.642609	-1.116109	18.491897
N49	6.973366	0.442365	18.730806

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Continuation of Table S1

Atom	*X*	*Y*	*Z*
N50	9.452712	0.056754	21.266169
N51	9.426560	2.232269	21.682229
H52	9.579949	3.005165	22.074609
N53	8.017376	3.959160	18.956714
C54	7.852090	-1.561353	17.445247
C55	8.271728	-2.625000	16.666761
H56	7.772224	-2.899227	15.907143
C57	9.420508	-3.271724	17.019436
H58	9.682567	-4.052351	16.546429
C59	10.226592	-2.790770	18.080713
H60	11.044797	-3.222711	18.297926
C61	9.837099	-1.769658	18.740558
H62	10.394817	-1.441862	19.436515
C63	8.101407	0.014523	19.206999
C64	8.829011	0.689955	20.320284
C65	8.773432	2.038578	20.482807
C66	9.791466	0.989740	22.148671
H67	10.222213	0.824599	22.979896
C68	8.393619	3.093937	19.653938

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Table S2

Cartesian atomic coordinates for model supramolecular associate 4.

Atom	*X*	*Y*	*Z*
Re1	8.300477	2.243187	0.271087
O2	8.949953	0.916137	1.158362
O3	6.656187	1.874869	-0.201585
O4	9.275468	2.491075	-1.129779
O5	8.299322	3.646935	1.266676
Re6	5.756060	4.104449	9.585219
O7	6.136347	4.760516	8.042341
O8	5.400963	5.392027	10.677990
O9	7.108932	3.207972	10.177036
O10	4.319458	3.119647	9.442906
Se11	3.749456	1.825593	7.091882
Se12	5.478852	0.067073	1.382061
N13	1.758844	0.072207	7.236001
N14	3.333607	0.756049	5.677477
N15	0.868550	-1.895745	5.107323
N16	1.618501	-2.022975	3.040324
H17	1.714004	-2.310500	2.213554
N18	3.377668	1.058740	2.652197
N19	4.354776	-1.013891	2.342298
C20	2.342597	1.032481	8.009245
C21	1.863137	1.291902	9.293973
H22	2.254447	1.975475	9.824458
C23	0.818681	0.545561	9.778379
H24	0.467907	0.721609	10.644187
C25	0.276669	-0.467281	9.000622
H26	-0.421644	-1.005327	9.354253
C27	0.726161	-0.701536	7.745981
H28	0.337449	-1.389118	7.218415
C29	2.338089	-0.025514	5.921185
C30	1.854974	-0.946899	4.905738
C31	2.317793	-1.010123	3.619505

Continuation of Table S2

Atom	*X*	*Y*	*Z*
C32	3.388987	-0.341610	2.864313
C33	0.761026	-2.504837	3.944448
H34	0.145356	-3.206574	3.768121
C35	4.399812	1.516348	1.877449
C36	4.517637	2.880436	1.599141
H37	5.239651	3.207908	1.075998
C38	3.567000	3.738162	2.100095
H39	3.633762	4.670443	1.928131
C40	2.498332	3.242886	2.864313
H41	1.831644	3.837919	3.186939
C42	2.412447	1.912458	3.145629
H43	1.698066	1.577491	3.674700

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Table S3

Crystal data and structure refinement for all compounds studied.

Compound	**3**	**4**
CCDC	2528228	2528229
Empirical formula	$C_{40}H_{24}Cl_4N_{20}OSe_4$	$C_{15}H_{11}N_6O_8Re_2Se_2$
Formula weight	1258.43	933.62
Temperature, K	150	100.00
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a, Å	7.0800(9)	8.1950(2)
b, Å	10.3859(14)	8.4069(3)
c, Å	17.124(2)	15.3073(5)
α, °	106.384(4)	96.037(2)
β, °	94.116(4)	97.6890(10)
γ, °	103.254(4)	98.9240(10)
Volume, Å^3	1163.2(3)	1023.88(6)
Z	1	2
d_{calc}, g/cm^3	1.796	3.028
μ, mm^{-1}	3.443	15.427
F(000)	616.0	850.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Index ranges	$-8 \le h \le 8$, $-12 \le k \le 10$, $-20 \le l \le 20$	$-10 \le h \le 10$, $-11 \le k \le 11$, $-19 \le l \le 20$
Reflections collected	7149	9500
Independent reflections	4019 [R_{int} = 0.0395]	4892 [R_{int} = 0.0389,]
Goodness-of-fit on F^2	1.044	1.091
Final R indexes [$I>=2\sigma(I)$]	R_1 = 0.0762, wR_2 = 0.1992	R_1 = 0.0370, wR_2 = 0.0762
Final *R* indexes [all data]	R_1 = 0.1049, wR_2 = 0.2239	R_1 = 0.0454, wR_2 = 0.0799

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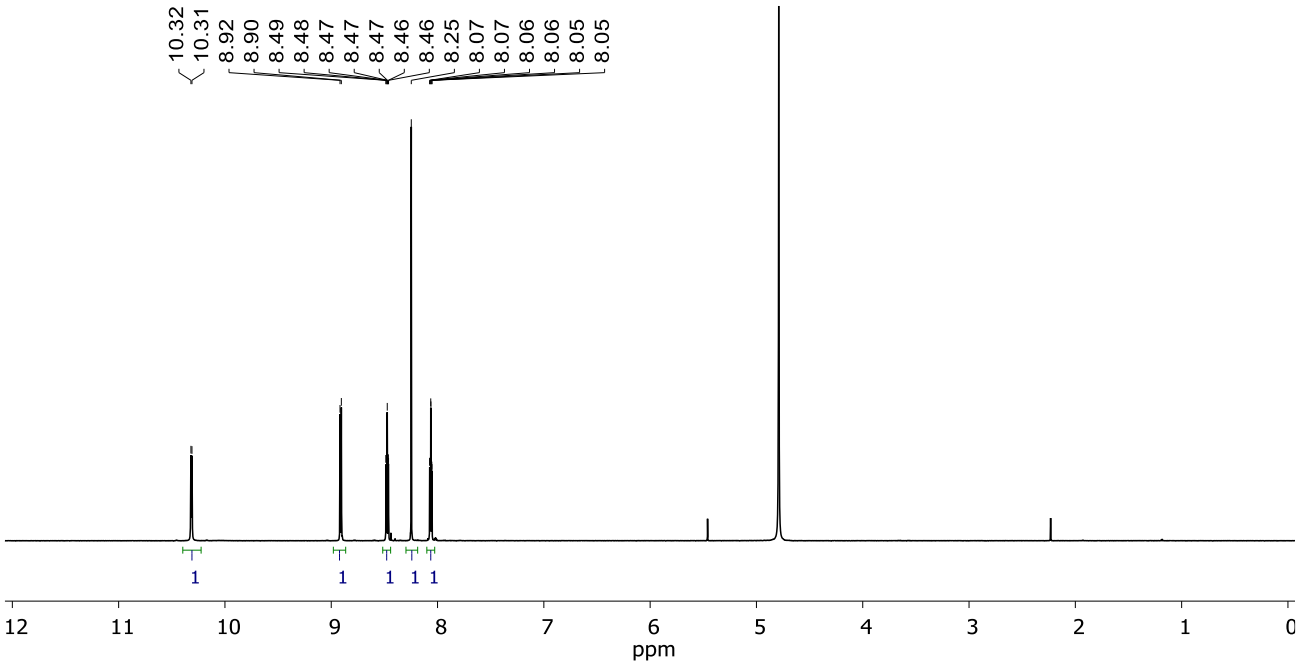

Figure S1. ^{1}H NMR spectrum (700 MHz, D_2O) of compound 3.

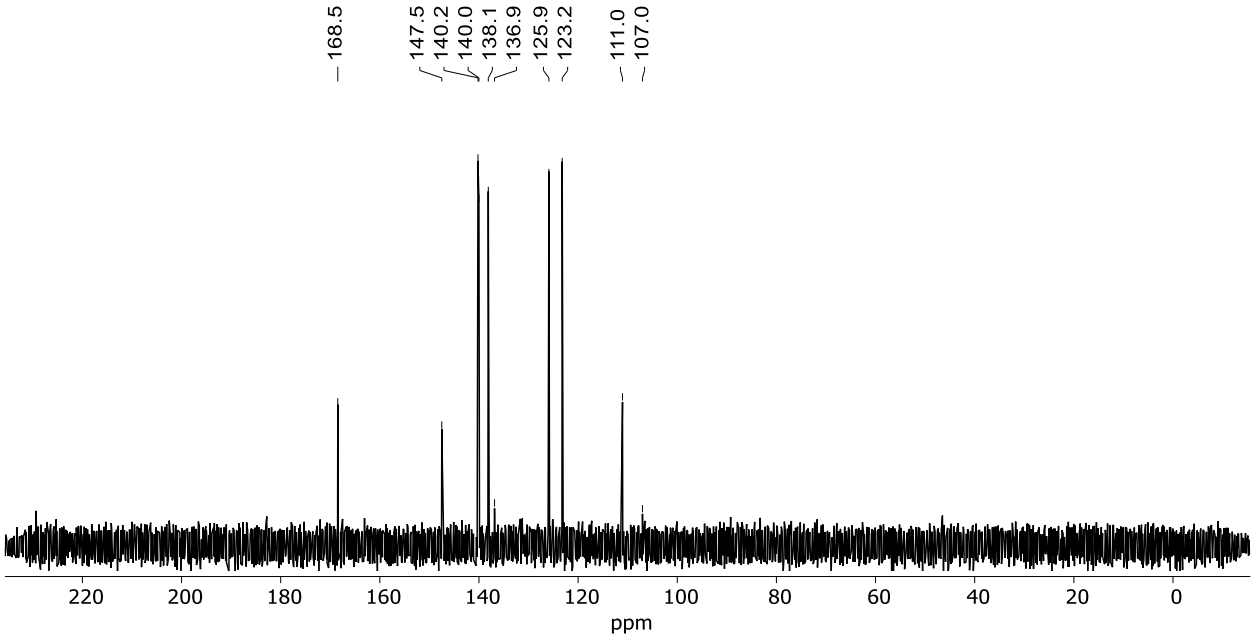

Figure S2. ^{13}C NMR spectrum (176 MHz, D_2O) of compound 3.