ELECTRONIC SUPPLEMENTARY INFORMATION

Charge-Displacement Analysis as a Tool to Study Chalcogen Bonded Adducts and Predict their Association Constants in Solution†

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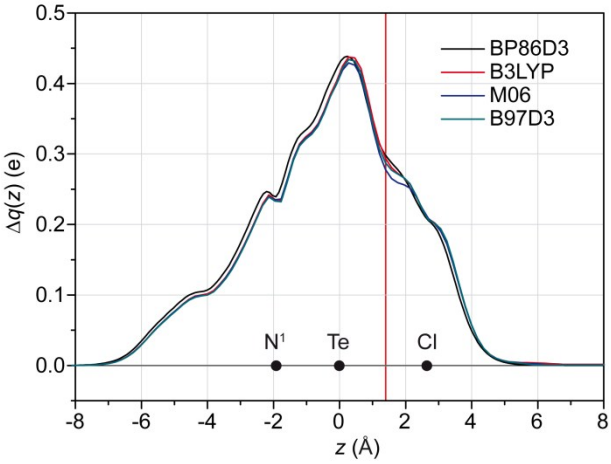

Figure S1. Charge Displacement function for **3a**Cl calculated with different XC functionals. The black dots represent the *z* coordinate of the atoms. The red vertical line identifies a suitable boundary between the two fragments.

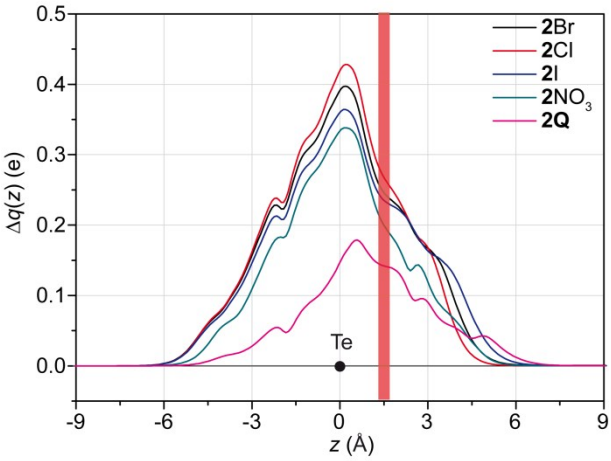

Figure S2. Charge Displacement function for the **2X** adducts. The black dot represent the *z* coordinate of the tellurium, always placed at the origin. The red vertical band identifies the range of the inter-fragment boundaries.

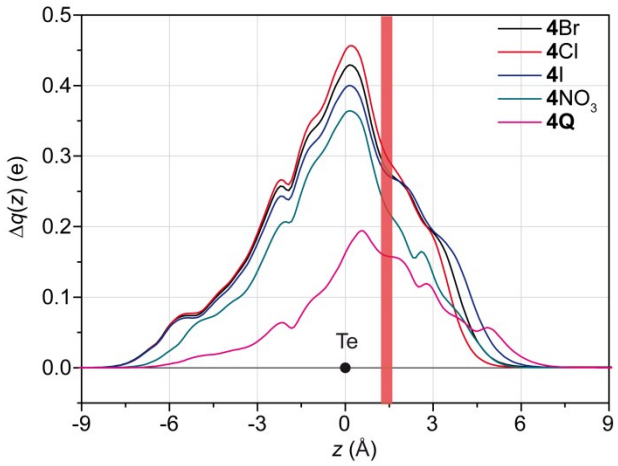

Figure S3. Charge Displacement function for the **4X** adducts. The black dot represent the *z* coordinate of the tellurium, always placed at the origin. The red vertical band identifies the range of the inter-fragment boundaries.

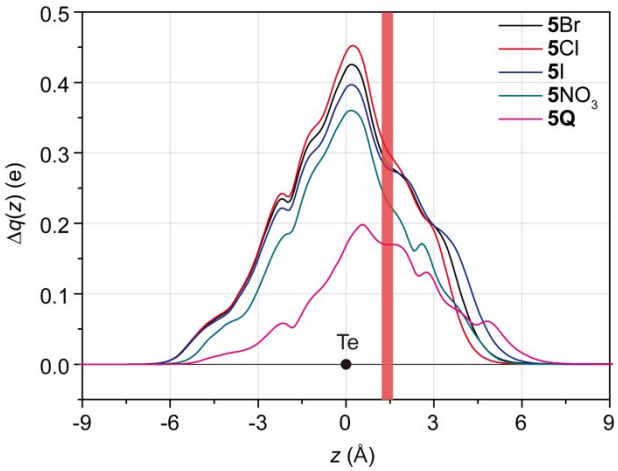

Figure S4. Charge Displacement function for the **5X** adducts. The black dot represent the *z* coordinate of the tellurium, always placed at the origin. The red vertical band identifies the range of the inter-fragment boundaries.

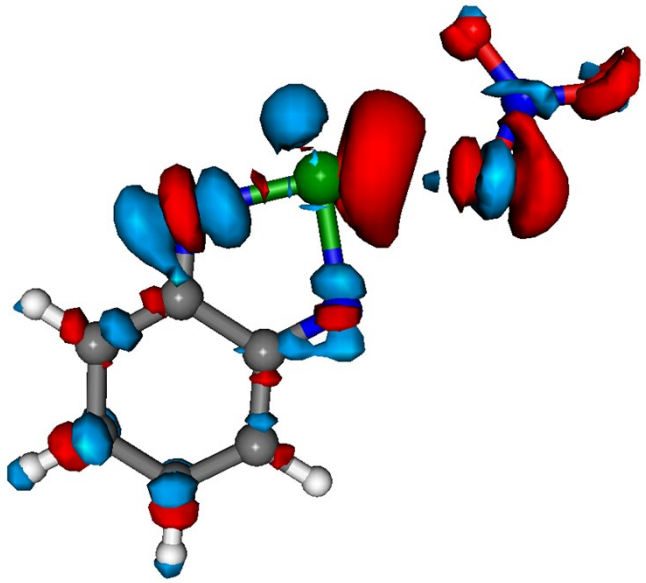

Figure S5. 3D contour plot of the change of electronic density upon formation of the adduct **2**NO_3. Blue (red) isosurfaces identify regions in which the electron density increases (decreases). Density value at the isosurfaces: ±0.002 au.

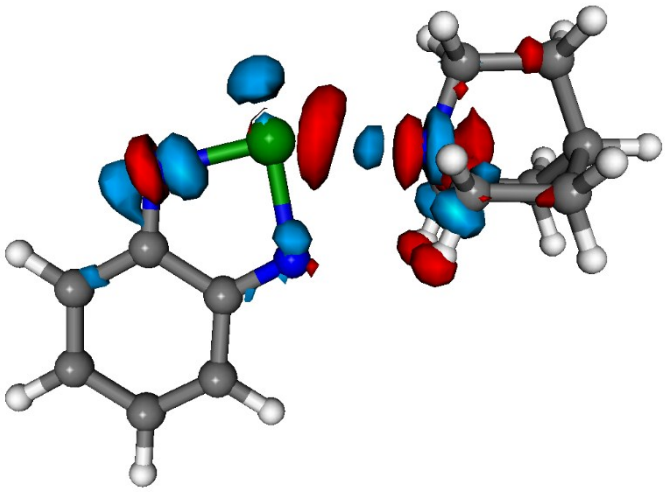

Figure S6. 3D contour plot of the change of electronic density upon formation of the adduct **2Q**. Blue (red) isosurfaces identify regions in which the electron density increases (decreases). Density value at the isosurfaces: ±0.002 au.

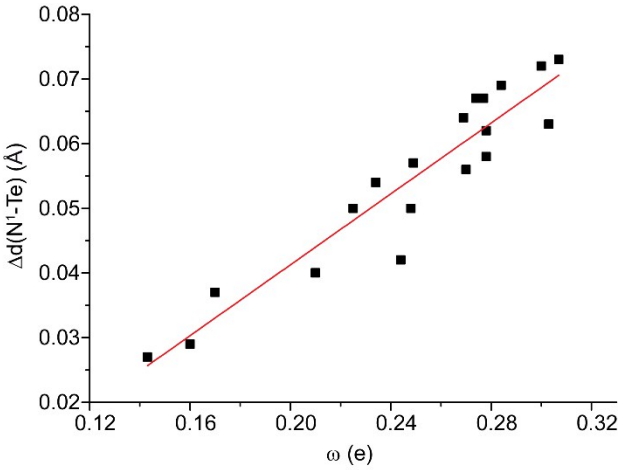

Figure S7. Linear correlation between ω and the lengthening of N^1-Te for the **2-5X** adducts ($r^2 = 0.8889$). Adduct **3aQ** has been excluded from the fitting procedure since its value of ω is affected not only by the Te···X interaction (see main text).

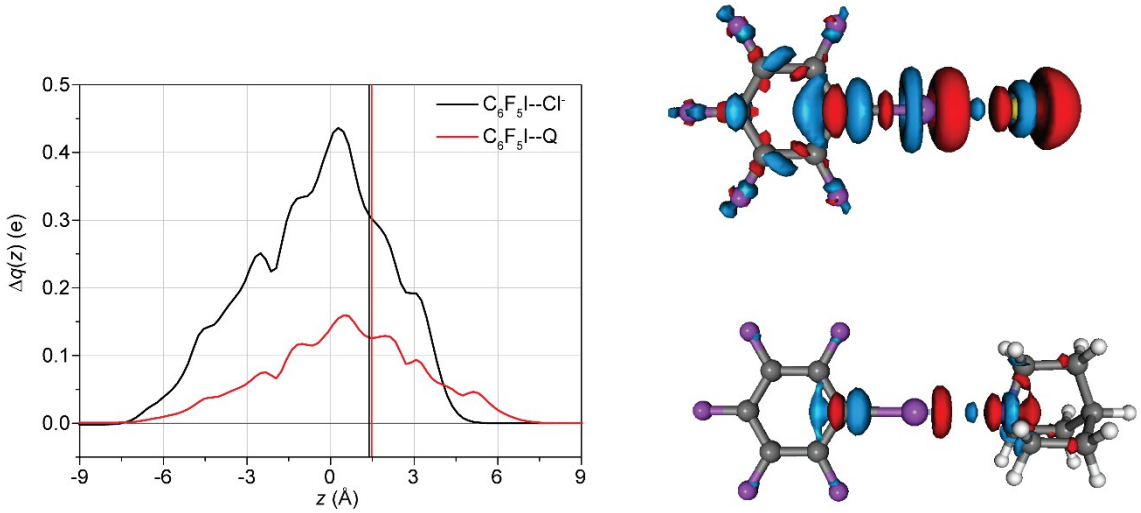

Figure S8. Charge Displacement functions for the $IC_6F_5\cdots Cl^-$ and $IC_6F_5\cdots$**Q** adducts. The iodine is always placed at the origin, while the anion is always placed on the +*z* semiaxis. The black and red vertical lines identify the inter-fragment boundaries for $IC_6F_5\cdots Cl^-$ and $IC_6F_5\cdots$**Q**, respectively. Aside are shown the 3D contour plots of the change of electronic density upon formation of the adduct for $IC_6F_5\cdots Cl^-$ (top) and $IC_6F_5\cdots$**Q** (down), respectively. Blue (red) isosurfaces identify regions in which the electron density increases (decreases). Density value at the isosurfaces: ±0.002 au.

Table S1. List of ω and q_H values, in electrons, for all the compounds studied.

Compound	ω (e)	q_H [a]	Compound	ω (e)	q_H [a]
2Br	0.249	-0.250	**3a**Br	0.277	-0.288
2Cl	0.278	-0.276	**3a**Cl	0.300	-0.306
2I	0.234	-0.241	**3a**I	0.269	-0.281
2NO_3	0.210	-0.217	**3a**NO_3	0.225	-0.230
2Q	0.143	-0.143	**3aQ**	0.141	-0.163
4Br	0.278	-0.284	**5**Br	0.284	-0.287
4Cl	0.303	-0.302	**5**Cl	0.307	-0.305
4I	0.270	-0.278	**5**I	0.274	-0.283
4NO_3	0.244	-0.240	**5**NO_3	0.248	-0.247
4Q	0.160	-0.160	**5Q**	0.170	-0.172
6aSPh	0.376	-0.370	**6b**SPh	0.330	-0.336

[a] q_H is the charge of the telluradiazole as computed by the Hirshfeld charge analysis.

XYZ Coordinates of optimized compounds (B97D3/def2-TZVP/ECP on I)

$C_6F_5I\cdots Cl^-$

Cl	0.0000	-0.0000	-2.7570
I	0.0000	0.0000	0.0000
C	0.0000	0.0001	2.2732
C	0.0000	0.0002	5.1071
C	0.0003	-1.1848	3.0063
C	-0.0003	1.1850	3.0062
C	-0.0003	1.2063	4.4039
C	0.0003	-1.2059	4.4041
F	0.0006	-2.3875	2.3807
F	0.0006	-2.3729	5.0927
F	-0.0006	2.3734	5.0925
F	-0.0006	2.3877	2.3805
F	0.0000	0.0003	6.4587

$C_6F_5I\cdots Q$

I	0.0000	0.0000	0.0000
C	-0.0074	0.0070	2.1631
C	-0.0246	0.0174	4.9846
C	-0.0153	-1.1858	2.8901
C	-0.0080	1.2052	2.8814
C	-0.0166	1.2236	4.2792
C	-0.0239	-1.1939	4.2881
F	-0.0155	-2.3767	2.2609
F	-0.0317	-2.3522	4.9680
F	-0.0173	2.3868	4.9506
F	-0.0009	2.3914	2.2435
F	-0.0330	0.0224	6.3248
N	0.0000	-0.0000	-2.7594
C	0.2042	1.3837	-3.2453
C	-1.3004	-0.5127	-3.2455
C	-1.3465	-0.5356	-4.8091
C	0.2066	1.4357	-4.8091
C	-0.0016	0.0017	-5.3402
H	-0.0023	0.0024	-6.4362
H	1.1542	1.7397	-2.8308
H	-1.4356	-1.5158	-2.8255
H	-2.1705	0.0871	-5.1798
H	-0.5959	2.0890	-5.1743
H	-0.5984	1.9995	-2.8239
H	-2.0814	0.1341	-2.8300
H	-1.5109	-1.5571	-5.1751
H	1.1582	1.8366	-5.1801
C	1.1374	-0.8940	-4.8110
H	2.1033	-0.5232	-5.1768
H	1.0110	-1.9185	-5.1831
C	1.0952	-0.8680	-3.2473
H	0.9287	-1.8694	-2.8344
H	2.0305	-0.4818	-2.8265