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Supporting Information

Chalcogen-bonded donor-acceptor complexes of 5,6-dicyano-[1,2,5]selenadiazolo[3,4-*b*]pyrazine with halide ions

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Contents

- 1 UV/Vis spectroscopy and titrations
- 2 XRD data
- 3 ⁷⁷Se NMR data
- 4 ESI-MS data
- 5 DFT data
- 6 References

Reaction $1 + Cl^{-} \leftrightarrow [1-Cl]^{-}$ in THF



Figure S1. Left: UV/Vis spectrum of 1 in THF (C = 5.1×10^{-5} M) and its changes upon addition of $[Bu_4N]^+[Cl]^-$ in the concentration range 4.04×10^{-5} –0.0097 M. Right: Concentration dependence of the optical density at 436 nm (circles) and its best fit with the following parameters: $K_{eq} = (1.05 \pm 0.12) \times 10^3$ L·mol⁻¹ and ϵ (436 nm) = $(1.20 \pm 0.02) \times 10^4$ M⁻¹cm⁻¹.

Reaction 1 +Br⁻ \leftrightarrow [1–Br]⁻ in THF



Figure S2. Left: UV/Vis spectrum of 1 in THF (C = = 1.77×10^{-5} M) and its changes upon addition of $[Bu_4N]^+[Br]^-$ in the concentration range $2.4 \times 10^{-4} - 0.0124$ M. Right: Concentration dependence of the optical density at 496 nm (circles) and its best fit with the following parameters: $K_{eq} = 420 \pm 30 \text{ L} \cdot \text{mol}^{-1}$ and ϵ (496 nm) = $(1.40 \pm 0.03) \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$.



Figure S3. Left: UV/Vis spectrum of 1 in MeCN (C = 1.50×10^{-5} M) and its changes upon addition of $[Et_4N]^+[Br]^-$ in the concentration range 0.004 – 0.078 M. Right: Concentration dependence of the optical density at 488 nm (circles) and its best fit with the following parameters: $K_{eq} = 15.1 \pm 1.0 \text{ L} \cdot \text{mol}^{-1}$ and ϵ (488 nm) = $(0.93 \pm 0.04) \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$.

Comparison of solution and solid-state UV/Vis spectra



a) UV/Vis spectrum of **1** in MeCN (red) and in a mixture with BaSO₄ (black)



b) UV/Vis spectrum of [1–Cl][–] in MeCN (red) and in a mixture with BaSO₄ (black)



c) UV/Vis spectra of 1 (black) and [1–Cl]⁻ (calculated from its accumulation curve for the upmost; red) in MeCN



d) UV/Vis spectrum in the form of Kubelka-Munk function of 1 (red) and [1-Cl]⁻ (black) as a mixture with BaSO₄

of Kubelka-Munk function of 1 (red) and $[1-Br]^-$ (black) as a mixture with BaSO₄

e) UV/Vis spectrum in the form f) UV/Vis spectrum in the form of Kubelka-Munk function of 1 (red) and $[1-I]^-$ (black) as a mixture with BaSO₄

Figure S4. A comparison of UV/Vis spectra of 1 and [1-X]- (X = Cl, Br, I) in solution and the solid state (BaSO₄ matrix) obtained from diffuse reflectance spectra of polycrystalline samples with Kubelka-Munk function.



Figure S5. UV/Vis spectra: A: 1 MeCN (solid line) and THF (dashed line). B: [1-Cl]⁻ in MeCN (solid line) and THF (dashed line). C): [1-Br]- in MeCN (solid line) and THF (dashed line). The spectra and extinction coefficients for $[1-X]^-$ (X = Cl, Br, I) were calculated from titration curves assuming the absence of side reactions.

2. XRD data

Compound	$[Et_4N]^+$ [1–Cl]-·thf	$[Et_4N]^+[1-Br]^- \cdot 0.5Et_2O$	$[Et_4N]^+[1-I]^-\cdot 0.5Et_2O$	[K(18-c-6)] ⁺ [1–Br] ⁻
Empirical formula	C ₁₈ H ₂₈ ClN ₇ OSe	C ₁₆ H ₂₅ BrN ₇ O _{0.5} Se	C ₃₂ H ₅₀ I ₂ N ₁₄ OSe ₂	C ₁₈ H ₂₄ BrKN ₆ O ₆ Se
Formula weight	472.88	482.30	1058.58	618.40
Temperature/K	200.01	296.15	296.15	173(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	C2/c	C2/c	P-1
a/Å	7.0780(3)	16.5590(7)	16.8201(8)	7.5052(5)
b/Å	15.0011(8)	19.9679(9)	20.0393(11)	10.9758(8)
c/Å	21.4924(11)	13.5371(7)	13.7957(8)	16.5976(17)
α/°	90	90	90	106.379(7)
β/°	91.892(2)	112.668(2)	112.564(2)	92.267(8)
$\gamma^{/\circ}$	90	90	90	104.840(7)
Volume/Å ³	2280.77(19)	4130.3(3)	4294.1(4)	1258.75(19)
Ζ	4	8	4	2
$\rho_{calc}g/cm^3$	1.377	1.551	1.637	1.632
µ/mm ⁻¹	1.786	3.770	3.203	3.288
F(000)	976.0	1944.0	2088.0	620.0
Crystal size/mm ³	$0.392 \times 0.314 \times 0.142$	$0.8\times0.6\times0.4$	$0.793 \times 0.102 \times 0.1$	$0.58 \times 0.43 \times 0.25$
Radiation	MoKa ($\lambda = 0.71073$)	MoKa ($\lambda = 0.71073$)	MoKa ($\lambda = 0.71073$)	MoKa ($\lambda = 0.71073$)
2θ range for data collection/°	4.664 to 62.564	5.224 to 55.014	4.066 to 52.038	5.498 to 51.08
Index ranges	$-8 \le h \le 10, -20 \le k$ $< 21, -31 \le 1 \le 30$	$-20 \le h \le 21, -24 \le k \le$ 25 $-17 \le 1 \le 17$	$-20 \le h \le 20, -24 \le k$ $< 24, -16 \le 1 \le 17$	$-9 \le h \le 9, -13 \le k \le$ 13 $-20 \le 1 \le 19$
Reflections collected	50168	37529	23349	10614
Independent	$6518 [R_{int} = 0.0486,$	$4718 [R_{int} = 0.0491, R_{\sigma} =$	$4210 [R_{int} = 0.0441,$	$4522 [R_{int} = 0.0246,$
reflections	$R_{\sigma} = 0.0282$]	0.0321]	$R_{\sigma} = 0.0283$]	$R_{\sigma} = 0.032$]
Data/restr./param.	6518/18/266	4718/0/237	4210/0/237	4522/0/301
Goodness-of-fit on F^2	1.062	1.052	1.074	1.027
Final R indexes $[I \ge$	$R_1 = 0.0316, wR_2 =$	$R_1 = 0.0284, wR_2 =$	$R_1 = 0.0400, wR_2 =$	$R_1 = 0.0226, wR_2 =$
2σ (I)]	0.0856	0.0606	0.1007	0.0570
Final R indexes [all	$R_1 = 0.0451, WR_2 = 0.0050$	$R_1 = 0.0589, WR_2 = 0.0731$	$R_1 = 0.05/3, WR_2 = 0.1183$	$R_1 = 0.0310, WR_2 = 0.0504$
Largest diff	0.68/0.55	0.0751	0.1105	0.0394
peak/hole / e Å ⁻³		0.55/-0.55	1.25/-0.85	0.34/-0.41
ĊCDC	216813 6	2168137	2168138	2168139

 Table S1 Crystallographic data of compounds synthesized

Compound	[K(18-c-6)] ⁺ [1 –I] ⁻	$[Ph_4P]^+[1-C1]^-$	$[BnNMe_3]^+[1-Br]^-$	$[Et_4N]^+[1_2-Cl]^-$
Empirical formula	C ₁₈ H ₂₄ IKN ₆ O ₆ Se	C ₃₀ H ₂₀ ClN ₆ PSe	C ₁₆ H ₁₆ BrN ₇ Se	C ₂₀ H ₂₀ ClN ₁₃ Se ₂
Formula weight	665.39	609.90	465.23	635.86
Temperature/K	296.15	296.15	296.15	200.04
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	$P2_1/n$	P-1	P2 ₁	P-1
a/Å	7.8062(4)	6.9738(2)	9.8387(14)	9.8914(9)
b/Å	22.5996(14)	14.0802(6)	6.5947(7)	12.6394(10)
c/Å	14.9943(9)	14.7332(7)	14.4796(19)	22.800(2)
α/\circ	90	103.557(2)	90	92.513(3)
β/°	102.719(2)	94.675(2)	92.018(5)	94.141(3)
γ/°	90	93.3900(10)	90	111.522(3)
Volume/Å ³	2580.3(3)	1397.12(10)	938.9(2)	2637.2(4)
Z	4	2	2	4
$\rho_{calc}g/cm^3$	1.713	1.450	1.646	1.601
μ/mm^{-1}	2.856	1.528	4.141	2.942
F(000)	1312.0	616.0	460.0	1264.0
Crystal size/mm ³	$0.9\times0.45\times0.3$	$0.8 \times 0.3 \times 0.12$	$0.6 \times 0.17 \times 0.03$	$0.1\times0.1\times0.05$
Radiation	MoK α ($\lambda = 0.71073$)	MoKa ($\lambda = 0.71073$)	MoKa ($\lambda = 0.71073$)	MoK α ($\lambda = 0.71073$)
20 range for data collection/°	4.556 to 55.038	4.602 to 59.244	4.926 to 55.178	4.03 to 53.616
Index ranges	$-10 \le h \le 8, -29 \le k \le$ 29, -19 $\le l \le 19$	$-8 \le h \le 9, -19 \le k \le$ 18, -20 $\le 1 \le 20$	$-9 \le h \le 12, -7 \le k \le 8, -18 \le 1 \le 18$	$-12 \le h \le 12, -16 \le k$ $\le 15, -28 \le 1 \le 28$
Reflections collected	34295	26226	9256	36951
Independent	5915 [$R_{int} = 0.0437, R_{\sigma}$	6573 [R _{int} = 0.0291,	$3864 [R_{int} = 0.0340,$	11155 [$R_{int} = 0.0663$,
reflections	= 0.0400]	$R_{\sigma} = 0.0298$]	$R_{\sigma} = 0.0508$]	$R_{\sigma} = 0.0720$]
Data/restr./param.	5915/0/298	6573/0/352	3864/1/227	11155/0/657
Goodness-of-fit on F^2	1.068	1.024	1.034	1.000
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0360, wR_2 = 0.0690$	$R_1 = 0.0362, wR_2 = 0.0872$	$R_1 = 0.0309, wR_2 = 0.0626$	$R_1 = 0.0397, wR_2 = 0.0893$
Final R indexes [all data]	$R_1 = 0.0678, wR_2 = 0.0813$	$R_1 = 0.0613, wR_2 = 0.1000$	$R_1 = 0.0560, wR_2 = 0.0691$	$R_1 = 0.0688, wR_2 = 0.1007$
Largest diff. peak/hole / e Å ⁻³	0.44/-0.59	0.59/-0.43	0.45/-0.51	0.47/-0.66
CCDC	2168140	2168141	2168142	2168143

Table S1 (continued)



Figure S6. Packing of $[Et_4N]^+[1_2-Cl]^-$ salt.



Figure S7. Fragments of packing of $[Et_4N]^+[1_2-Cl]^-$ depicting two surroundings of Cl atoms in the lattice, featuring tetrafurcate and pentafurcate chalcogen bonding.

Figure S8. ⁷⁷Se NMR spectrum of 1 in MeCN-d₃



Figure S9. ⁷⁷Se NMR spectrum of 1 in the saturated solution of $[Bu_4N]^+[Cl]^-$ in MeCN-d₃



Figure S10. ⁷⁷Se NMR spectrum of 1 in the saturated solution of $[Bu_4N]^+[Br]^-$ in MeCN-d₃



Figure S11. Experimental (for $\sim 6 \times 10^{-2}$ M solution of **1** in MeCN saturated with [Ph₄P]⁺[Cl]⁻; above) and calculated (below) ESI-MS spectra of [1–Cl]⁻; m/z, found / calcd. for C₆³⁵ClN₆⁸⁰Se: 270.904 / 270.904.



Figure S12. Experimental (for $\sim 6 \times 10^{-2}$ M solution of 1 in MeCN saturated with $[Bu_4N]^+[Br]^-$; above) and calculated (below) ESI-MS spectra of $[1-Br]^-$; m/z, found / calcd. for $C_6^{79}BrN_6^{80}Se$: 314.855 / 314.853.



Figure S13. Experimental (for ~6×10⁻² M solution of 1 in MeCN saturated with $[Bu_4N]^+[I]^-$; above) and calculated (below) ESI-MS spectra of $[1-I]^-$; m/z, found / calcd. for $C_6^{127}IN_6^{80}Se$: 362.842 / 362.840.

5. DFT data

5.1 QTAIM (Quantum Theory of Atoms In Molecules) and NCI (Non-Covalent Interaction) analyzes.

The electronic density distribution for complexes $[1-C1]^-$, $[1-Br]^-$ and $[1-I]^-$ was calculated for the XRD geometries at the B97-D3/def2-tzvp level of theory. A very powerful wavefunction analysis program – Multiwfn,⁹ was used for topological analysis of electronic density distribution and creation of the corresponding images. Figure S14 shows the gradient line map with contour lines of the electronic density for three complexes under study. This figure also shows all BCPs and bond paths; topological descriptors were calculated for BCPs lying on the Se–X⁻ bond paths.



Figure S14. Gradient line maps with contour lines of ρ on molecular plane for complexes [1–Cl]⁻ (a), [1–Br]⁻ (b) and [1–I]⁻ (c) plotted by Multiwfn program. Blue points correspond to BCPs, blue lines represent interbasin paths, brown lines represent bond paths.

For a more detailed understanding of the nature of Se_X^- bonding interactions, the reduced density gradients (RDGs(r)) were calculated and the regions of weak interactions were distinguished

$$RDG(r) = \frac{|\nabla \rho(r)|}{2(3\pi^2)^{1/3} \rho(r)^{4/3}}$$

Color-filled RDG maps were built using Multiwfn and VMD¹⁰ programs (Figure S15) and show that all complexes under study have four regions of non-covalent interactions: two regions of strong repulsion in the middle of the rings (filled by red), one region of weak repulsion between carbon atoms of CN-groups (filled by brown) and the most interesting for us blue or green discs between Se and halide. The green color of RDG isosurfaces in complexes with Br⁻ and I⁻ corresponds to very low ρ and the dominance of Van der Waals (or electrostatic) interactions. The blue color of RDG isosurface in the case of complex with Cl⁻ indicates much stronger attractive interaction. These findings fully agree with the previous data (Table 2) for Se–X⁻ bonds: the orbital contribution to the energy of the Se–Cl bond is sufficiently higher than for two other bonds, and the electron density at the BCP for Se–Cl bond is also noticeably higher.



Figure S15. The colour-filled reduced density gradient (RDG) maps (isosurface with RDG=0.5) for noncovalent interactions (NCI) in the complexes of **1** with halide ions.

To estimate the energy difference between the optimized and flat structures of complex $[1-Br]^-$, we, in addition to a full optimization, performed also a partial optimization with a fixed dihedral $\angle Br1-Se2-N4-C10$ angle, the same angle was chosen as in XRD structure.



In the case of the bromide complex, the difference between single-point energies of partially and fully optimized structures at the B97-D3/def2-tzvp level in the gas phase and in THF solution was calculated and found to be 5.04 and 2.53 kcal·mol⁻¹, respectively. Similar value (4.75 kcal·mol⁻¹) was predicted at the ω B97M-D3BJ/def2-tzvp level in the gas phase.

Table S2 Gas-phase calculated and experimental $E-X^-$ bond distances (r, Å) and $N-E-X^-$ bond angles (\angle, \circ) and the sums of covalent $(\sum r_{cov}^{i})^{1,2}$ and van-der-Waals $(\sum r_{VdW}^{i})^{3,4}$ radii of atoms E and X (E = Se, Te; X = S, F, Cl, Br, I). Experimental and computational data for $[1-X]^-$ are from this paper, Experimental and computational data for $[2-X]^-$ are from Refs^{5,6,7}. For complex $[3-X]^-$ experimental results are from Refs⁸ and computational data from Ref.^{5,6}

		N N N N Se [1-X] [−]	, x]		e X	NC N NC N [3 -X] ⁻	-
Compound	B97-D3/ r(E–X ⁻)	/def2-tzvp ∠N–E–X ⁻	r(E–X ⁻)	XRD ∠N–E–X ⁻	$\sum_{\substack{r_{EX}^{calc} - \sum_{j} r_{cov}^{i}}} r_{cov}^{i}$	$\frac{\sum_{v_{dW}}^{i} r_{v_{dW}}^{i}}{\sum_{v_{dW}}^{i} r_{v_{dW}}^{calc} - r_{Ex}^{calc}}$	$r_{EX/}^{calc} \sum r_{VdW}^{i}$
[2 –SPh] [–]	2.738 2.741 ^a	166.2 165.6 ^a	2.688	166.0	2.37 (0.37)	3.86 (1.12)	0.71
[3 –SPh] [–]	2.683	176.1	2.722	175.2	2.18 (0.50)	3.70 (1.02)	0.73
[2 −F] [−]	2.080	167.5	2.132	164.5	2.06 (0.02)	3.53 (1.4)	0.59
[3 −F] [−]	1.989	175.2	_	_	1.87 (0.12)	3.37 (1.38)	0.59
[1 –F] [–]	1.937	103.0	-	-	1.87 (0.07)	3.37 (1.43)	0.57
[2 -Cl] ⁻	2.651	170.2	2.859^{b}	172.4^{b}	2.34 (0.31)	3.81 (1.16)	0.70
[3 −Cl] ⁻	2.609	178.7	2.893 – 3.089	173.8 – 177.0	2.15 (0.46)	3.65 (1.04)	0.72
[1 -Cl] ⁻	2.586	106.4	2.980^{b} 2.964^{c}	175.6 ^b 172.2 ^c	2.01 (0.50)	3.55 (0.96)	0.73
[2 –Br] [–]	2.854	170.9	$2.982 - 3.110^d$	165.1 – 167.9 ^d	2.49 (0.36)	3.91 (1.06)	0.73
[3 −Br] ⁻	2.817	179.9	3.123, 3.223	178.8, 168.8	2.30 (0.52)	3.75 (0.93)	0.75
[1–Br] [–]	2.816, 2.794 ^e	108.0 107.3 ^e	3.327	167.6	2.30 (0.52)	3.75 (0.93)	0.75
[2 –I] [–]	3.095	171.0	3.391	172.4	2.68 (0.42)	4.04 (0.96)	0.77
[3 –I] [–]	3.084	179.7	3.355	174.2	2.49 (0.59)	3.88 (0.80)	0.79
[1 –I] [–]	3.073	108.4	3.586	166.3	2.49 (0.58)	3.88 (0.27)	0.81

^{*a*} DKH2 Hamiltonian. ^{*b*} [Et₄N]⁺ salt. ^{*c*} [PPh₄]⁺ salt.^{*d*} Two polymorphs. ^{*e*} Optimization was performed with *Gaussian16* suite of programs.

5.2 TD-DFT calculations of the UV-Vis spectra of anionic complex [1-Br]⁻ with different geometries: experimental XRD geometry and geometry optimized at the ωB97M-D3BJ/def2-TZVP level.

In the experimental geometry of the $[1-Br]^-$ anionic complex, the Br–Se–N angle is close to 180° (167.8°) and the Br atom is almost in the plane of the heterocycle. In the optimized geometry, the Br–Se–N angle is close to 90° (106°) and is almost in the plane perpendicular to the heterocycle plane. Calculation demonstrates that the electronic structures of $[1-Br]^-$ in these geometries are qualitatively different. For the experimental geometry, the LUMO is localized exclusively on the heterocycle and coincides with LUMO of **1**. At the same time, the three highest occupied MOs are practically degenerate and localized on the Br atom and are mainly its 4p-AOs. The situation is different in the case of optimized geometry. Both HOMO

and LUMO are delocalized over the entire complex and consist mainly of HOMO or LUMO of 1 and 4p-AO of the Br atom. In turn, HOMO-1 and HOMO-2 are practically degenerate and localized on the Br atom. As described in the main text, calculations with the experimental geometry reproduce the solid-state spectrum well, given that, as in case of 1 (transition c), the energy of the transition labeled i is significantly overestimated.



Figure S16. Experimental electronic absorption spectrum of $[1-Br]^-$ in acetonitrile (red spectrum) and its solid-state counterpart (black spectrum) in the form of Kubelka-Munk function. Vertical bars indicate the positions and oscillator strengths (f) of the electronic transitions calculated at the TD-M06-HF/def2-TZVP level of theory. Red bars represent the calculations with experimental geometry, blue bars represent the calculations with geometry optimized at the ω B97M-D3BJ/def2-TZVP level. Marks d – k indicate the electron promotions (see Fig. S17), which made the main contribution to the marked electronic transitions.



Figure S17. Diagrams of molecular orbitals calculated at the M06-HF/def2-TZVP level for heterocycle 1 (left), its anionic complex with Br⁻ with XRD geometry ($[1-Br]^-$, middle) and the same complex with geometry optimized at the ω B97M-D3BJ/def2-TZVP level (right), and electron promotions induced by UV and visible light excitations calculated by the TD–M06-HF/def2-TZVP method. Only one unoccupied (LUMO) orbital is present for 1 and its complex.

For the optimized geometry, a completely different spectrum was predicted, namely, only one intense band in the near UV and visible region (at about 400 nm) corresponding to the transition of electron from HOMO to LUMO. As mentioned above, both HOMO and LUMO are delocalized throughout the entire complex. Taking into account that the UV-Vis spectrum recorded for $[1-Br]^-$ in solutions is very close to the solid-state spectrum and consists of two bands, it can be assumed that the optimization of this complex has led to an incorrect structure. It should be expected that the $[1-Br]^-$ anionic complex in solutions has a geometry similar to that in the crystal, namely, with the Br atom lying almost in the plain of the heterocycle.

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