Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Organomercury(II) and -tellurium(II) compounds with the pincer ligand 2,6-$[O(CH_2CH_2)_2NCH_2]_2C_6H_3$ – stabilization of an unusual organotellurium(II) cationic species

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1,3-[O(CH$_2$CH$_2$)$_2$NCH$_2$]$_2$C$_6$H$_4$ (1)

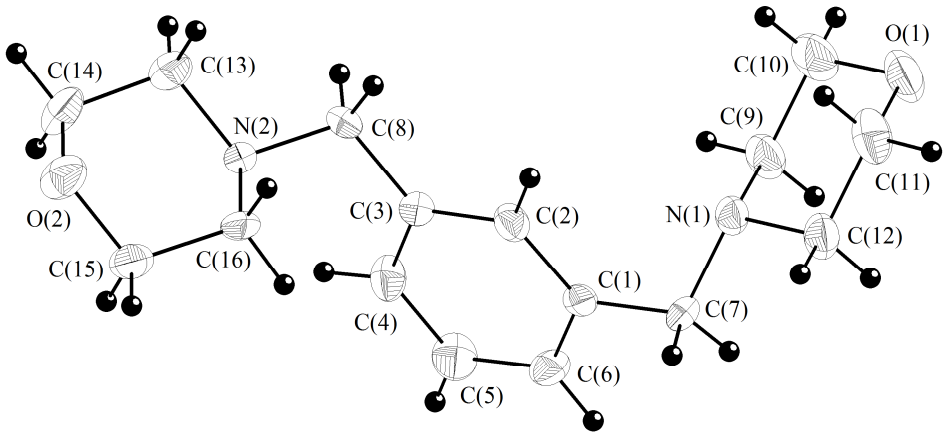

Figure S1. ORTEP representation at 30% probability and atom numbering scheme for the molecule of **1**.

Table S1 Selected bond distances (Å) and angles (°) for compound **1**

C(1)–C(2)	1.396(9)	C(4)–C(5)	1.384(10)
C(2)–C(3)	1.392(9)	C(5)–C(6)	1.386(10)
C(3)–C(4)	1.379(10)	C(1)–C(6)	1.384(10)
C(1)–C(7)	1.511(9)	C(3)–C(12)	1.512(9)
N(1)–C(7)	1.478(8)	N(2)–C(12)	1.468(8)
N(1)–C(8)	1.460(9)	N(2)–C(13)	1.467(8)
N(1)–C(11)	1.449(9)	N(2)–C(16)	1.474(8)
C(8)–C(9)	1.508(11)	C(13)–C(14)	1.522(11)
C(10)–C(11)	1.508(11)	C(15)–C(16)	1.508(10)
O(1)–C(9)	1.441(10)	O(2)–C(14)	1.420(9)
O(1)–C(10)	1.436(11)	O(2)–C(15)	1.420(8)
C(3)–C(2)–C(1)	122.3(6)	C(6)–C(5)–C(4)	120.4(7)
C(4)–C(3)–C(2)	118.4(6)	C(5)–C(6)–C(1)	120.8(6)
C(3)–C(4)–C(5)	120.3(7)	C(6)–C(1)–C(2)	117.6(6)
C(2)–C(1)–C(7)	121.2(6)	C(2)–C(3)–C(12)	121.5(6)
C(6)–C(1)–C(7)	121.2(6)	C(4)–C(3)–C(12)	120.1(6)
N(1)–C(7)–C(1)	114.1(5)	N(2)–C(12)–C(3)	113.6(5)
C(7)–N(1)–C(8)	111.4(6)	C(13)–N(2)–C(12)	111.8(5)
C(11)–N(1)–C(7)	110.0(5)	C(12)–N(2)–C(16)	112.0(5)
C(11)–N(1)–C(8)	108.5(5)	C(13)–N(2)–C(16)	108.6(5)
N(1)–C(8)–C(9)	109.3(7)	N(2)–C(13)–C(14)	109.9(6)
N(1)–C(11)–C(10)	110.4(6)	N(2)–C(16)–C(15)	109.4(6)
O(1)–C(9)–C(8)	111.7(7)	O(2)–C(14)–C(13)	110.9(6)
O(1)–C(10)–C(11)	111.9(7)	O(2)–C(15)–C(16)	112.1(6)
C(10)–O(1)–C(9)	108.3(6)	C(14)–O(2)–C(15)	110.0(5)

[2,6-{O(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]HgOAc (2)

- the crystal contains a 1:1 mixture of (S_{N1},R_{N2}) and (R_{N1},S_{N2}) isomers

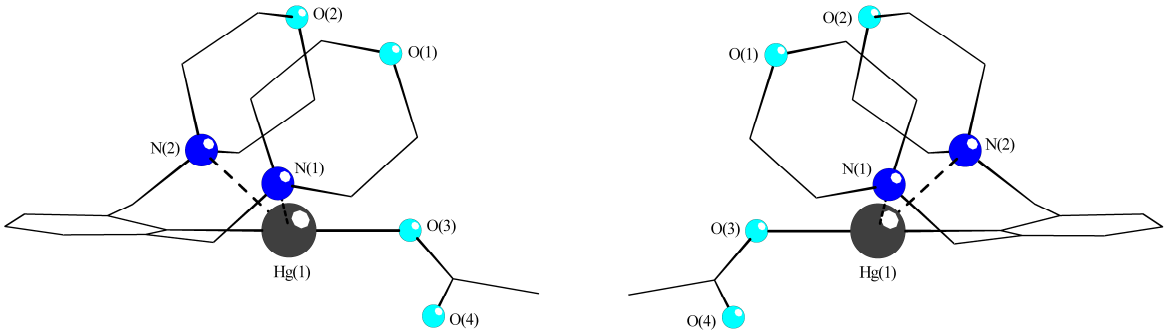

Figure S2. Molecular structure of (S_{N1},R_{N2})-**2** isomer (*left*) and (R_{N1},S_{N2})-**2** isomer (*right*) in the crystal of **2** (hydrogen atoms are not shown).

- the crystal of **2** contains pairs of isomers of same type, *i.e.* (S_{N1},R_{N2}) or (R_{N1},S_{N2}), respectively, connected through weak O(4)···H(12Aa) contacts. No further inter-dimer contacts are present.

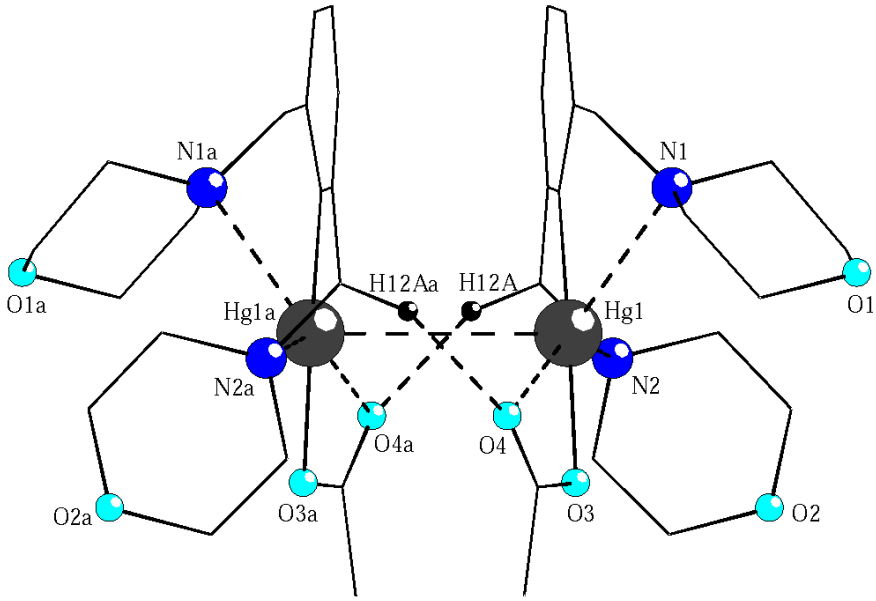

Figure S3. View along *c* axis of a dimer based on O···H$_{methylene}$ contacts between (S_{N1},R_{N2})-**2** isomers in the crystal of **2** (only hydrogen atoms involved in intermolecular contacts are shown) [symmetry equivalent atoms (1 – *x*, *y*, 0.5 – *z*) are given by ‘‘a’’].

- intramolecular distance	Hg(1)···O(4) 2.871(9) Å	$\sum r_{vdW}$(Hg,O) 2.90 Å
- intermolecular distance	O(4)···H(12Aa) 2.57 Å	$\sum r_{vdW}$(O,H) 2.60 Å
	Hg(1)···Hg(1a) 3.614(6) Å	$\sum r_{vdW}$(Hg,Hg) 3.00 Å

[2,6-{O(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$]HgCl (3)

- the crystal contains a 1:1 mixture of (R_{N1},R_{N2}) and (S_{N1},S_{N2}) isomers

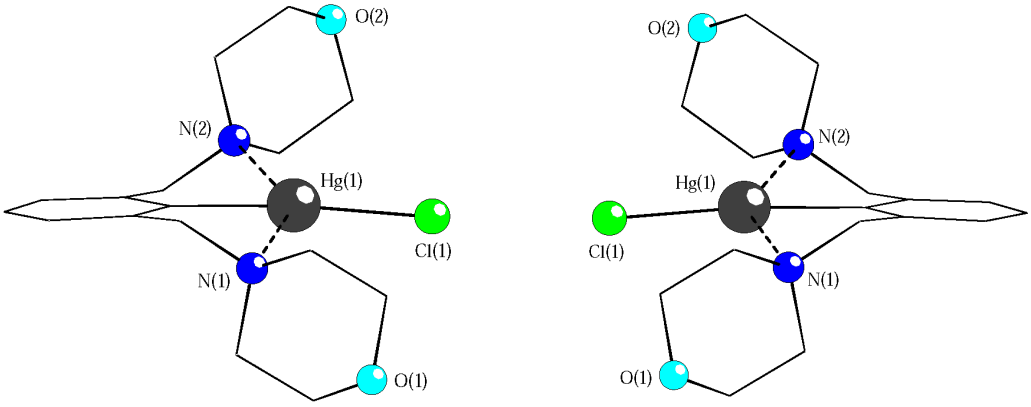

Figure S4. Molecular structure of (R_{N1},R_{N2})-**3** isomer (*left*) and (S_{N1},S_{N2})-**3** isomer (*right*) in the crystal of **3** (hydrogen atoms are not shown).

- the crystal of **3** contains parallel chains built from (R_{N1},R_{N2}) and (S_{N1},S_{N2}) isomers, respectively, connected through weak contacts between mercury and oxygen atoms [Hg(1)···O(1a) 2.878(5) Å] from only one pendant arm per ligand unit.

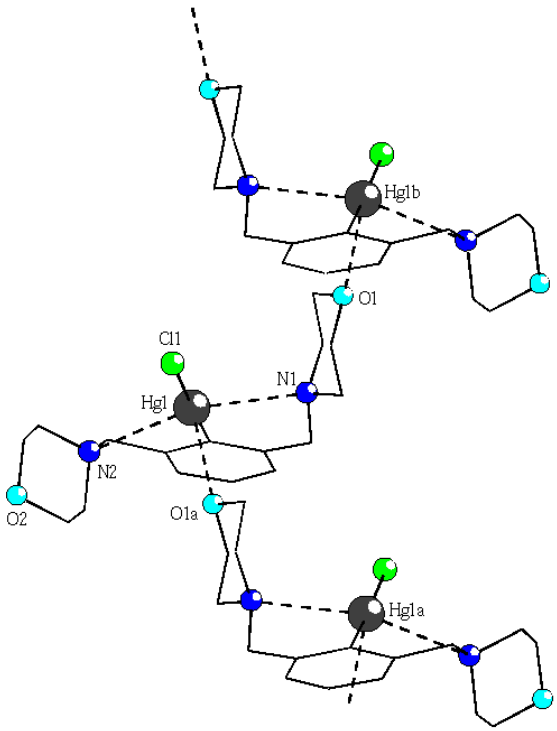

Figure S5. View of a chain polymer association based on Hg···O contacts between (R_{N1},R_{N2})-**3** isomers in the crystal of **3** (hydrogen atoms are not shown) [symmetry equivalent atoms (–0.5 – *x*, –0.5 + *y*, 0.5 – *z*) and (–0.5 – *x*, 0.5 + *y*, 0.5 – *z*) are given by ‘‘a’’ and ‘‘b’’, respectively].

- intermolecular distance Hg(1)···O(1a) 2.878(5) Å $\sum r_{vdW}$(Hg,O) 2.90 Å

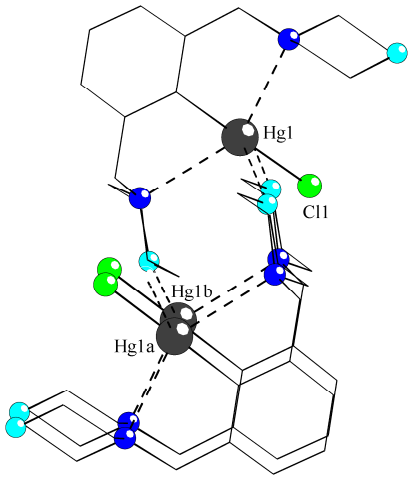

Figure S6. View along chain polymer association between (R_{N1},R_{N2})-**3** isomers in the crystal of **3** (hydrogen atoms are not shown) [symmetry equivalent atoms (–0.5 – *x*, –0.5 + *y*, 0.5 – *z*) and (–0.5 – *x*, 0.5 + *y*, 0.5 – *z*) are given by ‘‘a’’ and ‘‘b’’, respectively].

- weak inter-chain contacts between chlorine atoms and $H_{methylene}$ of the morpholinyl rings or aromatic hydrogen atoms results in a 3D supramolecular network.

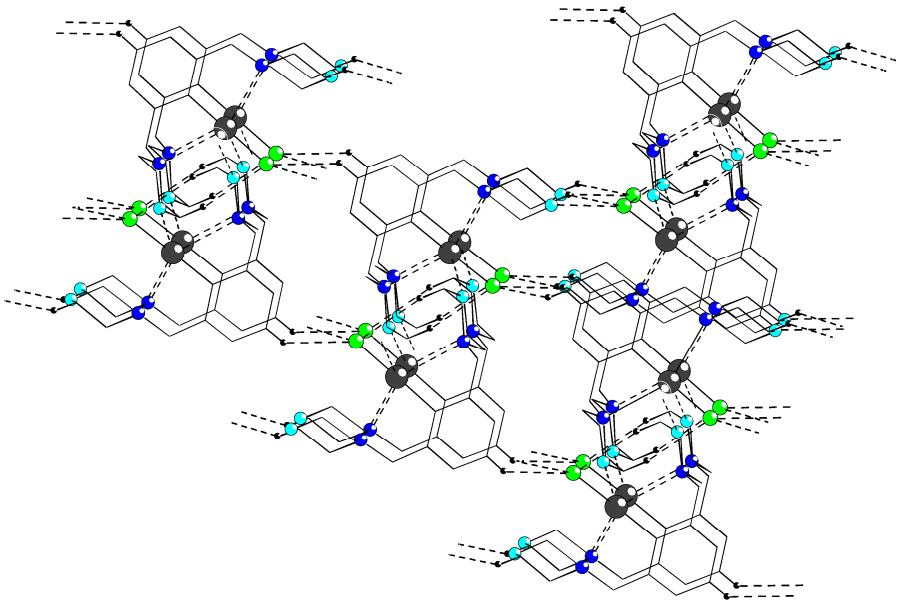

Figure S7. View of the 3D network built through weak chlorine-hydrogen contacts between chain polymers of (R_{N1},R_{N2})-**3** and (S_{N1},S_{N2})-**3** isomers, respectively, in the crystal of **3** (only hydrogen atoms involved in intra- and intermolecular contacts are shown) [symmetry equivalent atoms (–0.5 + *x*, 1.5 – *y*, –0.5 + *z*) and (–*x*, 2 – *y*, –*z*) are given by ‘‘a prime’’ and ‘‘b prime’’, respectively].

- intramolecular distance Cl(1)···H(10A) 2.91 Å $\sum r_{vdW}$(Cl,H) 3.01 Å
- intermolecular distances Cl(1)···H(15Bb’) 2.83 Å
  Cl(1)···H(4a') 2.98 Å

[2,6-{O(CH$_2$CH$_2$)$_2$NCH$_2$}$_2$C$_6$H$_3$Te]$_2$[Hg$_2$Cl$_6$] (4)

- the crystal contains a 1:1 mixture of (R_{N1},R_{N2}) and (S_{N1},S_{N2}) isomers of the cation

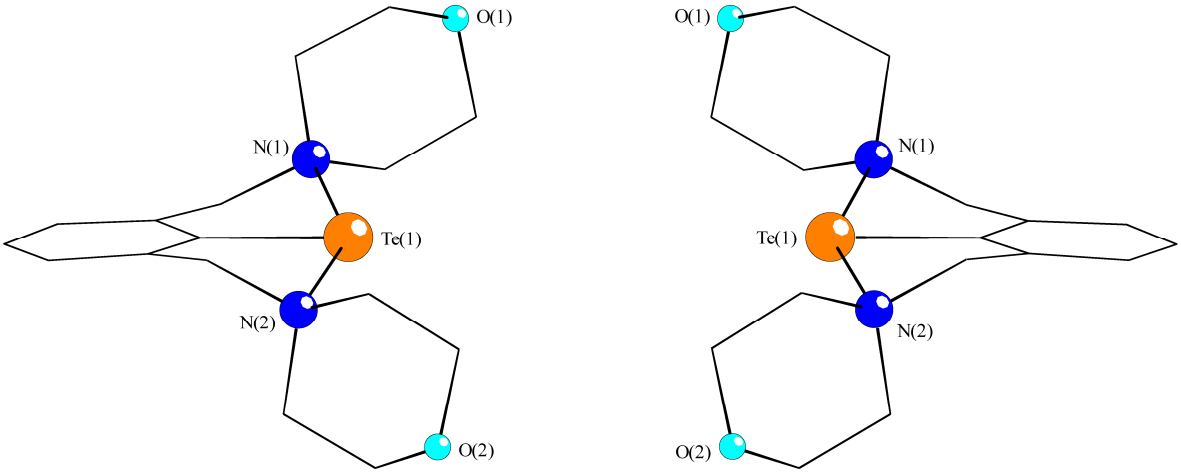

Figure S8. Structure of (R_{N1},R_{N2}) cation (*left*) and (S_{N1},S_{N2}) cation (*right*) in the crystal of **4** (hydrogen atoms are not shown).

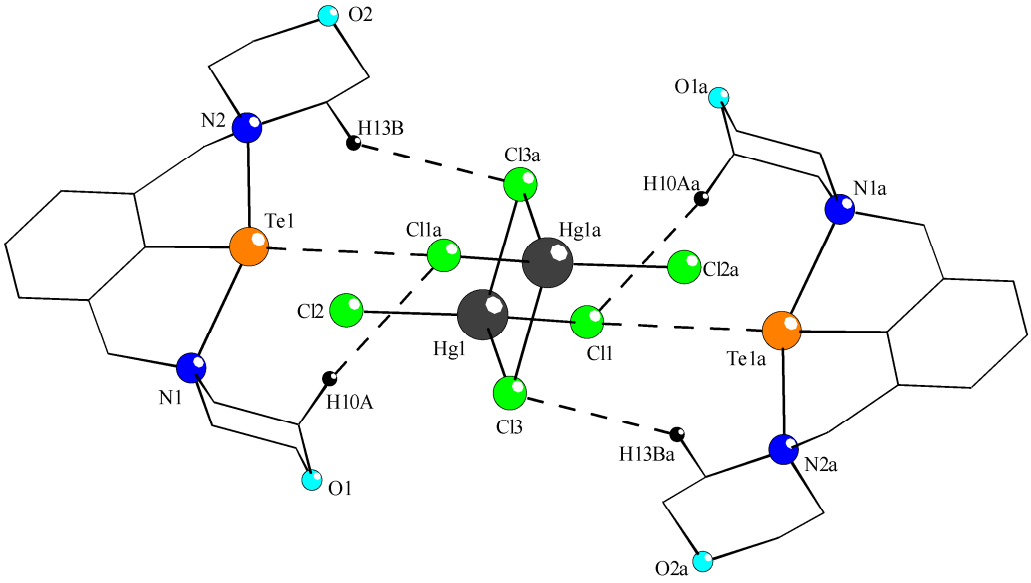

Figure S9. View of the Te···Cl and Cl···H$_{methylene}$ contacts between pairs of (R_{N1},R_{N2})-[RTe]$^+$ and (S_{N1},S_{N2})-[RTe]$^+$ cations and the [Hg$_2$Cl$_6$]$^{2-}$ dianion in the crystal of **4** (only hydrogen atoms involved in cation-anion contacts are shown) [symmetry equivalent atoms (1 – *x*, –*y*, –*z*) are given by ‘‘prime’’].

- cation-anion distances

Te(1)···Cl(1a) 3.869(3) Å
Cl(1)···H(10Aa) 2.92 Å
Cl(3)···H(13Ba) 2.98 Å

$\sum r_{vdW}$(Te,Cl) 3.90 Å
$\sum r_{vdW}$(Cl,H) 3.01 Å

- additional weak Cl···H contacts between anions and cations result in stacked layers with no inter-layers contacts.

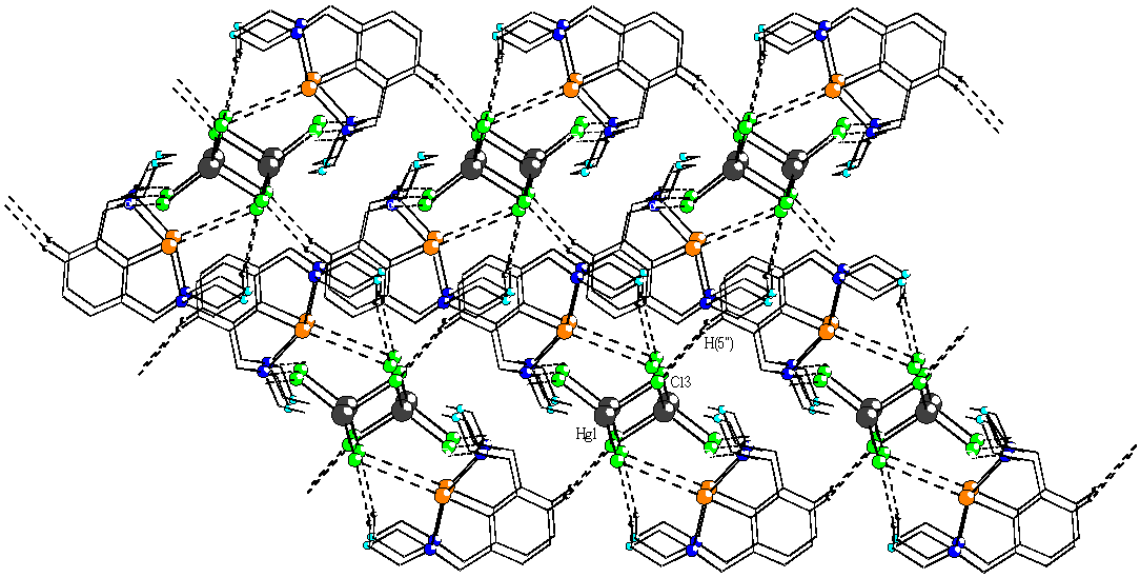

Figure S10. View along *a* axis of the layers built through weak chlorine-hydrogen contacts between $[RTe]_2[Hg_2Cl_6]$ units in the crystal of **4** (only hydrogen atoms involved in intra- and inter-units contacts are shown) [symmetry equivalent atoms (*x*, *y*, –1 + *z*) are given by ‘‘double prime’’].

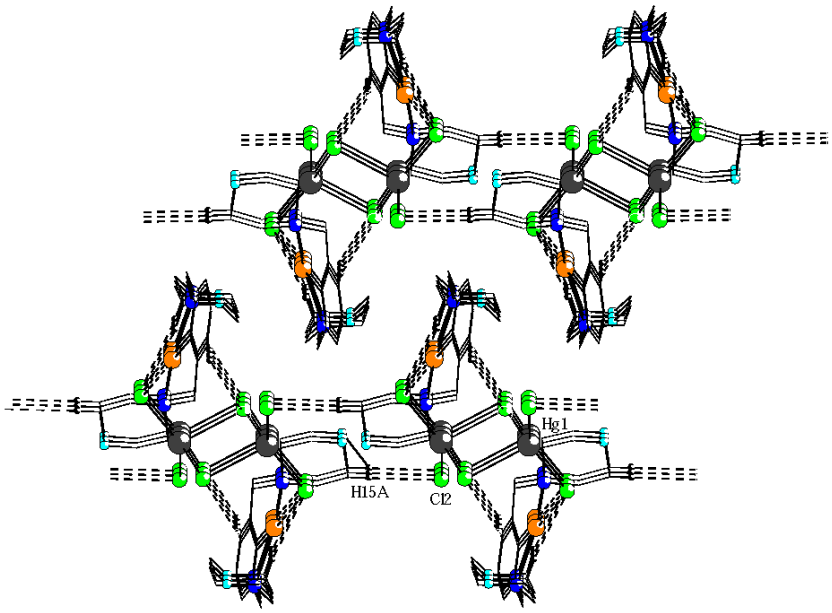

Figure S11. View along *c* axis of the layers built through weak chlorine-hydrogen contacts between $[RTe]_2[Hg_2Cl_6]$ units in the crystal of **4** (only hydrogen atoms involved in intra- and inter-units contacts are shown) [symmetry equivalent atoms (–0.5 + *x*, 1.5 – *y*, –0.5 + *z*) are given by ‘‘prime’’].

- cation-anion distances Cl(2)···H(15A’) 2.93 Å Cl(3)···H(5’’) 2.91 Å $\sum r_{vdW}$(Cl,H) 3.01 Å

[1,3-{O(CH$_2$CH$_2$)$_2$NHCH$_2$}$_2$C$_6$H$_4$][HgCl$_4$]·H$_2$O (5·H$_2$O)

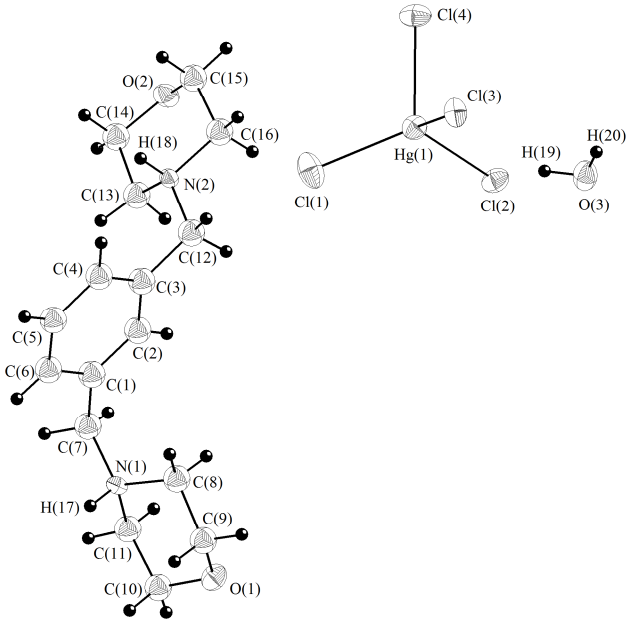

Figure S12. ORTEP representation at 30% probability and atom numbering scheme for the dication and the dianion in the crystal of **5**·H$_2$O.

Table S2. Selected bond distances (Å) and angles (°) for compound **5**·H$_2$O

C(1)–C(2)	1.373(9)	C(4)–C(5)	1.375(9)
C(2)–C(3)	1.387(9)	C(5)–C(6)	1.390(10)
C(3)–C(4)	1.372(9)	C(1)–C(6)	1.389(10)
C(1)–C(7)	1.510(9)	C(3)–C(12)	1.503(9)
N(1)–C(7)	1.485(8)	N(2)–C(12)	1.491(8)
N(1)–C(8)	1.495(8)	N(2)–C(13)	1.494(8)
N(1)–C(11)	1.508(8)	N(2)–C(16)	1.503(8)
N(1)–H(17)	0.853(19)	N(2)–H(18)	0.86(2)
C(8)–C(9)	1.496(9)	C(13)–C(14)	1.520(9)
C(10)–C(11)	1.481(10)	C(15)–C(16)	1.504(9)
O(1)–C(9)	1.432(8)	O(2)–C(14)	1.420(8)
O(1)–C(10)	1.400(10)	O(2)–C(15)	1.386(8)
Hg(1)–Cl(1)	2.411(2)	Hg(1)–Cl(3)	2.5130(18)
Hg(1)–Cl(2)	2.4475(18)	Hg(1)–Cl(4)	2.5614(19)
O(3)–H(19)	0.89(6)	O(3)–H(20)	0.89(6)
C(3)–C(2)–C(1)	121.4(6)	C(6)–C(5)–C(4)	121.4(7)
C(4)–C(3)–C(2)	119.3(6)	C(5)–C(6)–C(1)	118.6(6)
C(3)–C(4)–C(5)	119.8(6)	C(6)–C(1)–C(2)	119.6(6)
C(2)–C(1)–C(7)	119.5(7)	C(2)–C(3)–C(12)	119.3(6)
C(6)–C(1)–C(7)	120.9(6)	C(4)–C(3)–C(12)	121.4(6)
N(1)–C(7)–C(1)	113.9(5)	N(2)–C(12)–C(3)	112.7(5)

C(7)–N(1)–C(8)	115.7(5)	C(13)–N(2)–C(12)	113.5(5)
C(11)–N(1)–C(7)	111.5(5)	C(12)–N(2)–C(16)	112.8(5)
C(11)–N(1)–C(8)	107.8(5)	C(13)–N(2)–C(16)	109.5(5)
C(7)–N(1)–H(17)	109(4)	C(12)–N(2)–H(18)	110(4)
C(8)–N(1)–H(17)	111(4)	C(13)–N(2)–H(18)	103(4)
C(11)–N(1)–H(17)	101(4)	C(16)–N(2)–H(18)	107(4)
N(1)–C(8)–C(9)	111.6(5)	N(2)–C(13)–C(14)	110.3(5)
N(1)–C(11)–C(10)	112.7(6)	N(2)–C(16)–C(15)	109.5(5)
O(1)–C(9)–C(8)	110.7(6)	O(2)–C(14)–C(13)	112.2(6)
O(1)–C(10)–C(11)	112.5(6)	O(2)–C(15)–C(16)	113.0(5)
C(10)–O(1)–C(9)	110.4(5)	C(14)–O(2)–C(15)	109.8(5)
Cl(1)–Hg(1)–Cl(2)	119.23(7)	Cl(2)–Hg(1)–Cl(3)	107.35(6)
Cl(1)–Hg(1)–Cl(3)	111.48(6)	Cl(2)–Hg(1)–Cl(4)	104.28(6)
Cl(1)–Hg(1)–Cl(4)	111.40(9)	Cl(3)–Hg(1)–Cl(4)	101.43(6)
H(19)–O(3)–H(20)	109(7)		

- two polymeric chains of alternating water molecules and $[HgCl_4]^{2-}$ dianions are bridged by $[1,3\text{-}\{O(CH_2CH_2)_2NHCH_2\}_2C_6H_4]^{2+}$ dications

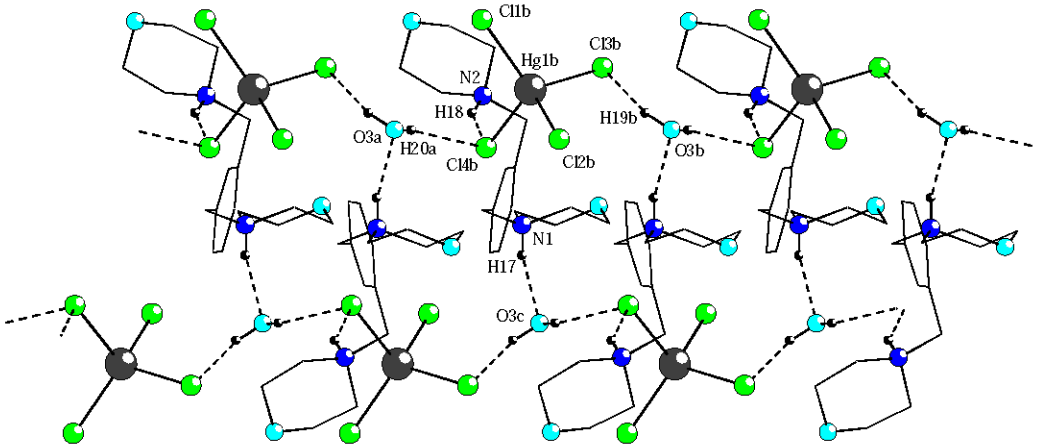

Figure S13. View along *b* axis of the polymeric chains of alternating water molecules and $[HgCl_4]^{2-}$ dianions bridged by $[1,3\text{-}\{O(CH_2CH_2)_2NHCH_2\}_2C_6H_4]^{2+}$ dications in the crystal of **5**·H_2O (only hydrogen atoms involved in hydrogen bonding are shown) [symmetry equivalent atoms (–0.5 + *x*, 1.5 – *y*, 1 – *z*), (0.5 + *x*, 1.5 – *y*, 1 – *z*) and (*x*, *y*, 1 + *z*) are given by ‘‘a’’, ‘‘b’’ and ‘‘c’’, respectively].

- hydrogen bonding

Cl(3b)···H(19b) 2.47 Å	$\sum r_{vdW}$(Cl,H) 3.01 Å
Cl(4b)···H(20a) 2.42 Å	
Cl(4b)···H(18) 2.37 Å	
O(3c)···H(17) 1.98 Å	$\sum r_{vdW}$(O,H) 2.60 Å

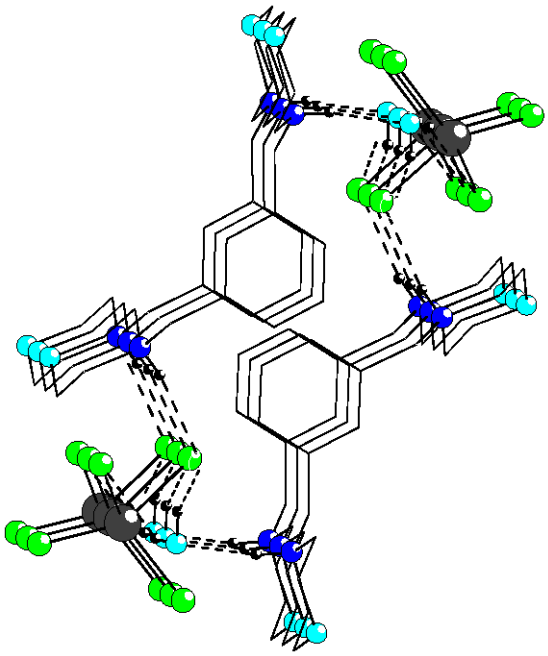

Figure S14. View along *a* axis of the polymeric chains of alternating water molecules and $[HgCl_4]^{2-}$ dianions bridged by $[1,3\text{-}\{O(CH_2CH_2)_2NHCH_2\}_2C_6H_4]^{2+}$ dications in the crystal of **5**·H_2O.

- **Table S3**. Comparison of selected experimental (X-ray) and theoretical (BP86/def2-TZVP) bond lengths (Å) and bond angles (°) of **3**.

	X-ray	**3b**	**%**
Hg(1)–C(1)	2.066(6)	2.079	0.6
Hg(1)–Cl(1)	2.3152(17)	2.332	0.7
Hg(1)–N(1)	2.840(5)	2.952	3.9
Hg(1)–N(2)	2.877(5)	3.011	4.6
C(2)–C(7)–N(1)	116.5(6)	114.0	–2.1
C(6)–C(12)–N(2)	114.5(5)	113.7	–0.7
C(1)–C(2)–C(7)–N(1)	41.5(9)	47.1	13.5
C(1)–C(6)–C(12)–N(2)	41.1(10)	50.0	21.6

Table S4. Comparison of selected experimental (X-ray) and theoretical (BP86/def2-TZVP) bond lengths (Å) and bond angles (°) of **4**, **4a**, **4b** and **4e**.

	X-ray	**4a**	**%**	**4b**	**%**	**4e**	**%**
Te(1)–C(1)	2.074(8)	2.108	1.6	2.095	1.0		
Te(1)–N(1)	2.392(7)	2.475	3.5	2.443	2.1		
Te(1)–N(2)	2.354(7)	2.448	4.0	2.443	3.6		
C(2)–C(7)–N(1)	110.7(7)	111.1	0.4	111.2	0.4		
C(6)–C(12)–N(2)	108.5(7)	110.7	2.1	111.2	2.4		
C(1)–C(2)–C(7)–N(1)	30.3(12)	35.9	18.5	33.9	10.6		
C(1)–C(6)–C(12)–N(2)	37.0(11)	36.8	–0.5	34.0	–8.9		
Te(1)···Cl(1a)	3.869(3)	3.240	–16.3				
Te(1)···Cl(2)	4.029(3)	3.950	–2.0				
Hg(1a)–Cl(1a)	2.373(3)	2.597	9.5			2.484	4.7
Hg(1a)–Cl(2a)	2.382(3)	2.412	1.3			2.486	4.4
Hg(1a)–Cl(3a)	2.586(3)	2.597	0.4			2.656	2.7
Hg(1a)–Cl(3)	2.748(3)	2.690	–2.1			2.703	–1.7
Cl(1a)–Hg(1a)–Cl(2a)	133.02(11)	113.4	–14.8			118.4	–11.0

Table S5. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of the anion **RHgCl** (**3a**); both nitrogen atoms coordinated to the mercury atom.

Atom	**x**	**y**	**z**
C	3.166177	3.850364	4.280954
C	3.309341	5.245680	4.373955
C	3.556041	5.824239	5.627922
H	3.678167	6.907899	5.700786
C	3.641970	5.033704	6.773474
H	3.829281	5.494798	7.744473
C	3.486672	3.651159	6.672920
H	3.548393	3.027090	7.567985
C	3.255176	3.044562	5.429818
C	3.146651	6.153557	3.164020
H	2.077384	6.198384	2.893004

H	3.441351	7.187418	3.447846
C	3.149961	1.529513	5.353321
H	4.048670	1.130231	4.851681
H	3.156052	1.115249	6.385352
C	5.325077	5.823069	2.127285
H	5.643877	5.240696	3.005436
H	5.612865	6.884251	2.300724
C	6.030300	5.307474	0.877638
H	7.113931	5.473103	0.952653
H	5.842458	4.221592	0.762850
C	4.181057	5.848850	–0.452452
H	3.928938	4.781626	–0.603044
H	3.909496	6.410559	–1.356683
C	3.425938	6.388356	0.757536
H	3.591011	7.486179	0.834312
H	2.345728	6.216521	0.626383
C	0.723426	1.338680	5.278120
H	0.643397	2.422678	5.452136
H	0.689724	0.832161	6.269057
C	–0.449634	0.861567	4.429143
H	–1.395690	0.994115	4.972122
H	–0.492657	1.446811	3.489238
C	0.876902	–0.795107	3.437807
H	0.887073	–0.263410	2.466936
H	0.899656	–1.877532	3.251459
C	2.084380	–0.370007	4.266511
H	2.134151	–0.991941	5.188248
H	3.007366	–0.543026	3.690605
N	3.869609	5.698632	1.975759
N	1.991118	1.058143	4.592910
O	5.595021	6.000948	–0.292394
O	–0.347821	–0.530977	4.129125
Hg	2.833943	2.971776	2.426777
Cl	2.486073	1.971967	0.348694

Table S6. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of **RHgCl** (**3b**); one nitrogen atom coordinated to the mercury atom.

Atom	**x**	**y**	**z**
C	2.092836	3.853501	5.571074
C	2.222225	5.254090	5.658736
C	3.477468	5.836182	5.446384
H	3.578212	6.923217	5.497905
C	4.591760	5.041681	5.167658
H	5.565513	5.505993	5.002725
C	4.458616	3.657563	5.099324
H	5.317419	3.022306	4.874951
C	3.208713	3.046214	5.296282
C	1.047092	6.144096	6.030813
H	0.829018	6.021398	7.106057

H	1.337978	7.206757	5.888301
C	3.125326	1.528287	5.268165
H	3.511923	1.135230	6.224821
H	2.054156	1.220820	5.219756
C	–0.101897	6.191555	3.883632
H	0.742868	5.651838	3.428999
H	0.090920	7.281266	3.771339
C	–1.398933	5.832253	3.167623
H	–1.367052	6.173326	2.123659
H	–1.542233	4.733487	3.178632
C	–2.625239	6.091755	5.144923
H	–2.802303	5.002216	5.224026
H	–3.495839	6.624623	5.550867
C	–1.365135	6.465488	5.918186
H	–1.255791	7.572060	5.932181
H	–1.452920	6.119686	6.960280
C	3.342764	1.170515	2.873287
H	3.277011	2.257957	2.715198
H	2.314188	0.750604	2.789369
C	4.228559	0.548675	1.799945
H	3.773511	0.665869	0.806771
H	5.218435	1.046969	1.801369
C	4.952670	–1.106172	3.293632
H	5.968697	–0.667549	3.354407
H	5.029923	–2.197823	3.391678
C	4.080655	–0.527109	4.402453
H	3.102272	–1.059017	4.410523
H	4.563035	–0.695614	5.378727
N	–0.188718	5.828954	5.306430
N	3.909606	0.914725	4.201597
O	–2.522906	6.474145	3.769674
O	4.393017	–0.856696	2.002662
Hg	0.190472	3.046824	5.812791
Cl	–1.914513	2.094050	6.104798

Table S7. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of **RHgCl** (**3c**); no nitrogen atom coordinated to the mercury atom.

Atom	**x**	**y**	**z**
C	2.530084	4.859333	4.333894
C	2.157891	5.165917	5.656670
C	2.915940	4.639723	6.712744
H	2.617611	4.879051	7.734983
C	4.017142	3.823499	6.459313
H	4.598335	3.418953	7.289984
C	4.376784	3.523208	5.146800
H	5.240961	2.892097	4.931992
C	3.641669	4.037677	4.068489
C	1.004669	6.102049	5.982276
H	1.410824	7.102309	6.213567

H	0.366665	6.233570	5.074166
C	4.040158	3.630464	2.658902
H	3.693909	2.598748	2.473450
H	3.499968	4.271977	1.920224
C	–0.571880	4.471944	6.861344
H	0.107776	3.664565	6.548720
H	–1.299471	4.644708	6.035616
C	–1.326851	4.050723	8.116769
H	–1.981371	3.194027	7.905397
H	–0.603783	3.762513	8.905572
C	–1.407163	6.269710	8.868195
H	–0.683173	6.064914	9.681983
H	–2.119023	7.033881	9.209445
C	–0.658248	6.747815	7.628685
H	–1.396421	7.066508	6.858263
H	–0.039550	7.622917	7.884641
C	6.025021	5.012415	2.408338
H	5.783448	5.510475	3.359767
H	5.572478	5.610971	1.584836
C	7.537322	4.965512	2.222830
H	7.946290	5.980342	2.123410
H	8.003945	4.476012	3.100701
C	7.376940	2.938137	1.057549
H	7.832029	2.372640	1.895107
H	7.672690	2.468683	0.109220
C	5.859266	2.937305	1.207582
H	5.404468	3.401386	0.303271
H	5.494451	1.899665	1.273438
N	0.214400	5.680370	7.131686
N	5.479546	3.651028	2.430076
O	–2.175621	5.096421	8.595531
O	7.899444	4.267603	1.029132
Hg	1.430719	5.648746	2.749844
Cl	0.213984	6.547629	0.987077

Table S8. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of the anion **[(RTe)(Hg_2Cl_6)]$^-$** (**4a**).

Atom	**x**	**y**	**z**
C	2.845973	4.441603	4.997332
C	3.062345	5.815302	5.111280
C	3.438469	6.343955	6.350393
H	3.624167	7.415682	6.456745
C	3.571204	5.496228	7.456536
H	3.862770	5.909420	8.423124
C	3.349801	4.119076	7.328175
H	3.476602	3.462820	8.192406
C	2.996985	3.581242	6.087049
C	2.817247	6.629560	3.867187
H	1.735776	6.829740	3.763389
H	3.342165	7.601588	3.898121

C	2.853029	2.112475	5.789735
H	3.803631	1.752391	5.351785
H	2.624118	1.518898	6.692179
C	4.714232	5.814408	2.535308
H	5.103130	5.208852	3.366746
H	5.104145	6.846669	2.621881
C	5.144306	5.211635	1.206952
H	6.236223	5.271206	1.115231
H	4.864012	4.145586	1.139700
C	3.167956	5.851001	0.159235
H	2.841056	4.794775	0.093162
H	2.777036	6.388034	–0.716599
C	2.633249	6.502518	1.430160
H	2.892691	7.578587	1.428292
H	1.539386	6.400364	1.490928
C	0.434404	2.095537	5.326314
H	0.349630	3.142812	5.650151
H	0.321398	1.441505	6.211613
C	–0.639235	1.748551	4.300487
H	–1.633036	1.849310	4.760504
H	–0.575677	2.447067	3.442382
C	0.765240	0.218064	3.232474
H	0.849003	0.857969	2.333438
H	0.816597	–0.828770	2.909646
C	1.899575	0.502618	4.202979
H	1.857963	–0.208316	5.049120
H	2.865284	0.391168	3.688499
N	3.222935	5.880620	2.648291
N	1.796326	1.882640	4.763137
O	4.588893	5.945694	0.108675
O	–0.519013	0.404051	3.856357
Te	2.327951	3.623025	3.125207
Cl	8.305857	–0.822290	1.992418
Cl	5.966593	2.291578	3.894199
Cl	5.693315	1.901801	–0.190185
Hg	6.360201	0.597112	2.093945
Cl	1.577956	2.401271	0.219405
Cl	2.797546	–0.590372	–2.444578
Cl	4.026655	–0.701723	1.700727
Hg	3.408992	0.707943	–0.506058

Table S9. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of the cation **[RTe]**$^{+}$ (**4b**); both nitrogen atoms coordinated to the tellurium atom.

Atom	**x**	**y**	**z**
C	3.256232	4.008011	4.622295
C	3.505127	5.374924	4.725814
C	3.901128	5.884494	5.967465
H	4.109297	6.950085	6.081715
C	4.011896	5.028335	7.068718
H	4.310479	5.431826	8.036197
C	3.743973	3.660598	6.943411
H	3.838718	3.004439	7.810781

C	3.372505	3.134241	5.701195
C	3.249951	6.214043	3.498185
H	2.180128	6.478908	3.448360
H	3.828197	7.152422	3.511636
C	3.160976	1.666704	5.421715
H	4.098658	1.224297	5.044766
H	2.867832	1.111596	6.327819
C	5.034317	5.390411	2.007763
H	5.504438	4.866149	2.851380
H	5.419939	6.424650	1.977891
C	5.340325	4.692617	0.688381
H	6.417680	4.742454	0.484650
H	5.045132	3.625782	0.742344
C	3.275577	5.331372	–0.211954
H	2.889867	4.290445	–0.190683
H	2.835286	5.838151	–1.080425
C	2.885353	6.063489	1.066492
H	3.191585	7.121720	0.995576
H	1.798422	6.020729	1.225111
C	0.751506	1.647793	4.895415
H	0.657694	2.676633	5.269894
H	0.619806	0.952068	5.742737
C	–0.293788	1.355356	3.826208
H	–1.297686	1.402305	4.267400
H	–0.233682	2.109622	3.016495
C	1.149864	–0.116867	2.715485
H	1.278488	0.577702	1.858832
H	1.202122	–1.143376	2.330183
C	2.252317	0.106529	3.743982
H	2.169759	–0.648079	4.545489
H	3.244435	0.019903	3.278689
N	3.559214	5.453497	2.250559
N	2.134668	1.462907	4.355930
O	4.684274	5.329959	–0.403617
O	–0.140364	0.044542	3.290007
Te	2.679016	3.232944	2.763084

Table S10. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of the cation **[RTe]**$^{+}$ (**4c**); one nitrogen atom coordinated to the tellurium atom.

Atom	**x**	**y**	**z**
C	3.440378	4.087452	4.679429
C	3.840382	5.419994	4.749578
C	4.284252	5.910891	5.985542
H	4.602581	6.951294	6.067473
C	4.323857	5.070101	7.101194
H	4.666467	5.460841	8.059381
C	3.946819	3.725604	6.998490
H	4.000046	3.074856	7.873529
C	3.513203	3.218291	5.769883

C	3.868857	6.218180	3.463458
H	4.896096	6.280317	3.068067
H	3.321355	5.535879	2.684143
C	3.200704	1.768054	5.508823
H	4.096828	1.260045	5.115268
H	2.879300	1.236228	6.418215
C	1.902818	7.625907	3.900184
H	1.729821	7.009839	4.794068
H	1.252075	7.247666	3.084058
C	1.554236	9.086733	4.188068
H	0.476288	9.189977	4.367786
H	2.100017	9.432142	5.087334
C	3.258296	9.854638	2.777144
H	3.849705	10.215404	3.640518
H	3.430643	10.524500	1.925043
C	3.676589	8.428384	2.419450
H	3.175516	8.129893	1.476292
H	4.764348	8.376872	2.264096
C	0.771624	1.874097	5.029303
H	0.744199	2.903156	5.412305
H	0.629833	1.176655	5.872289
C	–0.308411	1.639879	3.980745
H	–1.298549	1.731245	4.445413
H	–0.229334	2.400113	3.177970
C	1.037776	0.105052	2.828464
H	1.189395	0.799417	1.974565
H	1.029027	–0.918903	2.433336
C	2.171551	0.260381	3.834542
H	2.061996	–0.486643	4.638686
H	3.149568	0.127192	3.352634
N	3.309170	7.513700	3.505512
N	2.136494	1.617291	4.463270
O	1.865224	9.917493	3.074025
O	–0.229190	0.329772	3.429766
Te	2.670449	3.306523	2.883167

Table S11. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of the cation of **[RTe]**$^+$ (**4d**); no nitrogen atom coordinated to the tellurium atom.

Atom	**x**	**y**	**z**
C	0.101170	0.274599	0.098933
C	1.487199	0.343399	0.262202
C	2.118401	1.586420	0.133194
H	3.197738	1.667990	0.273743
C	1.363745	2.726697	–0.163786
H	1.860279	3.691707	–0.266192
C	–0.022839	2.639081	–0.330439
H	–0.600092	3.532233	–0.576223
C	–0.667539	1.403731	–0.194919
C	2.189602	–0.935801	0.664049

H	2.418931	–0.968408	1.741607
H	1.318354	–1.754622	0.566727
C	–2.143615	1.176546	–0.442084
H	–2.389926	1.161010	–1.516330
H	–2.287800	0.027988	–0.132221
C	3.279368	–1.327419	–1.529439
H	2.647031	–0.500239	–1.877587
H	2.839322	–2.280276	–1.883361
C	4.703571	–1.197596	–2.087264
H	4.692843	–1.338331	–3.175383
H	5.105432	–0.192100	–1.859784
C	5.640295	–2.093730	–0.134031
H	6.060468	–1.111164	0.152553
H	6.319863	–2.885066	0.206620
C	4.258521	–2.278222	0.509662
H	3.913631	–3.313041	0.321811
H	4.310440	–2.118062	1.595738
C	–2.925507	2.193990	1.678766
H	–1.860831	2.209412	1.946431
H	–3.410874	1.354480	2.214188
C	–3.608960	3.507071	2.084167
H	–3.633533	3.592995	3.177777
H	–3.047725	4.365791	1.669670
C	–5.028900	3.441765	0.220379
H	–4.500502	4.292294	–0.250273
H	–6.091075	3.487816	–0.051157
C	–4.422086	2.117300	–0.264608
H	–5.044716	1.282347	0.109937
H	–4.405371	2.076195	–1.362811
N	3.316335	–1.323615	–0.069618
N	–3.056535	1.990002	0.238855
O	5.552931	–2.204295	–1.549603
O	–4.959592	3.535498	1.638231
Te	–0.859352	–1.592772	0.302668

Table S12. Cartesian coordinates (Å) of the optimized structure (BP86/def2-TZVP) of the dianion **[Hg_2Cl_6]$^{2-}$** (**4e**).

Atom	**x**	**y**	**z**
Cl	8.333915	–1.750968	0.885590
Cl	6.600200	1.366764	3.232010
Cl	5.883125	1.273770	–0.964135
Hg	6.514037	–0.094459	1.222759
Cl	1.645447	1.751008	–0.885468
Cl	3.379020	–1.366687	–3.232067
Cl	4.096215	–1.273872	0.964069
Hg	3.465240	0.094445	–1.222759

Table S13. Cartesian coordinates (Å) of the optimized (H atoms only) structure (BP86/def2-TZVP) of the anion **[(RTe)(Hg$_2$Cl$_6$)]$^-$** (**4A**).

Atom	x	y	z
C	3.183252	4.090252	4.678322
C	3.359312	5.469550	4.769337
C	3.619561	6.012086	5.999147
H	3.766982	7.092144	6.095314
C	3.702121	5.215474	7.117909
H	3.896655	5.669286	8.091124
C	3.537300	3.850214	7.024796
H	3.628531	3.225240	7.916965
C	3.322097	3.255398	5.784558
C	3.172337	6.254173	3.499865
H	2.104144	6.516778	3.388019
H	3.748609	7.196269	3.505623
C	3.252234	1.779432	5.481080
H	4.220911	1.442653	5.067877
H	2.997327	1.164221	6.359286
C	5.021566	5.389276	2.218644
H	5.426751	4.862812	3.094295
H	5.401545	6.428419	2.214990
C	5.421209	4.683112	0.950961
H	6.513225	4.707111	0.840278
H	5.130709	3.615987	0.970809
C	3.467012	5.297721	–0.133625
H	3.088713	4.254243	–0.145146
H	3.088851	5.797340	–1.036936
C	2.998073	6.046130	1.094972
H	3.338251	7.097615	1.040730
H	1.898926	6.036325	1.165382
C	0.862322	1.662094	4.955369
H	0.729216	2.676389	5.364058
H	0.786572	0.944436	5.793382
C	–0.193763	1.335698	3.939028
H	–1.185729	1.316101	4.410307
H	–0.200043	2.075358	3.114832
C	1.335618	–0.072805	2.819808
H	1.407112	0.602806	1.942556
H	1.451470	–1.094794	2.439059
C	2.408439	0.217413	3.820403
H	2.363312	–0.519815	4.643262
H	3.400104	0.151693	3.345670
N	3.540587	5.443699	2.330117
N	2.235401	1.563381	4.402610
O	4.875426	5.325763	–0.194718
O	0.059642	0.019778	3.430623
Te	2.720250	3.254870	2.838250
Cl	8.038136	–1.799680	0.657717
Cl	6.300288	1.416295	3.035805
Cl	5.872721	1.309464	–0.937254

Hg	6.524345	–0.044991	1.167766
Cl	1.936271	1.788628	–0.654922
Cl	3.674120	–1.427346	–3.033010
Cl	4.101686	–1.320516	0.940049
Hg	3.450063	0.033939	–1.164972