Electronic Supplementary Information to

Can Modified DNA Base Pairs with Chalcogen Bonding Expand the Genetic Alphabet? A Combined Quantum Chemical and Molecular Dynamics Simulation Study

Karan Deep Sharma,[a,b] Preetleen Kathuria,[a] Stacey D. Wetmore*,[c] and Purshotam Sharma*,[a]

[a] Computational Biochemistry Laboratory, Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, 160014, India.

[b] Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, United States.

[c] Department of Chemistry and Biochemistry, University of Lethbridge, Alberta, T1K 3M4, Canada.

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Section S1. Trends in QM binding energies of the modified pairs.

a. G:C$_{XY}$ pairs. Our analysis reveals that the trend in chalcogen bond lengths of G:C$_{XY}$ pairs in the gas phase (i.e., G:C$_{SeF}$ < G:C$_{SeCl}$ < G:C$_{SeBr}$ < G:C$_{SF}$ < G:C$_{SCl}$ < G:C$_{SBr}$ (Figure 3)) inversely correlates with the gas-phase binding energies (i.e., G:C$_{SeF}$ > G:C$_{SeCl}$ > G:C$_{SeBr}$ > G:C$_{SF}$ > G:C$_{SCl}$ > G:C$_{SBr}$, Figures 3 and 7). Thus, Se-containing pairs possess enhanced binding energies and form shorter chalcogen bonds compared to S-containing pairs, which occurs mainly due to greater polarizability and a more prominent σ hole on Se compared to S. Further, the reduction in chalcogen bond length and increase in the gas-phase binding energy directly align with an increase in the electronegativity of the halogen atom covalently bonded to the chalcogen. The binding energies are up to 55.0 kJ mol^{-1} less in water due to bulk solvent screening (Figure 3 and S6). Furthermore, the trend in the binding energies of G:C$_{SeY}$ and G:C$_{SY}$ pairs correlates with the magnitude of $V_{S,max}$ at the σ hole of the C$_{SeY}$ (i.e., C$_{SeF}$ > C$_{SeCl}$ > C$_{SeBr}$) and C$_{SY}$ (C$_{SF}$ > C$_{SCl}$ > C$_{SBr}$, Figure 2).

b. G$_{XY}$:C pairs. As observed for G:C$_{XY}$ pairs, the trend in chalcogen bond length in G$_{XY}$:C pairs (i.e., G$_{SeF}$:C < G$_{SeCl}$:C < G$_{SeBr}$:C < G$_{SF}$:C < G$_{SCl}$:C < G$_{SBr}$:C) inversely correlates with the binding energies (i.e., G$_{SeF}$:C > G$_{SeCl}$:C > G$_{SF}$:C > G$_{SeBr}$:C > G$_{SCl}$:C > G$_{SBr}$:C, Figures 4 and 7). However, the binding energies are reduced by up to 47.0 kJ mol^{-1} in water due to bulk solvent screening. Furthermore, the trend in the binding energies of G$_{SeY}$:C pairs correlates with the magnitude of $V_{S,max}$ at the σ hole of the G$_{SeY}$ nucleobase (i.e., G$_{SeF}$ > G$_{SeCl}$ > G$_{SeBr}$, Figures S4). However, this trend changes in G$_{SY}$:C pairs (i.e., G$_{SCl}$ > G$_{SBr}$ > G$_{SF}$), mainly because of the out-of-plane location of the SF group in the optimized structure of the G$_{SF}$ monomer (Figure S4).

c. A$_{XY}$:T pairs. The trend in the chalcogen bond lengths of A$_{XY}$:T pairs in the gas phase (i.e., A$_{SeF}$:T < A$_{SeCl}$:T < A$_{SeBr}$:T < A$_{SF}$:T < A$_{SBr}$:T < A$_{SCl}$:T, Figure 5) largely shows an inverse correlation with the binding energies (i.e., A$_{SeF}$:T > A$_{SeCl}$:T > A$_{SeBr}$:T > A$_{SF}$:T > A$_{SCl}$:T > A$_{SBr}$:T, Figures 5 and 7). Similarly, as observed for G:C$_{XY}$ and G$_{XY}$:C pairs, the binding energies are reduced by up to

15.4 kJ mol^{-1} in water due to bulk solvent screening. Furthermore, the trend in binding energy of A_{XY}:T pairs correlates with the magnitude of $V_{S,max}$ at the σ hole formed on the A_{SeY} (i.e., A_{SeF} > A_{SeCl} > A_{SeBr}) and A_{SY} (i.e., A_{SF} > A_{SCl}> A_{SBr}) nucleobases (Figure S5).

d. G_{XY}:$C_{X'Y'}$ pairs. Each of the six categories (i.e., G_{XY}:C_{SeF}, G_{XY}:C_{SeCl}, G_{XY}:C_{SeBr}, G_{XY}:C_{SF}, G_{XY}:C_{SCl} and G_{XY}:C_{SBr}) of these pairs are described below:

1. G_{XY}:C_{SeF} pairs. These pairs possess a common O6(G_{XY})···Se–F(C_{SeF}) chalcogen bond, that has similar structural characteristics in all G_{XY}:C_{SeF} pairs (i.e., chalcogen bond length or angle remain in the range of 2.305 ± 0.007 Å or 169.8 ± 0.4° in the gas-phase and 2.309 ± 0.036 Å or 168.3 ± 0.6° in water, Figures 6 and S14). However, the chalcogen bond lengths or angles of the variable (Y–X(G_{XY})···O2(C_{SeF})) chalcogen bond change with the identity of the G_{XY}:C_{SeF} pair (by up to 0.287 Å or 11.6° in the gas phase and 0.426 Å or 12.8° in water, Figures 6 and S14). Furthermore, the characteristics of the Y–X(G_{XY})···O2(C_{SeF}) chalcogen bond of G_{XY}:C_{SeF} significantly differ from the replaced N2–H(G)···O2(C) hydrogen bond of canonical G:C (i.e., bond lengths or angles differ by 0.731 Å – 1.018 Å or 12.1° – 23.7° in the gas-phase and by 0.632 – 1.058 Å or 12.0 – 21.3° in water, Figures 6, S1 and S14).

The (Y–X(G_{XY})···O2(C_{SeF})) chalcogen bond lengths of these pairs in the gas phase (i.e., G_{SeF}:C_{SeF} < G_{SeCl}:C_{SeF} < G_{SeBr}:C_{SeF} < G_{SF}:C_{SeF} < G_{SBr}:C_{SeF} < G_{SCl}:C_{SeF}, Figures 6) largely show an inverse correlation with the binding energies (i.e., G_{SeF}:C_{SeF} > G_{SeCl}:C_{SeF} > G_{SF}:C_{SeF} > G_{SeBr}:C_{SeF} > G_{SCl}:C_{SeF} > G_{SBr}:C_{SeF}, Figures 6). Similarly, as observed for G:C_{XY} and G_{XY}:C pairs, the binding energies are reduced by up to 40.1 kJ mol^{-1} in water due to bulk solvent screening. Our calculations further reveal that G_{XY}:C_{SeF} pairs possess 7.1 – 58.2 kJ mol^{-1} lower binding energy compared to canonical G:C in gas phase (Figures 6 and S1). However, in water, G_{XY}:C_{SeF} possesses 1.6 kJ mol^{-1} – 12.9 kJ mol^{-1} lower binding energy compared to canonical G:C, except G_{SeCl}:C_{SeF} and G_{SeF}:C_{SeF}, which possess 0.3 kJ mol^{-1} and 13.9 kJ mol^{-1} higher binding energy than G:C (Figures 6 and S14).

2. G_{XY}:C_{SeCl} pairs. These pairs possess a common O6(G_{XY})···Se–Cl(C_{SeCl}) chalcogen bond, which exhibits similar structural characteristics in all G_{XY}:C_{SeCl} pairs (i.e., chalcogen bond length or angle remain in the range 2.438 ± 0.009 Å or 162.2 ± 0.5° in the gas phase and 2.497 ± 0.050 Å or 160.5 ± 1.1° in water, Figures S9 and S15). However, the chalcogen bond lengths or angles of the variable (Y–X(G_{XY})···O2(C_{SeCl})) chalcogen bond change with the identity of the G_{XY}:C_{SeCl} pair (by up to 0.295 Å or 11.3° in the gas-phase and 0.422 Å or 12.8° in water, Figures S9 and S15). In addition, the characteristics of the Y–X(G_{XY})···O2(C_{SeCl}) chalcogen bond of G_{XY}:C_{SeCl} significantly differ from the replaced N2–H(G)···O2(C) hydrogen bond of canonical G:C (i.e., bond lengths or angles differ by 0.693 Å – 0.988 Å or 11.6° – 22.9° in the gas phase and by 0.587 Å – 1.009 Å or 11.4° – 24.2° in water, Figures S9 and S15).

The (Y–X(G_{XY})···O2(C_{SeCl})) chalcogen bond lengths in the gas phase (i.e., G_{SeF}:C_{SeCl} < G_{SeCl}:C_{SeCL} < G_{SeBr}:C_{SeCl} < G_{SF}:C_{SeCl} < G_{SBr}:C_{SeCl} < G_{SCl}:C_{SeCl}, Figures S9) largely show an inverse correlation with the binding energies (i.e., G_{SeF}:C_{SeCl} > G_{SeCl}:C_{SeCl} > G_{SeBr}:C_{SeCl} > G_{SF}:C_{SeCl} > G_{SCl}:C_{SeCl} > G_{SBr}:C_{SeCl} Figures S9). Similarly, as observed for G:C_{XY} and G_{XY}:C pairs, the binding energies are reduced by up to 39.6 kJ mol^{-1} in water due to bulk solvent screening.

3. G_{XY}:C_{SeBr} pairs. These pairs possess a common O6(G_{XY})···Se–Br(C_{SeBr}) chalcogen bond, which has similar structural characteristics in all G_{XY}:C_{SeBr} pairs (i.e., chalcogen bond length or angle remain 2.476 ± 0.009 Å or 160.8 ± 0.5° in the gas-phase and 2.579 ± 0.053 Å or 159.1 ± 0.5° in water, Figures S10 and S16). However, the chalcogen bond lengths or angles of the variable (Y–X(G_{XY})···O2(C_{SeBr})) chalcogen bond change with the identity of the G_{XY}:C_{SeBr} pair (up to 0.290 Å or 8.6° in the gas-phase and 0.416 Å or 12.7° in water, Figures S10 and S16). Furthermore, the characteristics of the Y–X(G_{XY})···O2(C_{SeBr}) chalcogen bond of G_{XY}:C_{SeBr} significantly differ from the replaced N2–H(G)···O2(C) hydrogen bond of canonical G:C (i.e., bond lengths or angles differ by 0.689 Å – 0.979 Å or 11.4° – 23.0° in the gas-phase and by 0.575 Å – 0.991 Å or 11.3° – 24.0° in water, Figures S1, S10 and S16).

The (Y–X(G_{XY})···O2(C_{SeBr})) chalcogen bond lengths in the gas phase (i.e., G_{SeF}:C_{SeBr} < G_{SeCl}:C_{SeBr} < G_{SeBr}:C_{SeBr} < G_{SF}:C_{SeBr} < G_{SBr}:C_{SeBr} < G_{SCl}:C_{SeBr}, Figures S10) largely show an inverse correlation with the binding energies (i.e., G_{SeF}:C_{SeBr} > G_{SeCl}:C_{SeBr} > G_{SeBr}:C_{SeBr} > G_{SF}:C_{SeBr} > G_{SCl}:C_{SeBr} > G_{SBr}:C_{SeBr}, Figures S10). Similarly, as observed for G:C_{XY} and G_{XY}:C pairs, the binding energies are reduced by up to 38.8 kJ mol^{-1} in water due to bulk solvent screening.

4. G_{XY}:C_{SF} pairs. These pairs possess a common O6(G_{XY})···S–F(C_{SF}) chalcogen bond that remains similar in all G_{XY}:C_{SF} pairs (i.e., chalcogen bond length or angle remain 2.539 ± 0.023 Å or 163.4 ± 1° in the gas phase and 2.735 ± 0.155 Å or 160.4 ± 0.6° in water, Figures S11 and S17). However, the chalcogen bond lengths or angles of the variable (Y–X(G_{XY})···O2(C_{SF})) chalcogen bond change with the identity of the G_{XY}:C_{SF} pair (up to 0.394 Å or 11.2° in the gas phase and 0.573 Å or 12.8° in water, Figures S11 and S17). Furthermore, the characteristics of the Y–X(G_{XY})···O2(C_{SF}) chalcogen bond of G_{XY}:C_{SF} significantly differ from the replaced N2–H(G)···O2(C) hydrogen bond of canonical G:C (i.e., bond lengths or angles differ by 0.733 Å – 1.127 Å or 12.2° – 23.4° in the gas-phase and by 0.585 Å – 1.158 Å or 11.6° – 24.6° in water, Figures S1, S11 and S17).

The (Y–X(G_{XY})···O2(C_{SF})) chalcogen bond lengths in the gas phase (i.e. G_{SeF}:C_{SF} < G_{SeCl}:C_{SF} < G_{SeBr}:C_{SF} < G_{SF}:C_{SF} < G_{SBr}:C_{SF} < G_{SCl}:C_{SF}, Figures S11) largely show an inverse correlation with the binding energies (i.e., G_{SeF}:C_{SF} > G_{SeCl}:C_{SF} > G_{SF}:C_{SF} > G_{SeBr}:C_{SF} > G_{SCl}:C_{SF} > G_{SBr}:C_{SF}, Figures S11). Similarly, as observed for the G:C_{XY} and G_{XY}:C pairs, the binding energies are reduced by up to 37.7 kJ mol^{-1} in water due to bulk solvent screening.

5. G_{XY}:C_{SCl} pairs. These pairs possess a common O6(G_{XY})···S–Cl(C_{SCl}) chalcogen bond that possesses similar structural characteristics in all G_{XY}:C_{SCl} pairs (i.e., chalcogen bond length or angle remain in the range 2.741 ± 0.017 Å or 152.0 ± 0.4° in the gas-phase and 2.979 ± 0.043 Å or 152.8 ± 0.6° in water, Figures S12 and S18). However, the chalcogen bond lengths or angles of the variable (Y–X(G_{XY})···O2(C_{SCl})) chalcogen bond change with the identity of the G_{XY}:C_{SCl} pair

(by up to 0.457 Å or 12.0° in the gas-phase and 0.438 Å or 12.5° in water, Figures S12 and S18). Furthermore, the characteristics of the Y–X(G_{XY})···O2(C_{SCl}) chalcogen bond of G_{XY}:C_{SCl} significantly differ from the replaced N2–H(G)···O2(C) hydrogen bond of canonical G:C (i.e., bond lengths or angles differ by 0.696 Å – 1.153 Å or 11.1° – 23.1° in the gas-phase and by 0.548 Å – 0.986 Å or 10.9° – 23.4° in water, Figures S1, S12 and S18).

The (Y–X(G_{XY})···O2(C_{SCl})) chalcogen bond lengths in the gas phase (i.e., G_{SeF}:C_{SCl} < G_{SeCl}:C_{SCl} < G_{SeBr}:C_{SCl} < G_{SF}:C_{SCl} < G_{SBr}:C_{SCl} < G_{SCl}:C_{SCl}, Figures S12) largely shows an inverse correlation with the binding energies (i.e., G_{SeF}:C_{SCl} > G_{SeCl}:C_{SCl} > G_{SF}:C_{SCl} > G_{SeBr}:C_{SCl} > G_{SCl}:C_{SCl} > G_{SBr}:C_{SCl}, Figures S12). Similarly, as observed for G:C_{XY} and G_{XY}:C pairs, the binding energies are reduced by up to 31.2 kJ mol^{-1} in water due to bulk solvent screening.

6. G_{XY}:C_{SBr} pairs. These pairs possess a common O6(G_{XY})···S–Br(C_{SBr}) chalcogen bond that possesses similar structural characteristics in all G_{XY}:C_{SBr} pairs (i.e., chalcogen bond length or angle remain 2.757 ± 0.032 Å or 155.2 ± 3.1° in the gas-phase and 2.923 ± 0.041 Å or 150.6 ± 0.6° in water, Figures S13 and S19). However, the chalcogen bond lengths or angles of the variable (Y–X(G_{XY})···O2(C_{SBr})) chalcogen bond change with the identity of the G_{XY}:C_{SBr} pair (by up to 0.320 Å or 11.4° in the gas-phase and 0.438 Å or 12.5° in water, Figures S13 and S19). Furthermore, the characteristics of the Y–X(G_{XY})···O2(C_{SBr}) chalcogen bond of G_{XY}:C_{SBr} significantly differ from the replaced N2–H(G)···O2(C) hydrogen bond of canonical G:C (i.e., bond lengths or angles differ by 0.690 Å – 1.010 Å or 12.2° – 23.0° in the gas phase and by 0.555 Å – 1.007 Å or 11.7° – 25.0° in water, Figures S1, S13 and S19).

The (Y–X(G_{XY})···O2(C_{SBr})) chalcogen bond lengths in the gas phase (i.e., G_{SeF}:C_{SBr} < G_{SeCl}:C_{SBr} < G_{SeBr}:C_{SBr} < G_{SF}:C_{SBr} < G_{SBr}:C_{SBr} < G_{SCl}:C_{SBr}, Figures S13) largely shows an inverse correlation with the binding energies (i.e., G_{SeF}:C_{SBr} > G_{SeCl}:C_{SBr} > G_{SF}:C_{SBr} > G_{SeBr}:C_{SBr} > G_{SCl}:C_{SBr} > G_{SBr}:C_{SBr}, Figures S13). Similarly, as observed for G:C_{XY} and G_{XY}:C pairs, the binding energies are reduced by up to 34.0 kJ mol^{-1} in water due to bulk solvent screening.

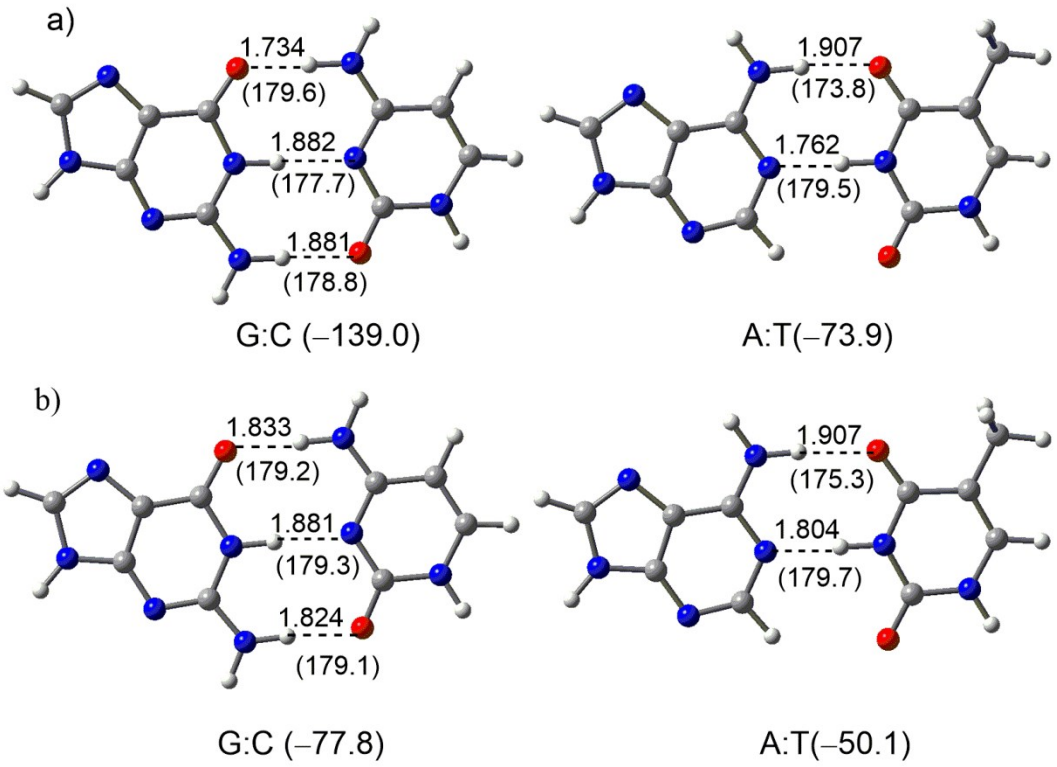

Figure S1. B3LYP-D3/6-31G(d,p) gas phase (a) or implicit solvent (water, b) optimized structures and B3LYP-D3/6-311+G(2df,p) or IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, in parentheses) for canonical G:C and A:T base pairs. Optimized hydrogen-bond distances (Å) and hydrogen-bond angles (deg., in parentheses) are shown.

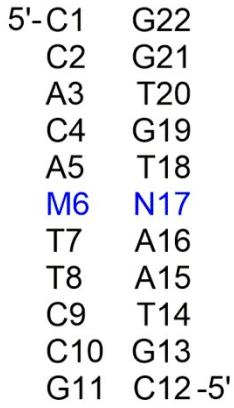

Figure S2. The 11-mer DNA sequence and numbering used in MD simulations, where the G:C_{XY} ,G_{XY}:C, G_{XY}:$C_{X'Y'}$ and A_{XY}:T (X= S, Se and Y= F, Cl, Br) modified base pairs were placed at the M:N position.

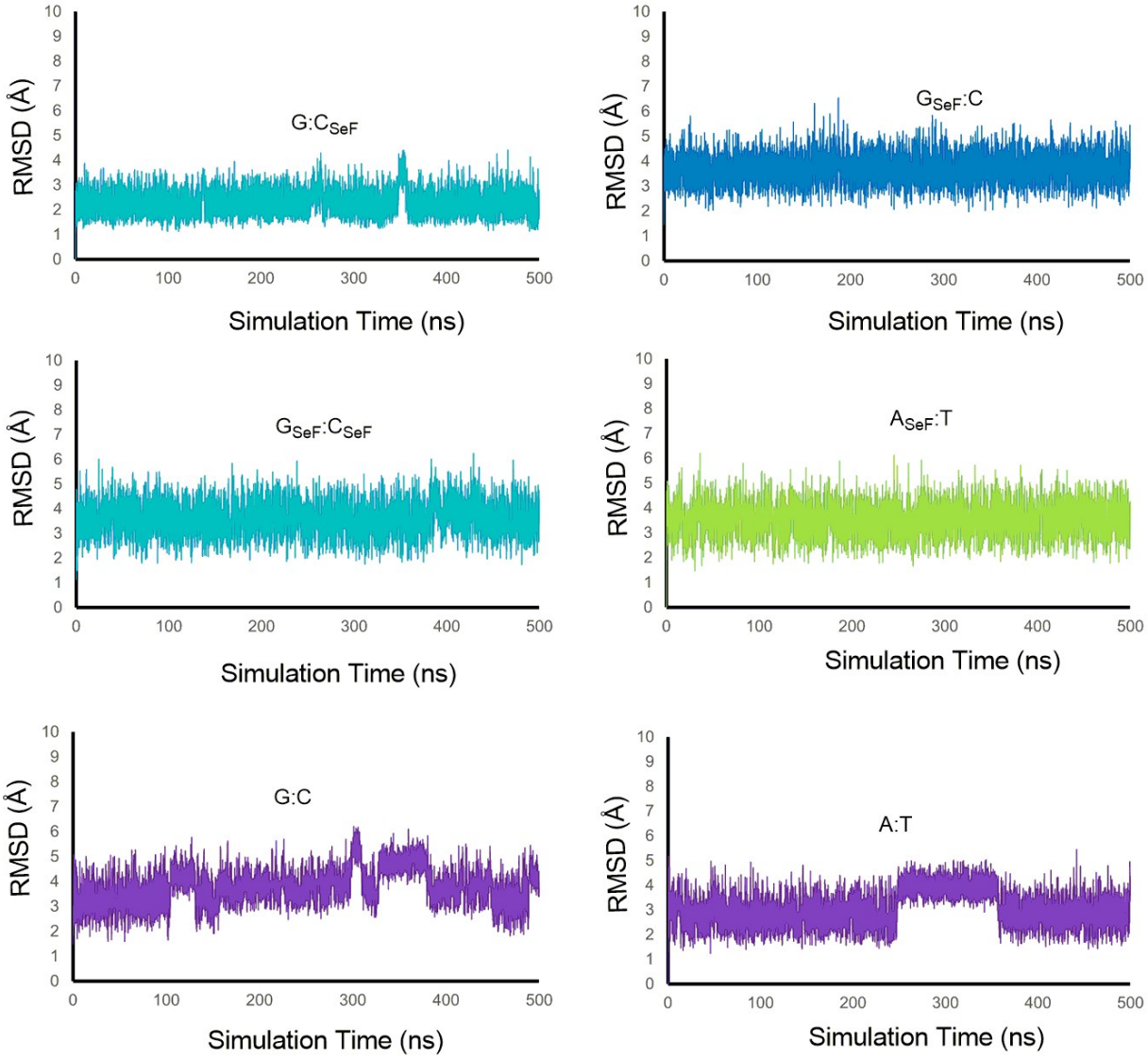

Figure S3. Plots of the backbone root-mean-square deviation (RMSD) with respect to the first production simulation frame versus time for DNA containing modified or canonical DNA base pairs during MD simulations.

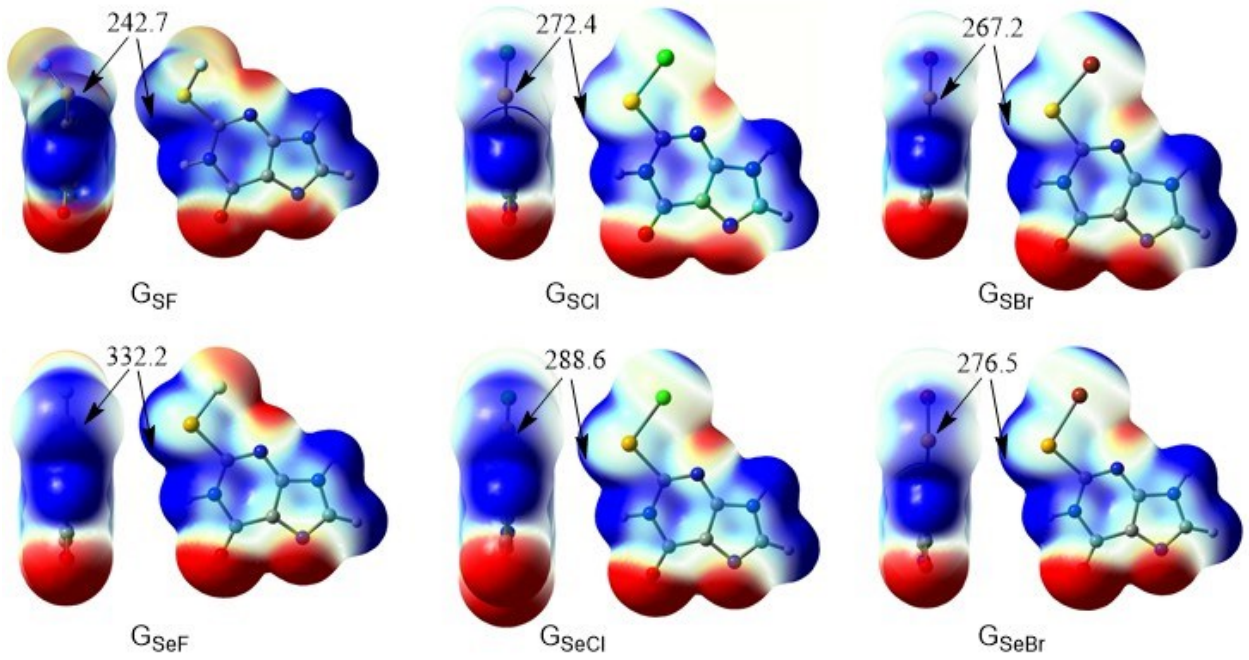

Figure S4. ESP maps on 0.002 electrons bohr^{-3} isodensity surfaces for the G_{XY} modified base (X= S, Se and Y= F, Cl, Br). Values of the maximum electrostatic potential at the σ hole are indicated ($V_{S,max}$, kJ mol^{-1}).

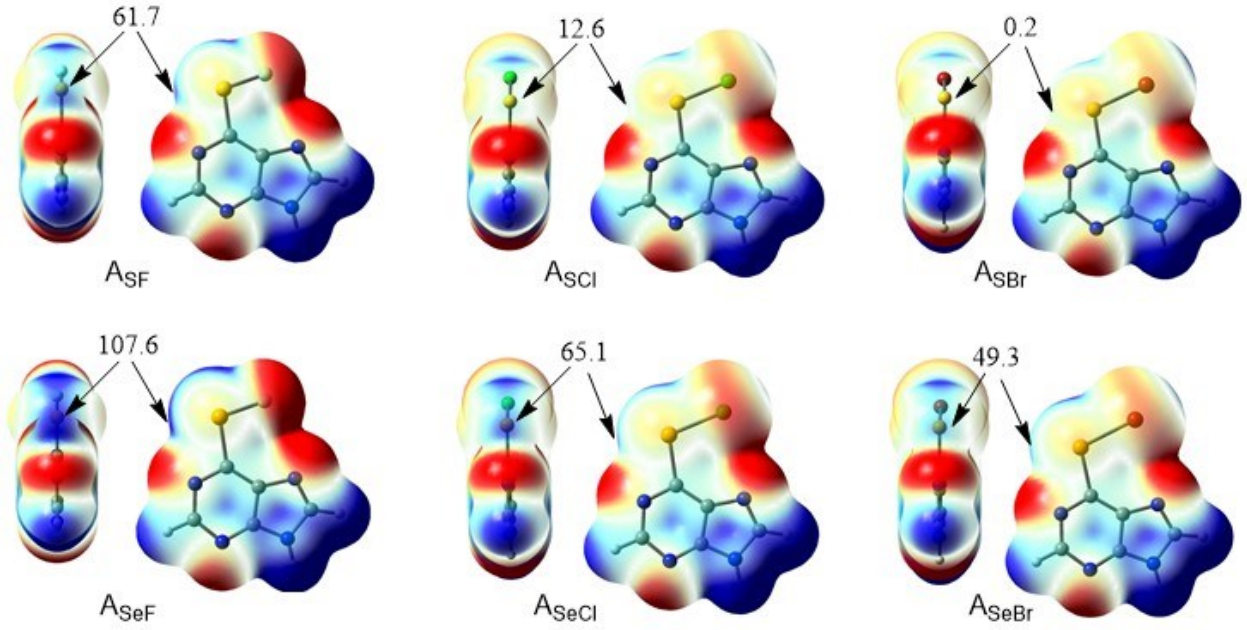

Figure S5. ESP maps on 0.002 electrons bohr^{-3} isodensity surfaces for the A_{XY} modified base (X= S, Se and Y= F, Cl, Br). Values of the maximum electrostatic potential at the σ hole are indicated ($V_{S,max}$, kJ mol^{-1}).

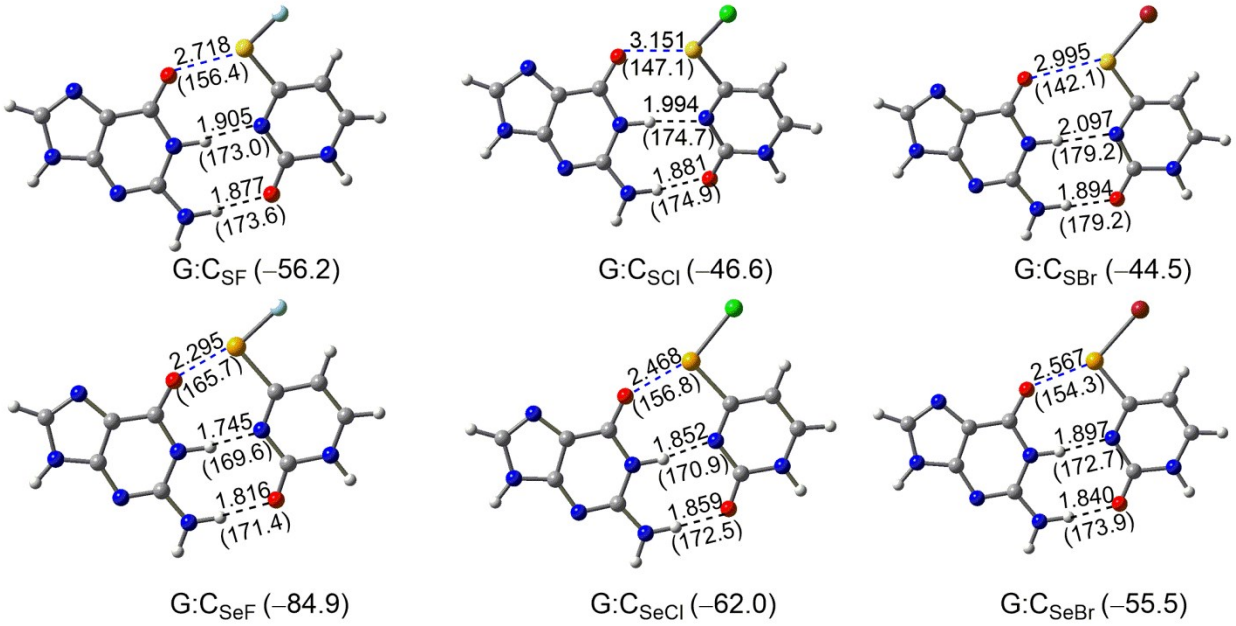

Figure S6. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) of G:C$_{XY}$ base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

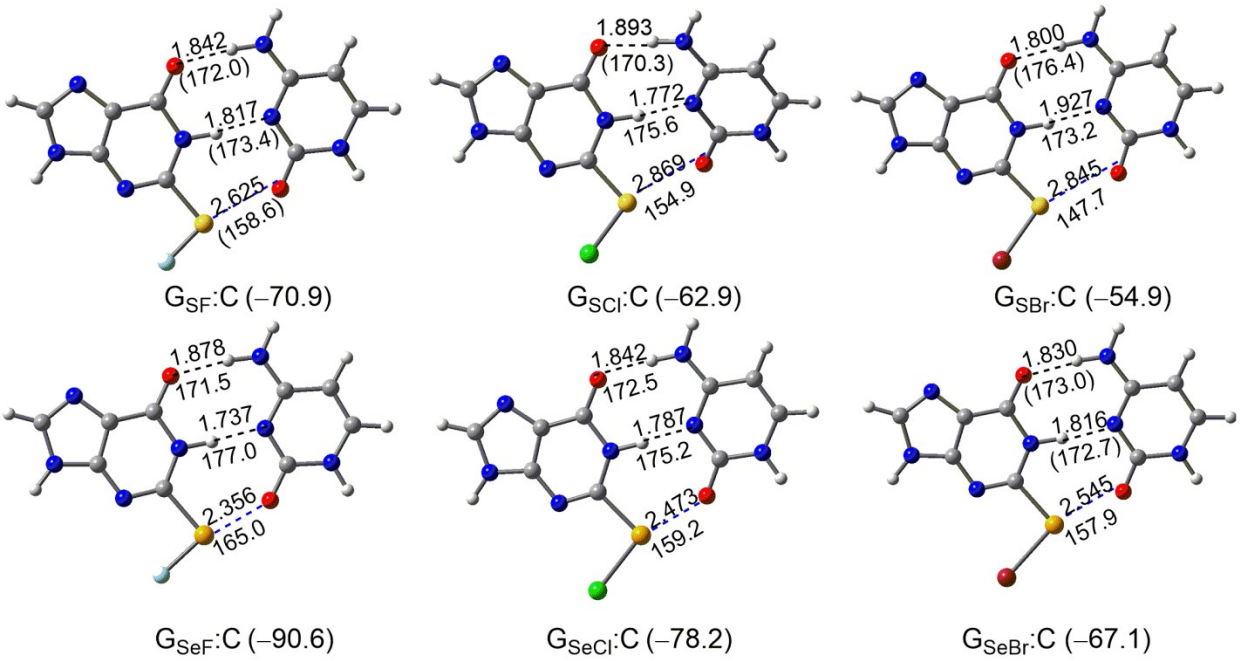

Figure S7. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) of G_{XY}:C base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

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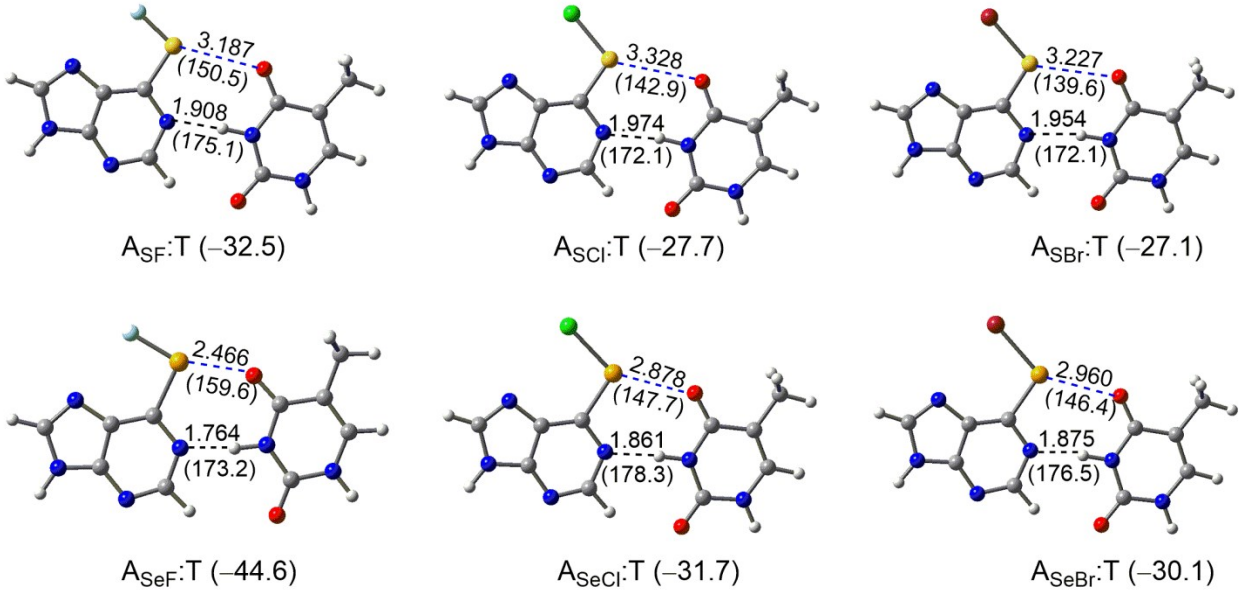

Figure S8 Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) of A$_{XY}$:T base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

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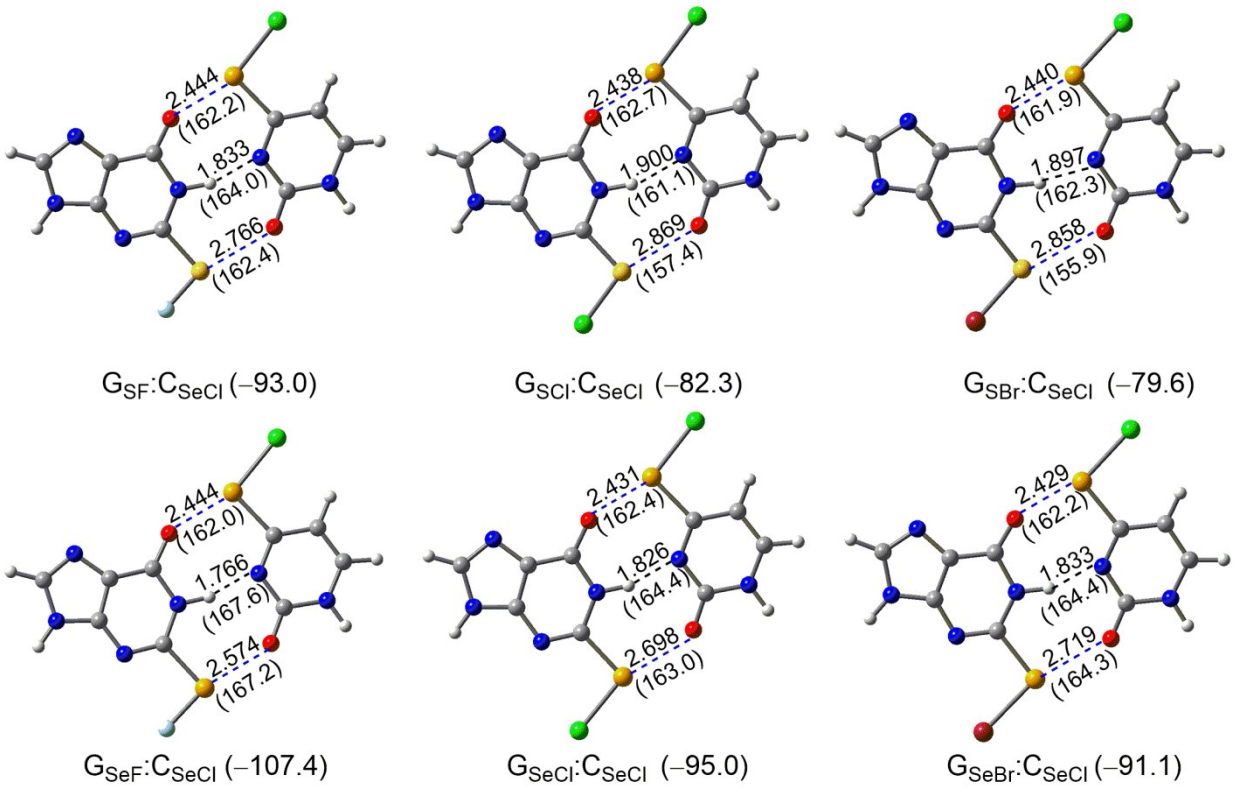


Figure S9. Gas-phase B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SeCl} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

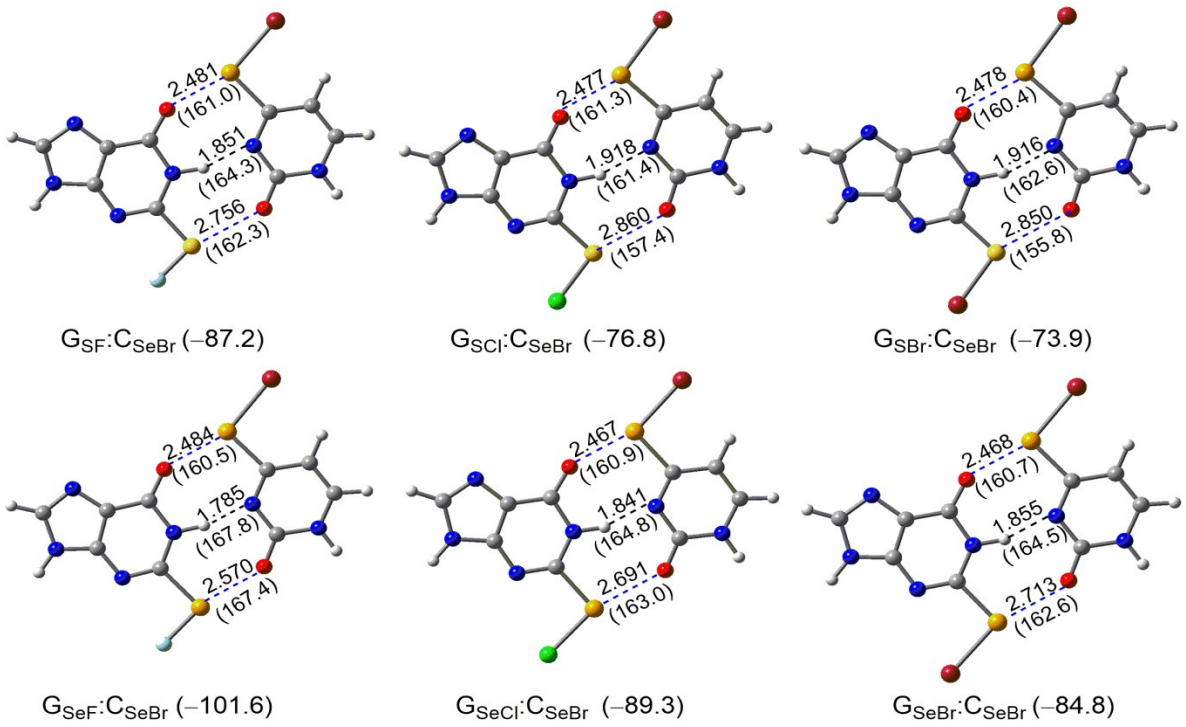


Figure S10. Gas-phase B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SeBr} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

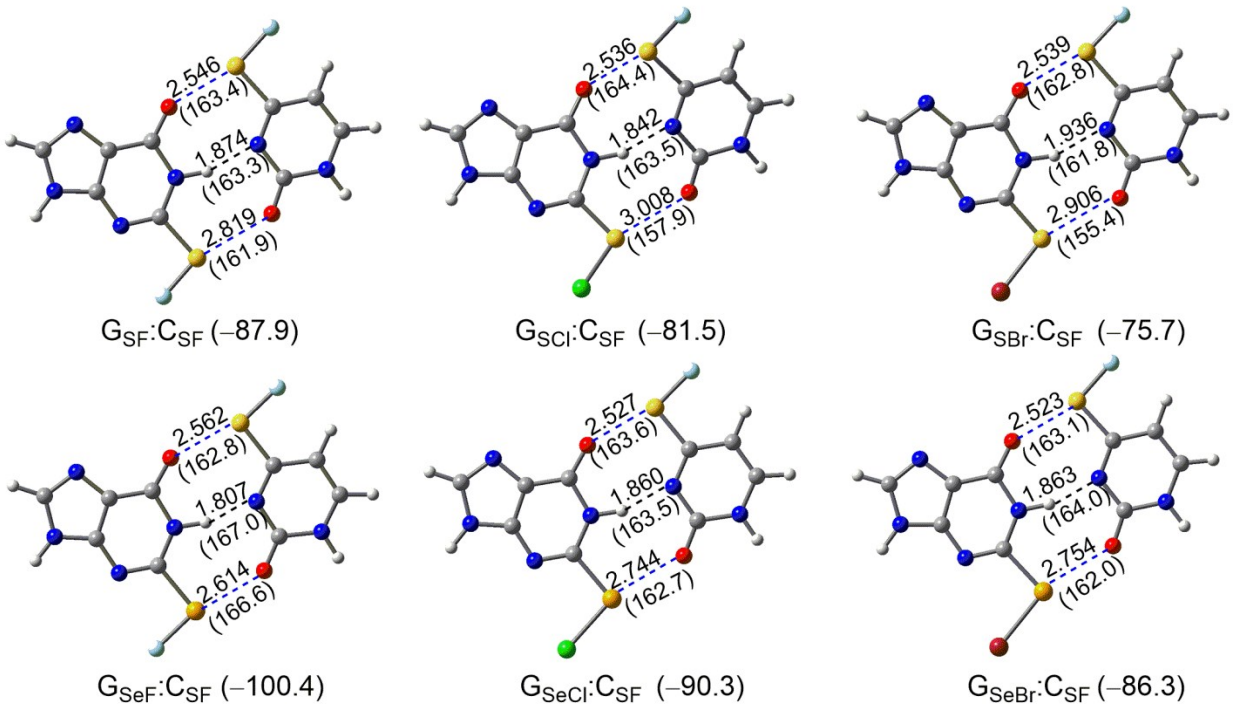


Figure S11. Gas-phase B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SF} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

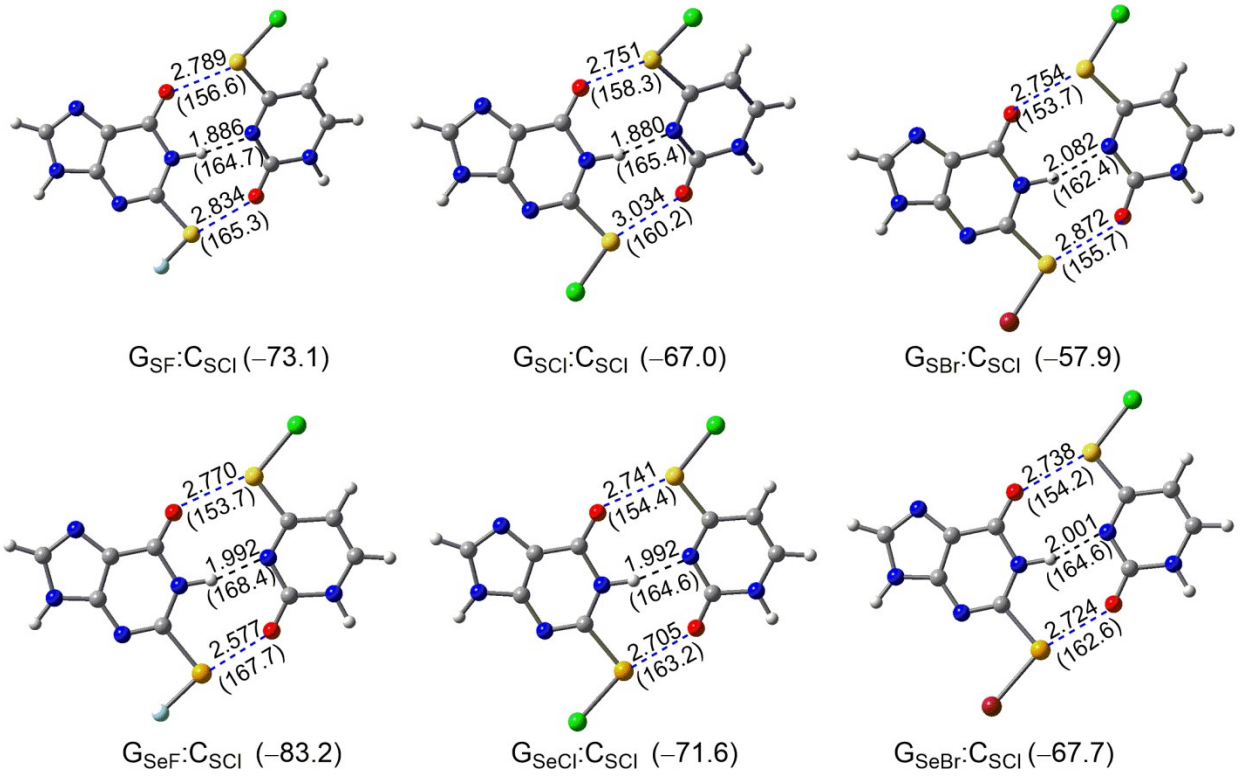
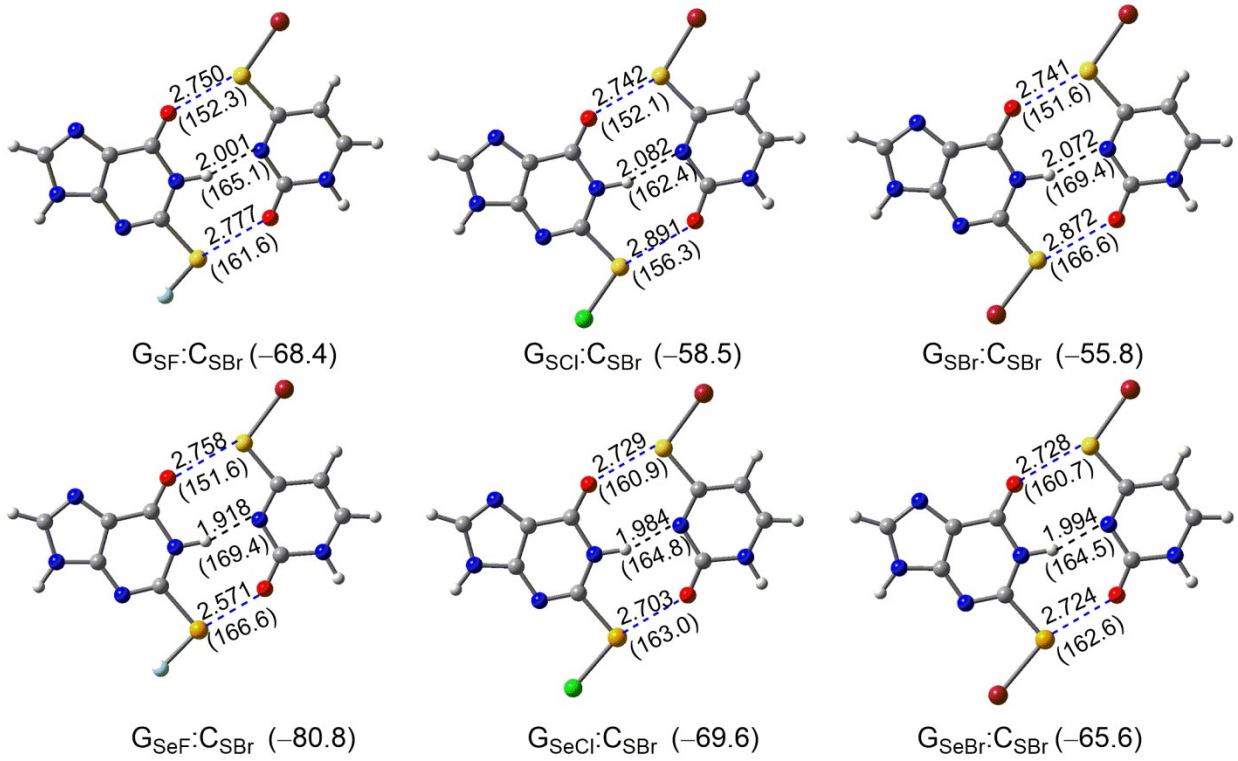


Figure S12. Gas-phase B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SCl} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.



G_{SF}:C_{SBr} (–68.4) G_{SCl}:C_{SBr} (–58.5) G_{SBr}:C_{SBr} (–55.8)

G_{SeF}:C_{SBr} (–80.8) G_{SeCl}:C_{SBr} (–69.6) G_{SeBr}:C_{SBr} (–65.6)

Figure S13. Gas-phase B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for selected G_{XY}:C_{SBr} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

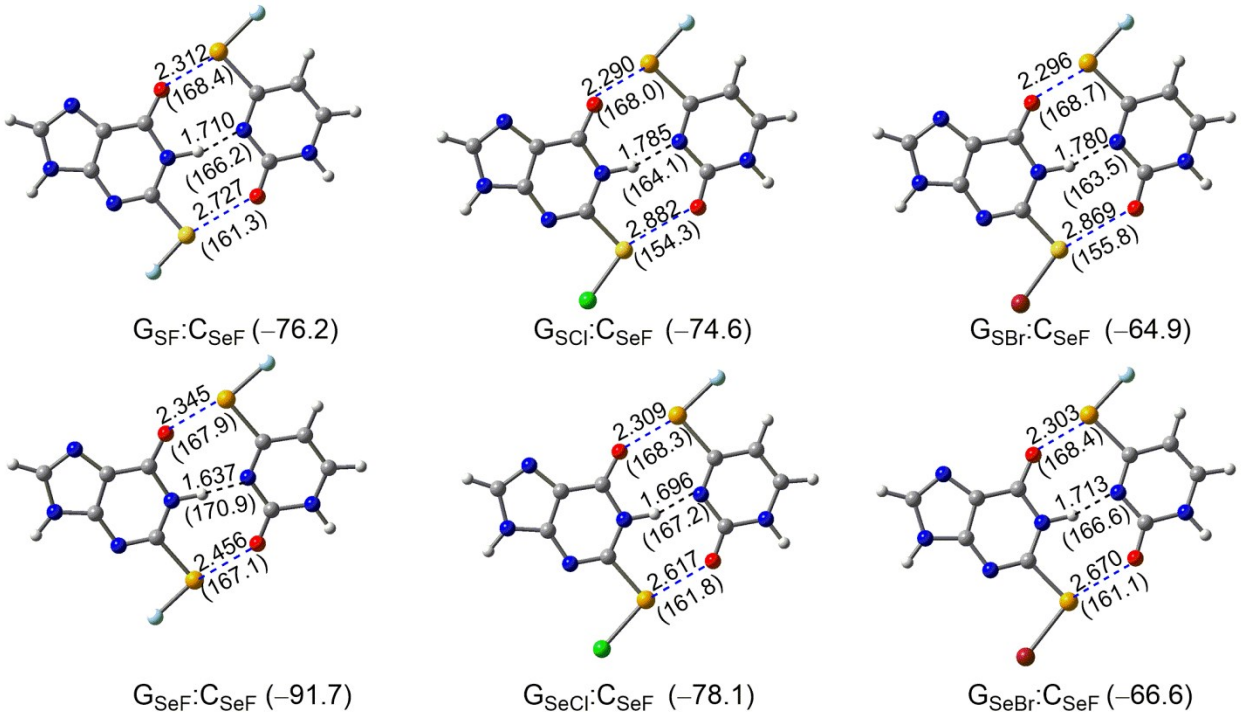


Figure S14. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SeF} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

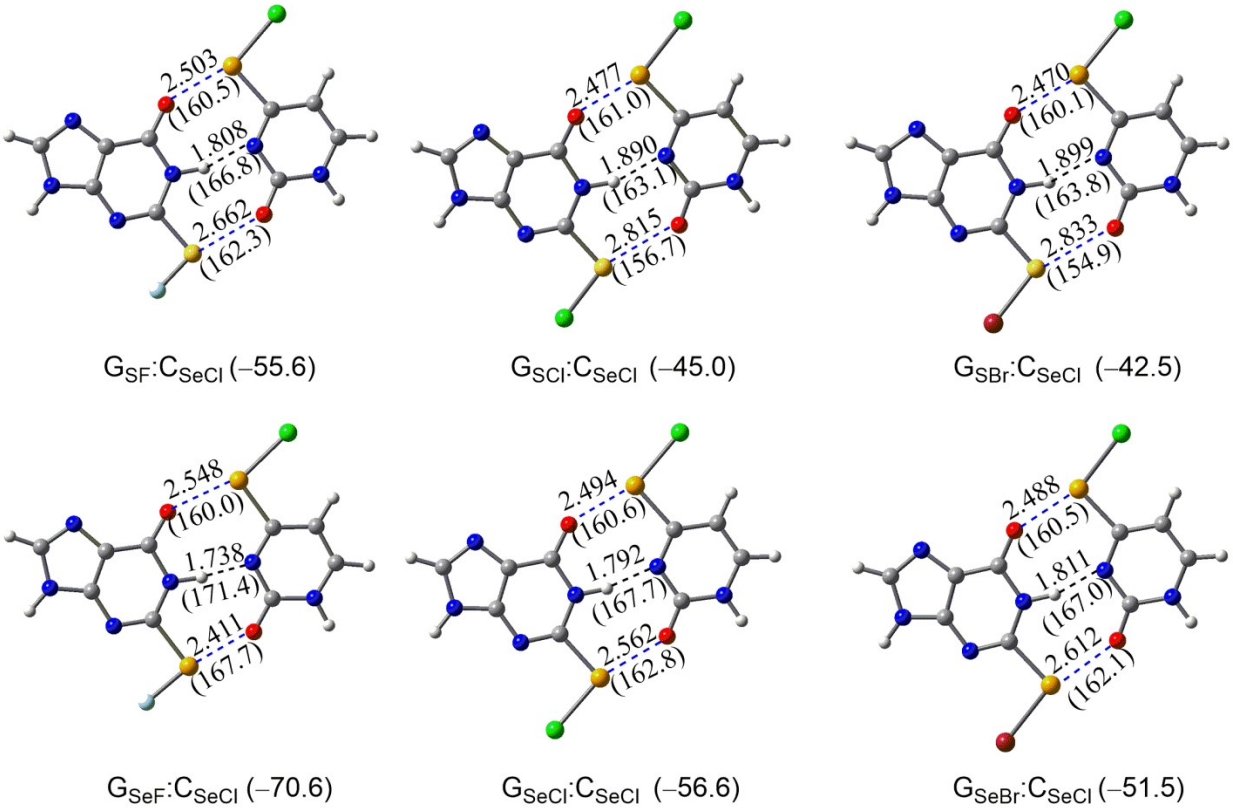


Figure S15. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SeCl} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

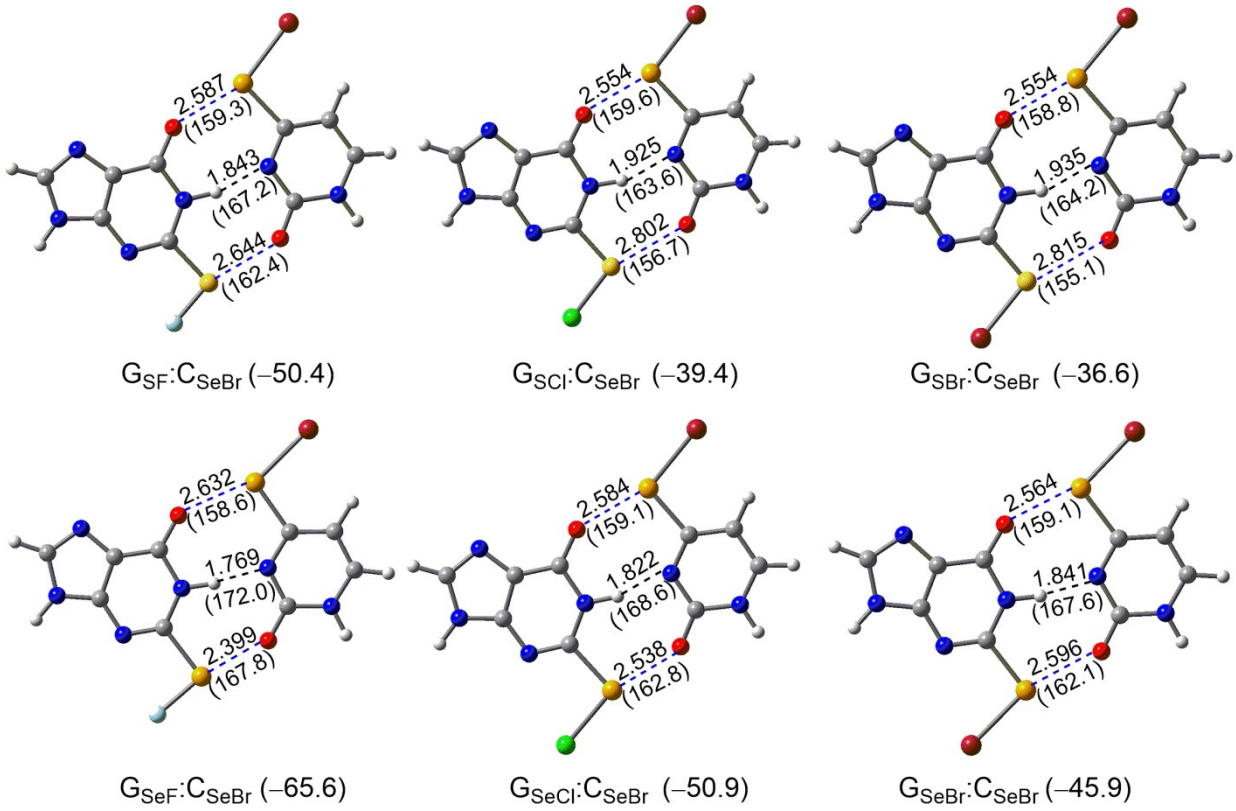


Figure S16. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G$_{XY}$:C$_{SeBr}$ double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.

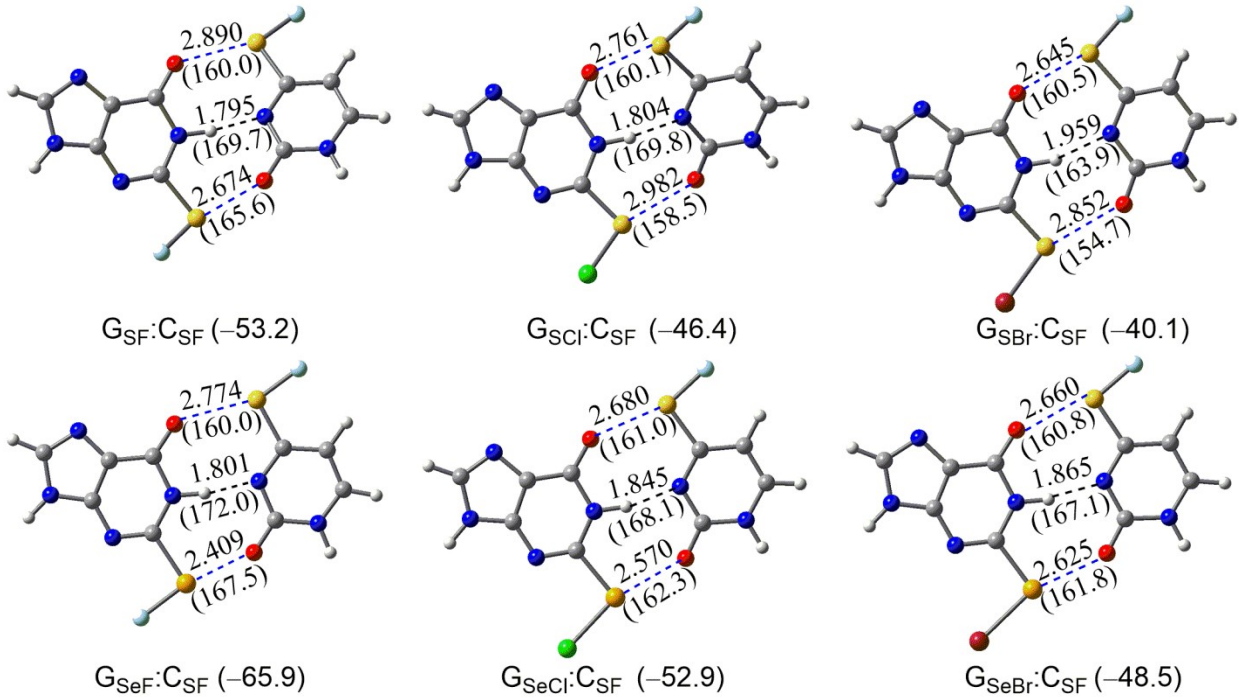
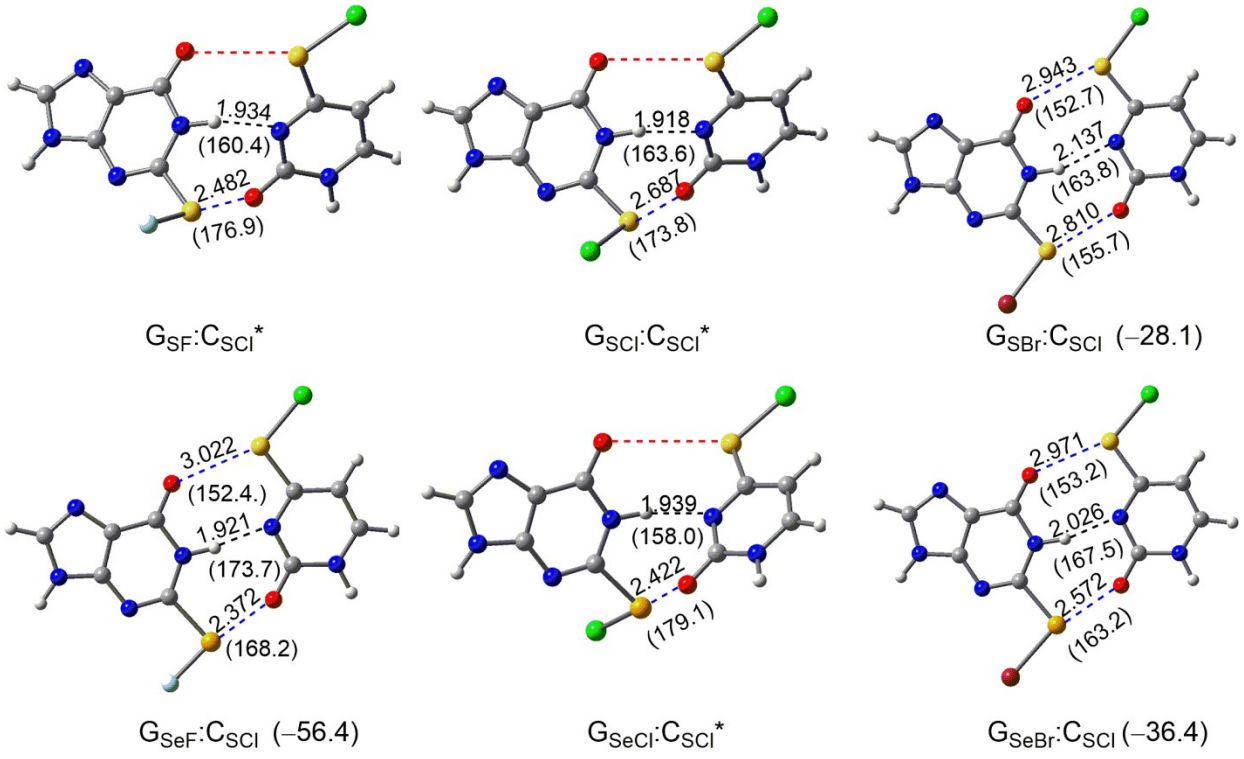


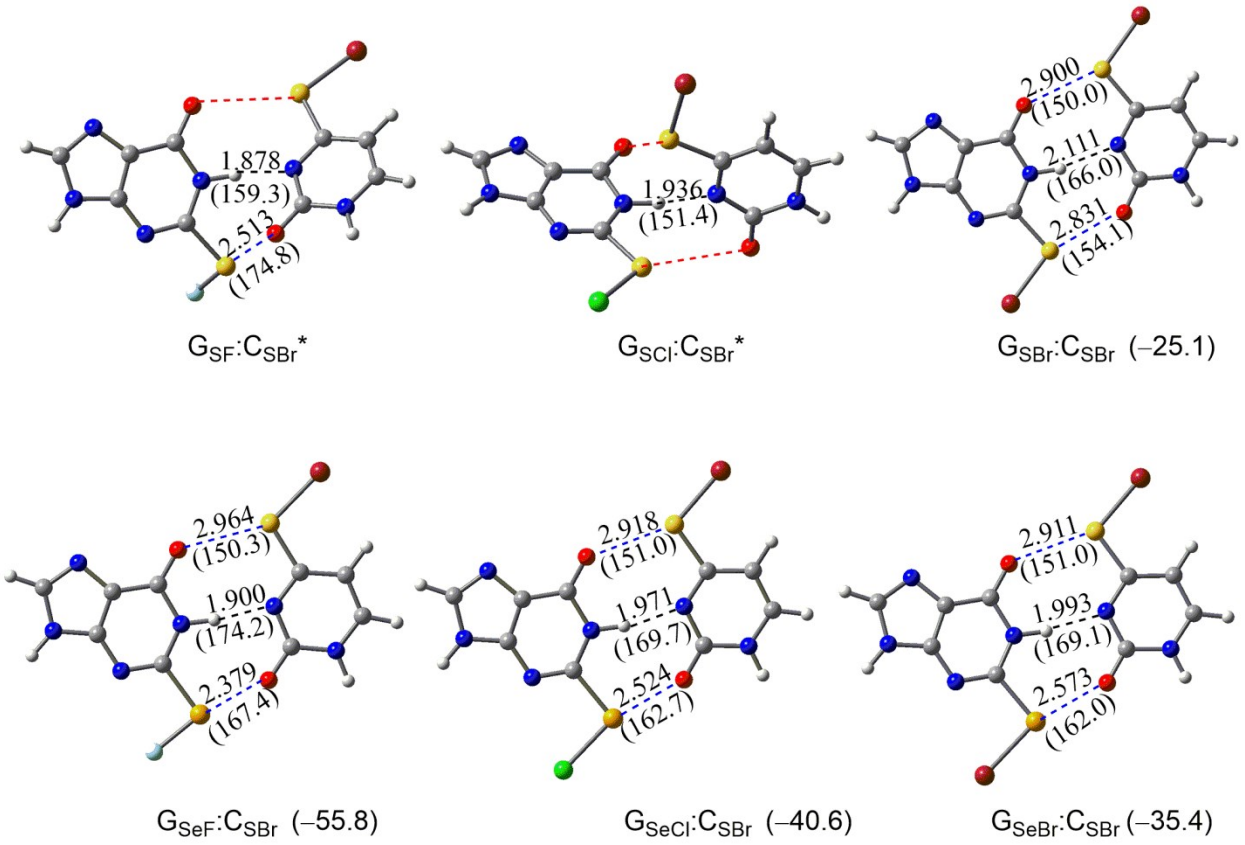
Figure S17. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SF} double-substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided.



G_{SF}:C_{SCl}* G_{SCl}:C_{SCl}* G_{SBr}:C_{SCl} (–28.1)

G_{SeF}:C_{SCl} (–56.4) G_{SeCl}:C_{SCl}* G_{SeBr}:C_{SCl} (–36.4)

Figure S18. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SCl} double substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided. Base pairs marked with an asterisk (*) are not considered for further analysis due to the absence of chalcogen bonding (red dotted line).



G_{SF}:C_{SBr}* G_{SCl}:C_{SBr}* G_{SBr}:C_{SBr} (–25.1)

G_{SeF}:C_{SBr} (–55.8) G_{SeCl}:C_{SBr} (–40.6) G_{SeBr}:C_{SBr} (–35.4)

Figure S19. Implicit solvent (water) phase IEFPCM-B3LYP-D3/6-31G(d,p) optimized structures and IEFPCM-B3LYP-D3/6-311+G(2df,p) binding energies (kJ mol^{-1}, parentheses) for G_{XY}:C_{SBr} double substituted base pairs. Optimized hydrogen-bond (black dotted lines) distances (Å) and angles (deg., parentheses), and chalcogen-bond (blue dotted lines) distances (Å) and angles (deg., parentheses) are provided. Base pairs marked with an asterisk (*) are not considered for further analysis due to the absence of chalcogen bonding (red dotted line).

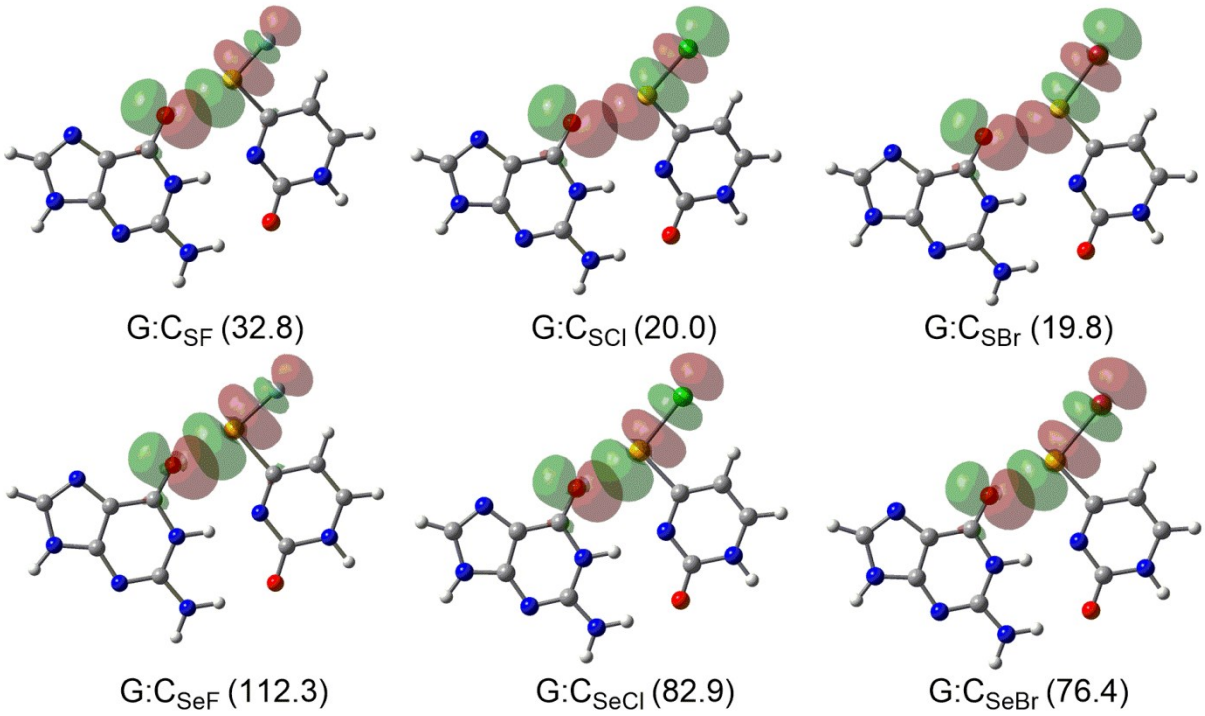


Figure S20. Overlap of donor (i.e., lone pair (n) of O6 (G)) and acceptor (σ^*_{X-Y}) NBOs associated with chalcogen bonds in the G:C$_{XY}$ pairs. The $E^{(2)}$ values corresponding to the orbital interaction are provided (kJ mol^{-1}, in parentheses).

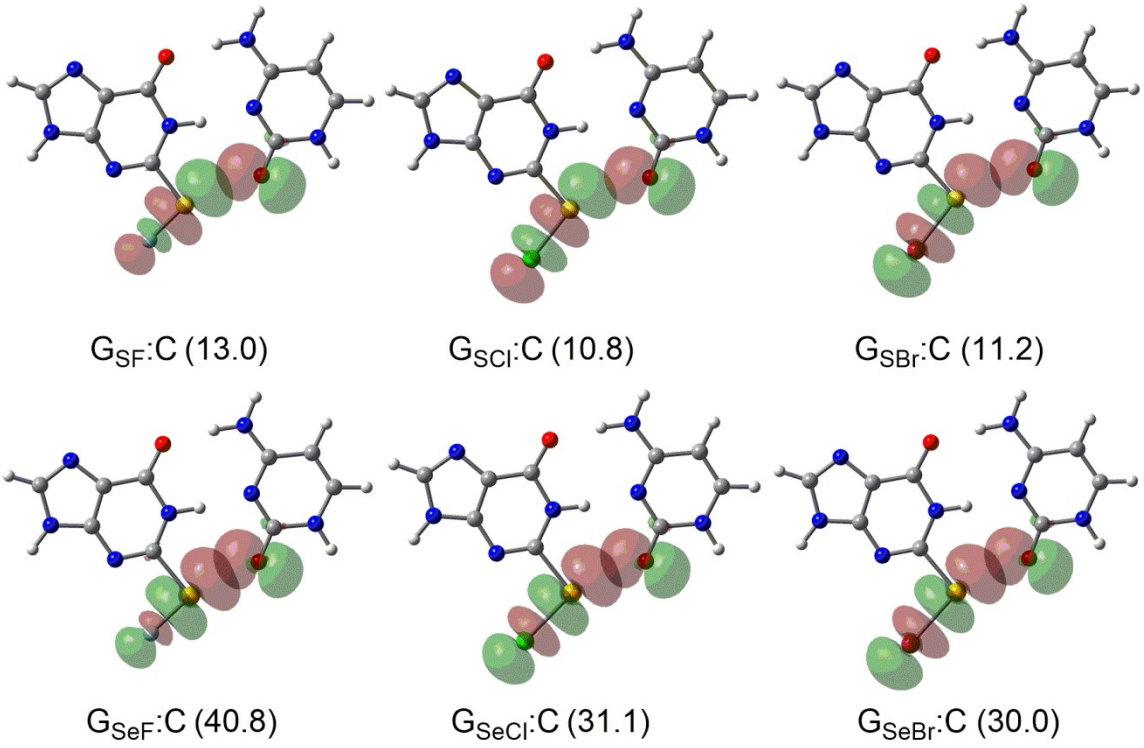


Figure S21. Overlap of donor (i.e., lone pair (n) of O2 (C)) and acceptor (i.e. σ^*_{X-Y} of G_{X-Y}) NBOs associated with chalcogen bonds in the G_{XY}:C pairs. The $E^{(2)}$ values corresponding to the orbital interaction are provided (kJ mol^{-1}, in parentheses).

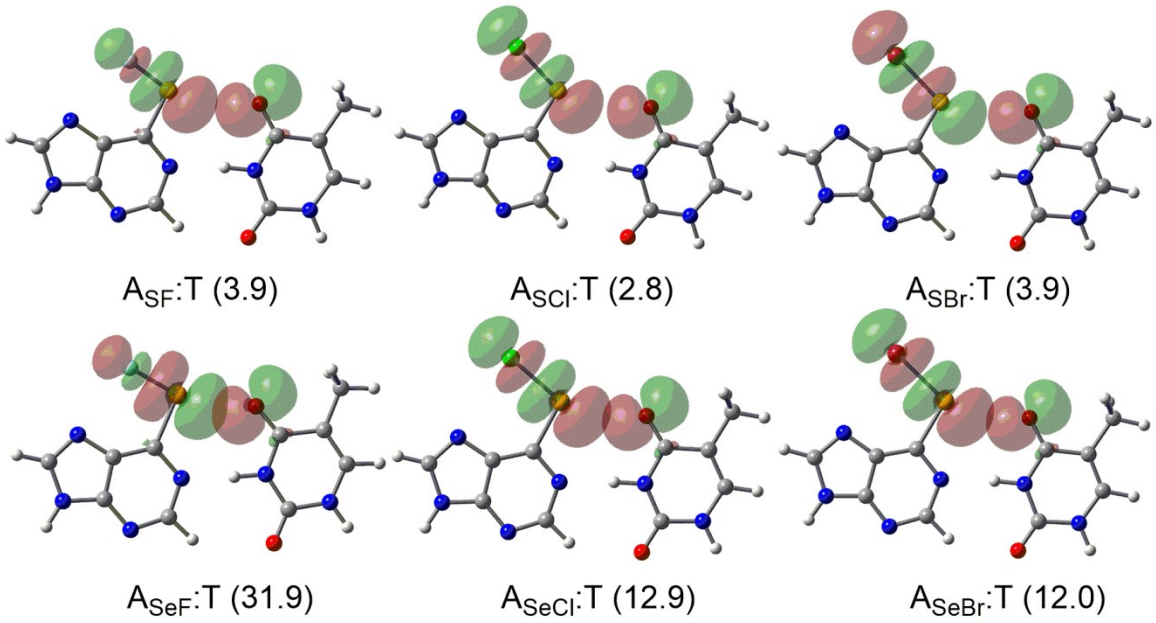


Figure S22. Overlap of donor (i.e., lone pair (n) of O4 (T)) and acceptor ($\sigma^*_{X–Y}$ of A_{X-Y}) NBOs associated with chalcogen bonds in the A_{XY}:T pairs. The $E^{(2)}$ values corresponding to the orbital interaction are provided (kJ mol^{-1}, in parentheses).

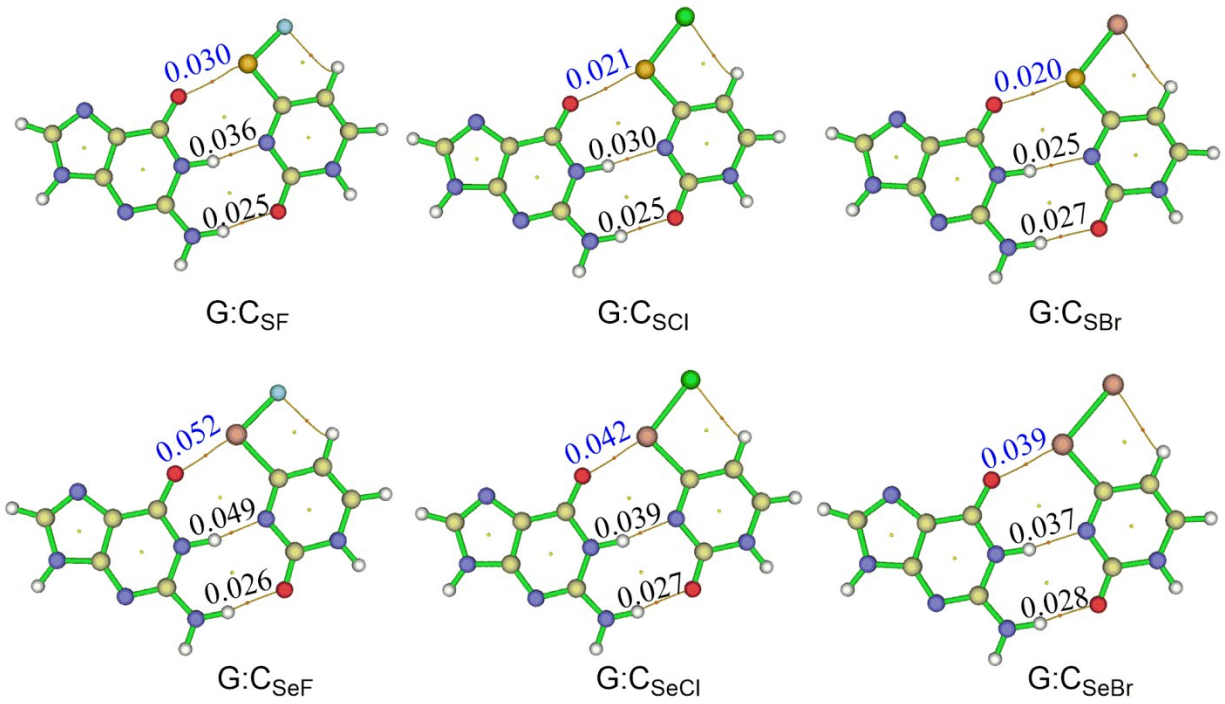


Figure S23. Bond critical paths (thin brown lines) and bond critical points (red dots) associated with intermolecular interactions in G:C_{XY} pairs. The electron densities ($\rho(r)$) at the hydrogen bond critical points (black) and chalcogen bond critical points (blue) are provided.

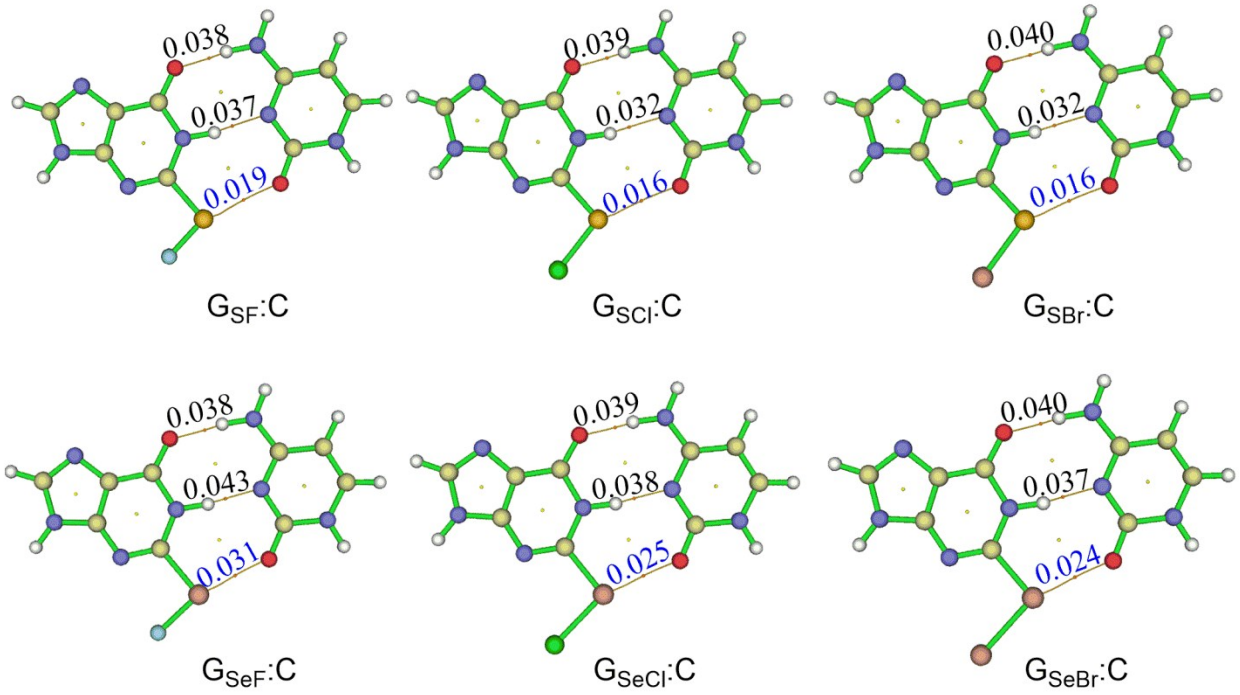


Figure S24. Bond critical paths (thin brown lines) and bond critical points (red dots) associated with intermolecular interactions in G_{XY}:C pairs. The electron densities ($\rho(r)$) at the hydrogen bond critical points (black) and chalcogen bond critical points (blue) are provided.

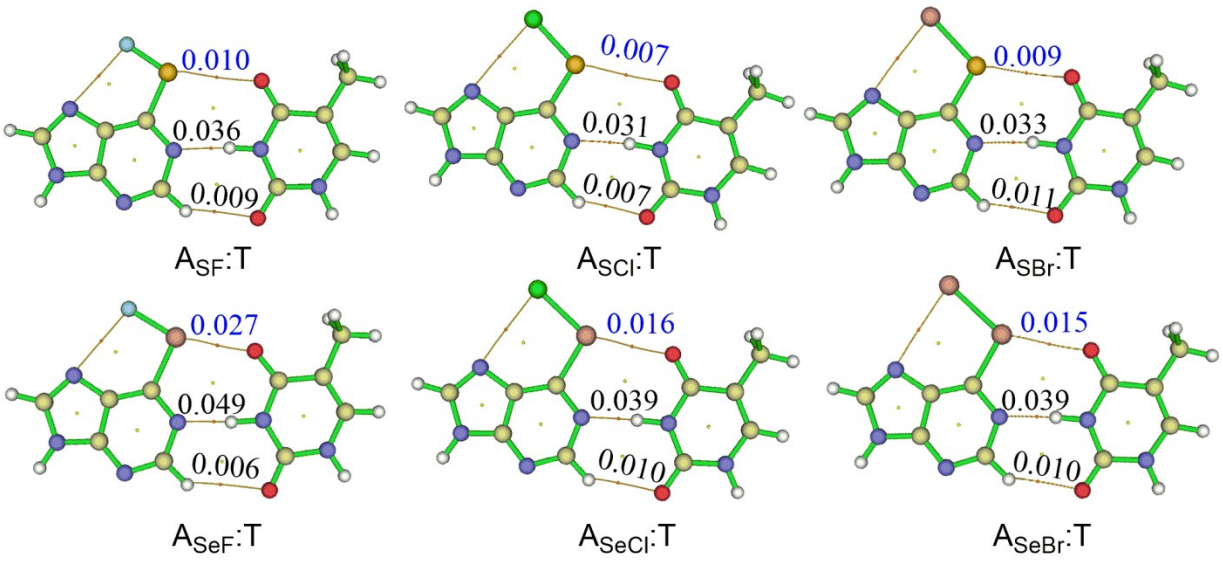


Figure S25. Bond critical paths (thin brown lines) and bond critical points (red dots) associated with intermolecular interactions in A_{XY}:T pairs. The electron densities ($\rho(r)$) at the hydrogen bond critical points (black) and chalcogen bond critical points (blue) are provided.

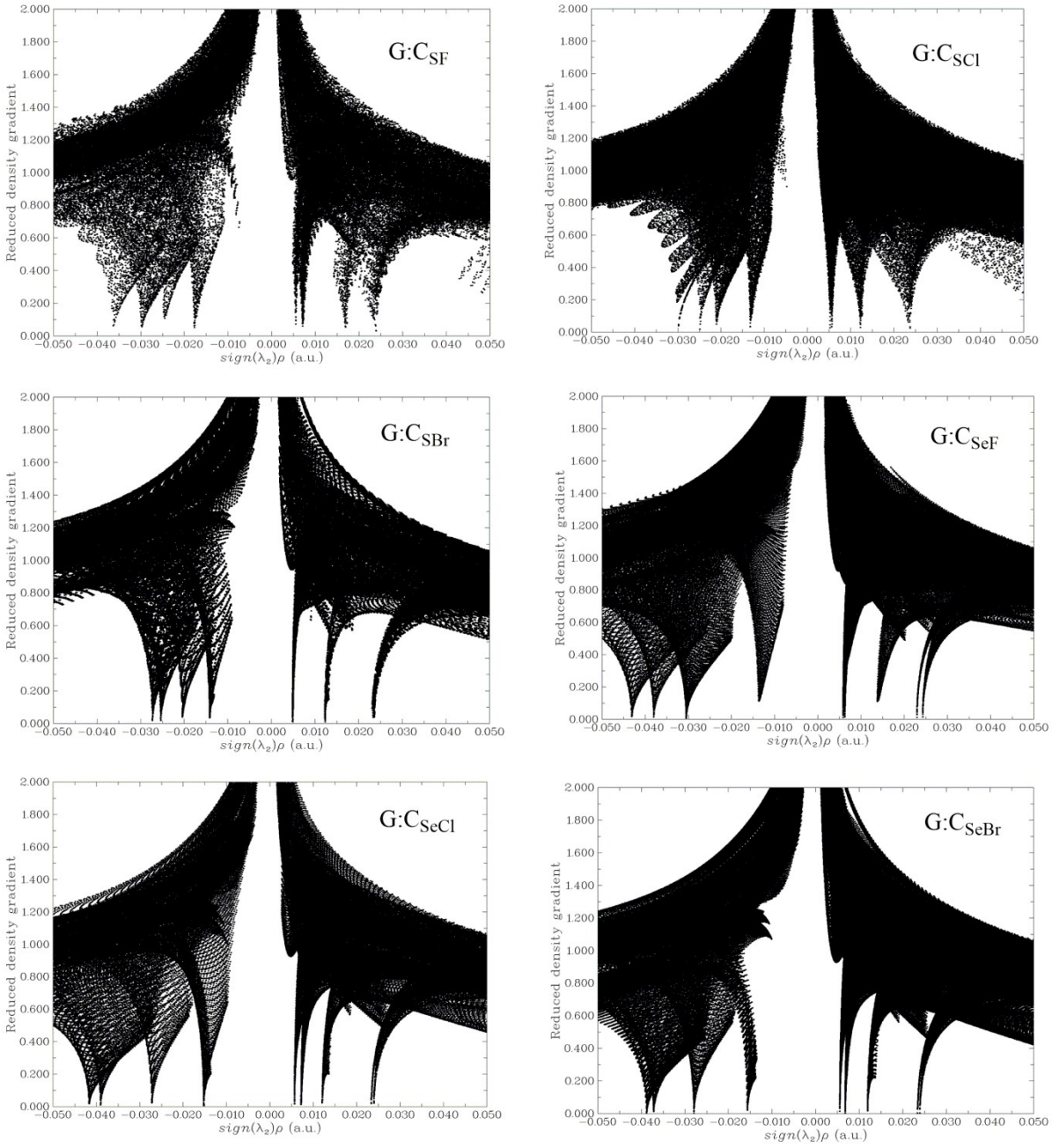


Figure S26. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G:C$_{XY}$ pairs.

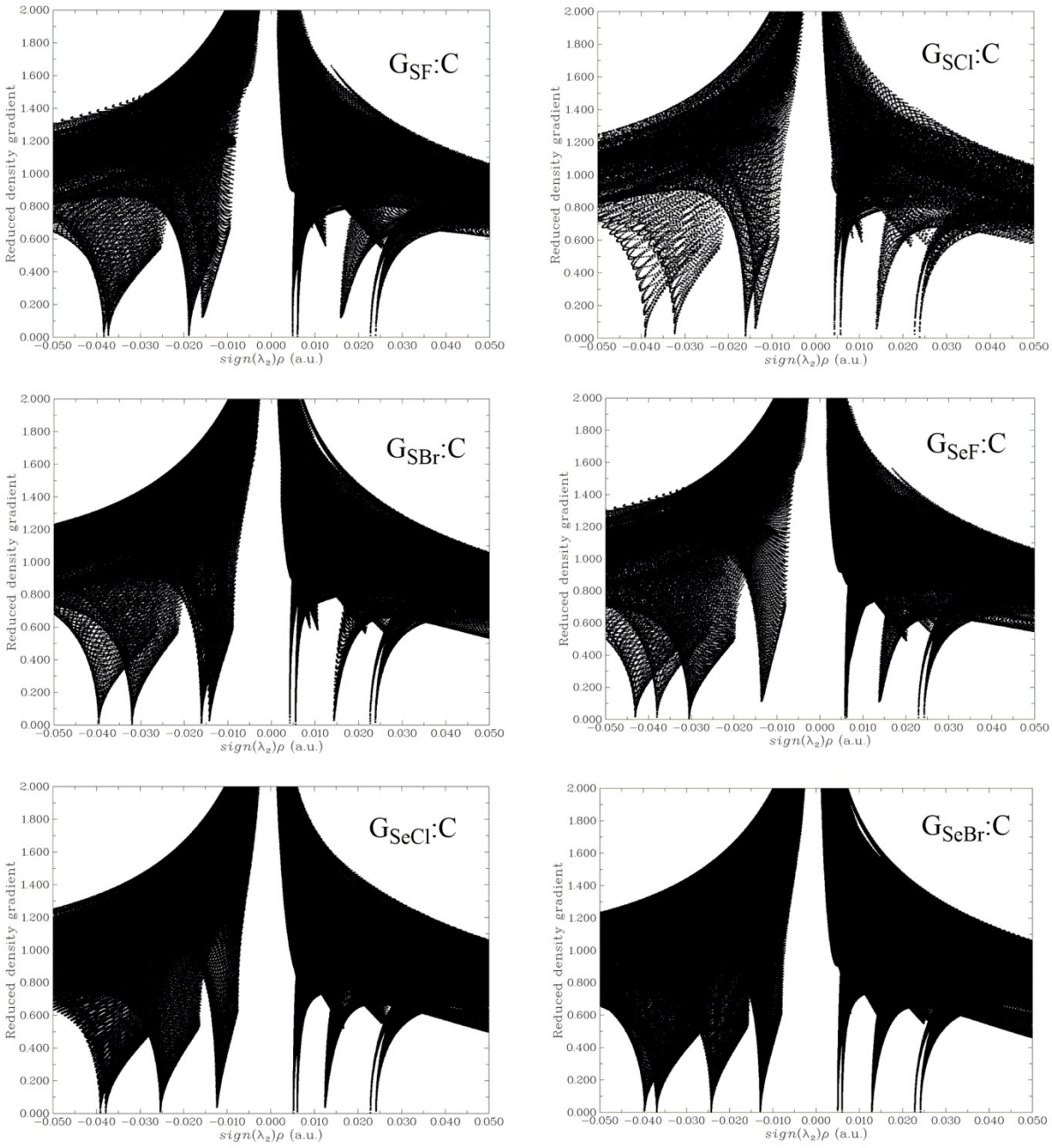


Figure S27. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C pairs.

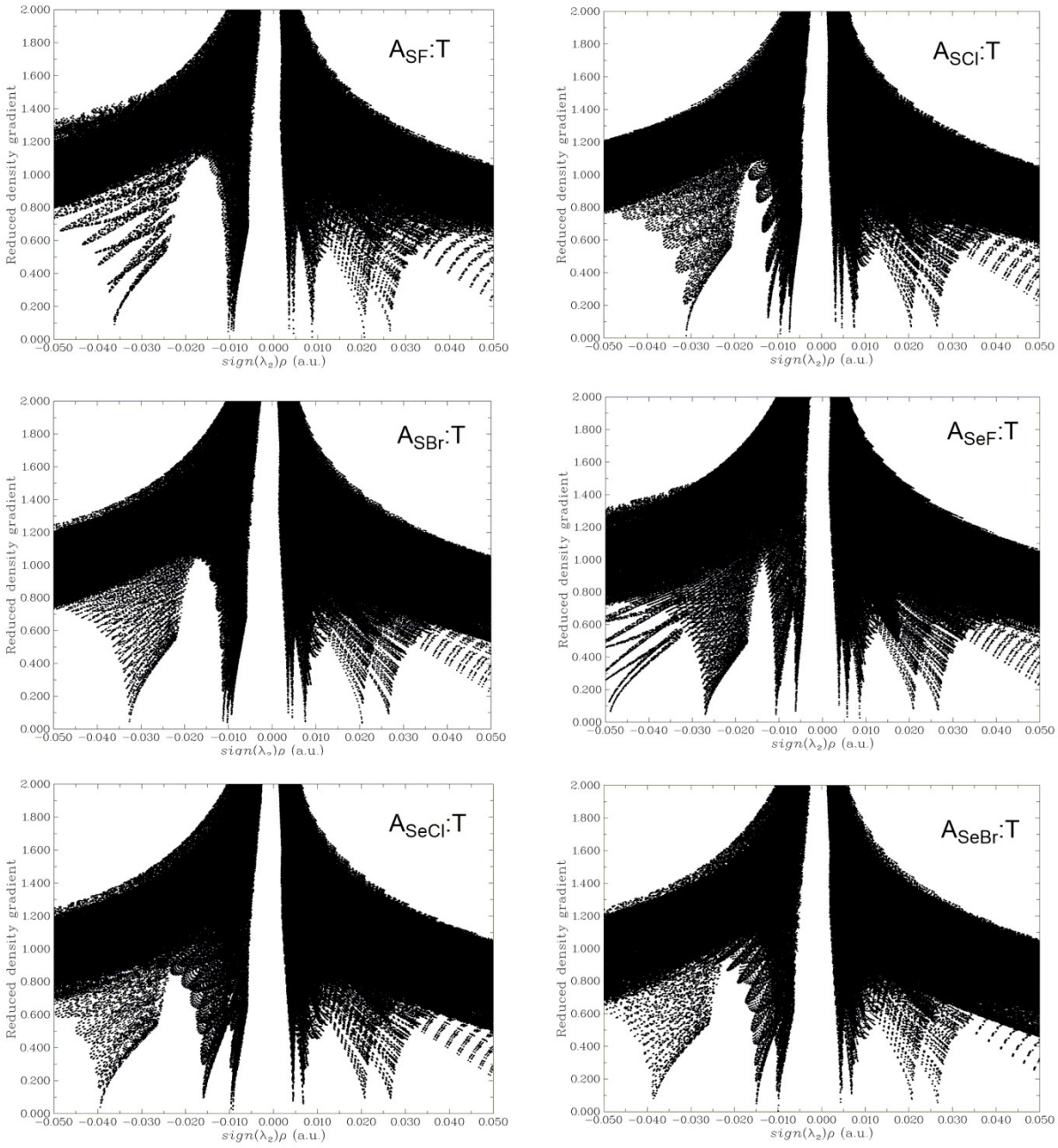


Figure S28. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for A_{XY}:T pairs.

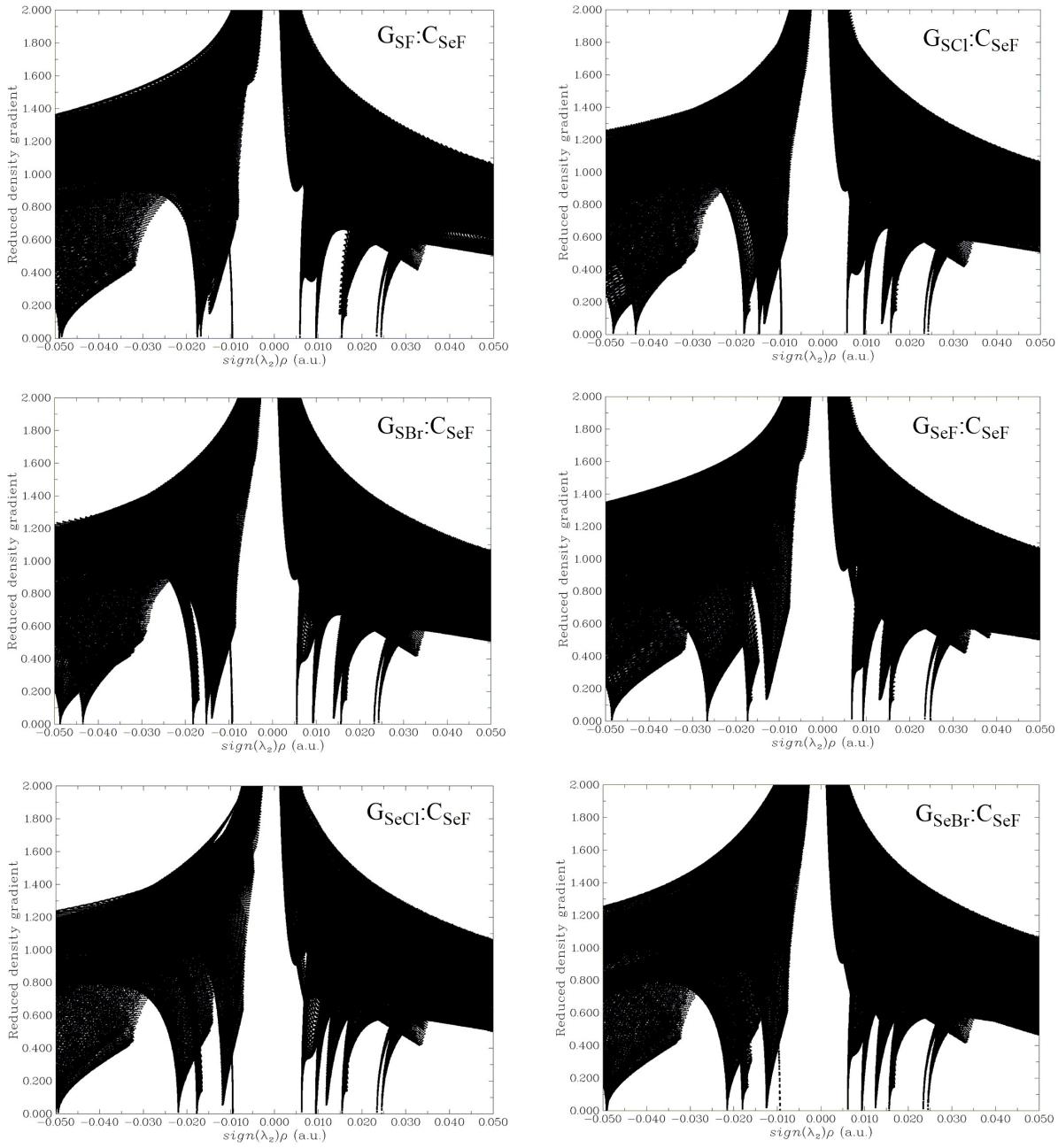


Figure S29. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C_{SeF} pairs.

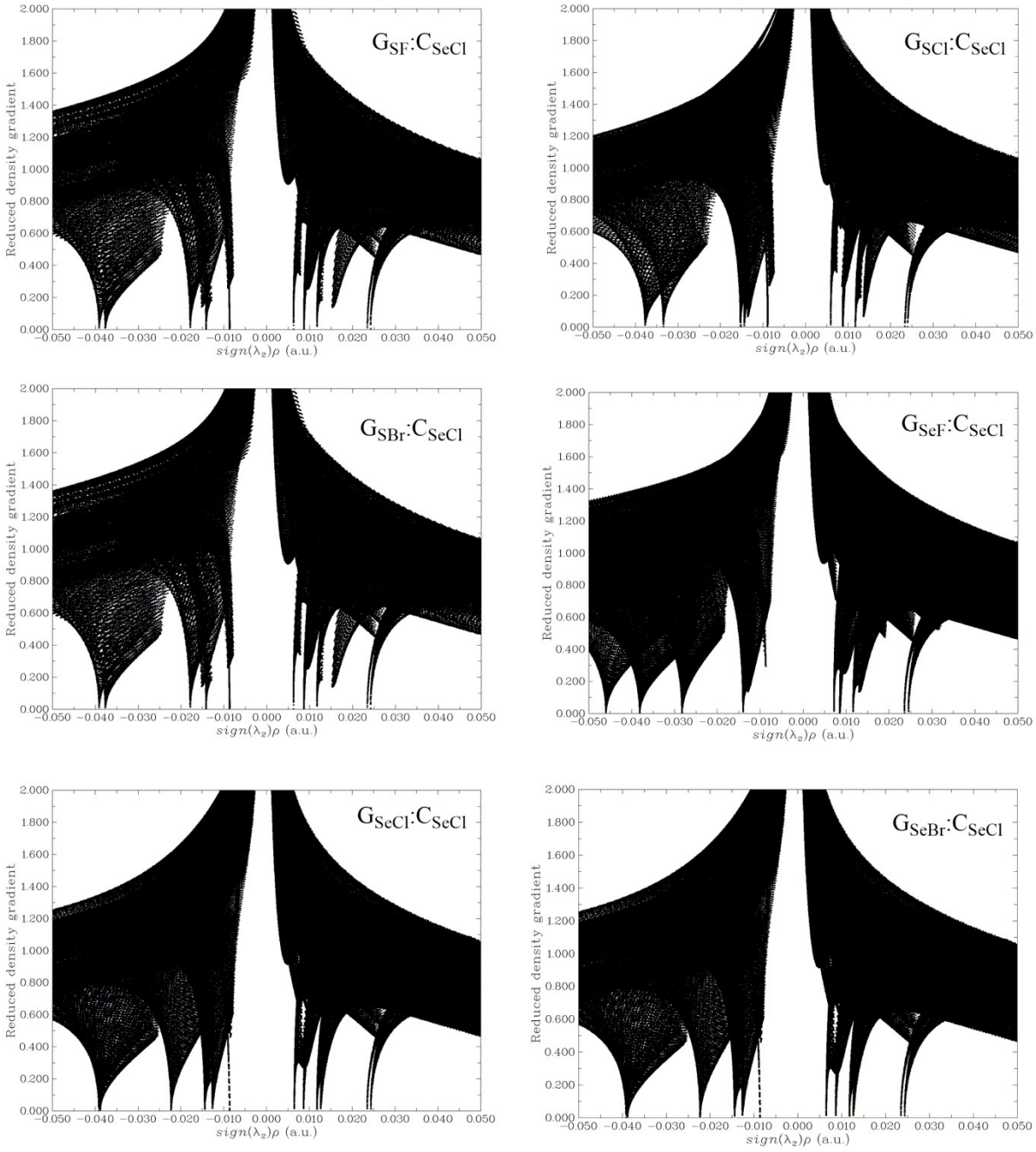


Figure S30. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C_{SeCl} pairs.

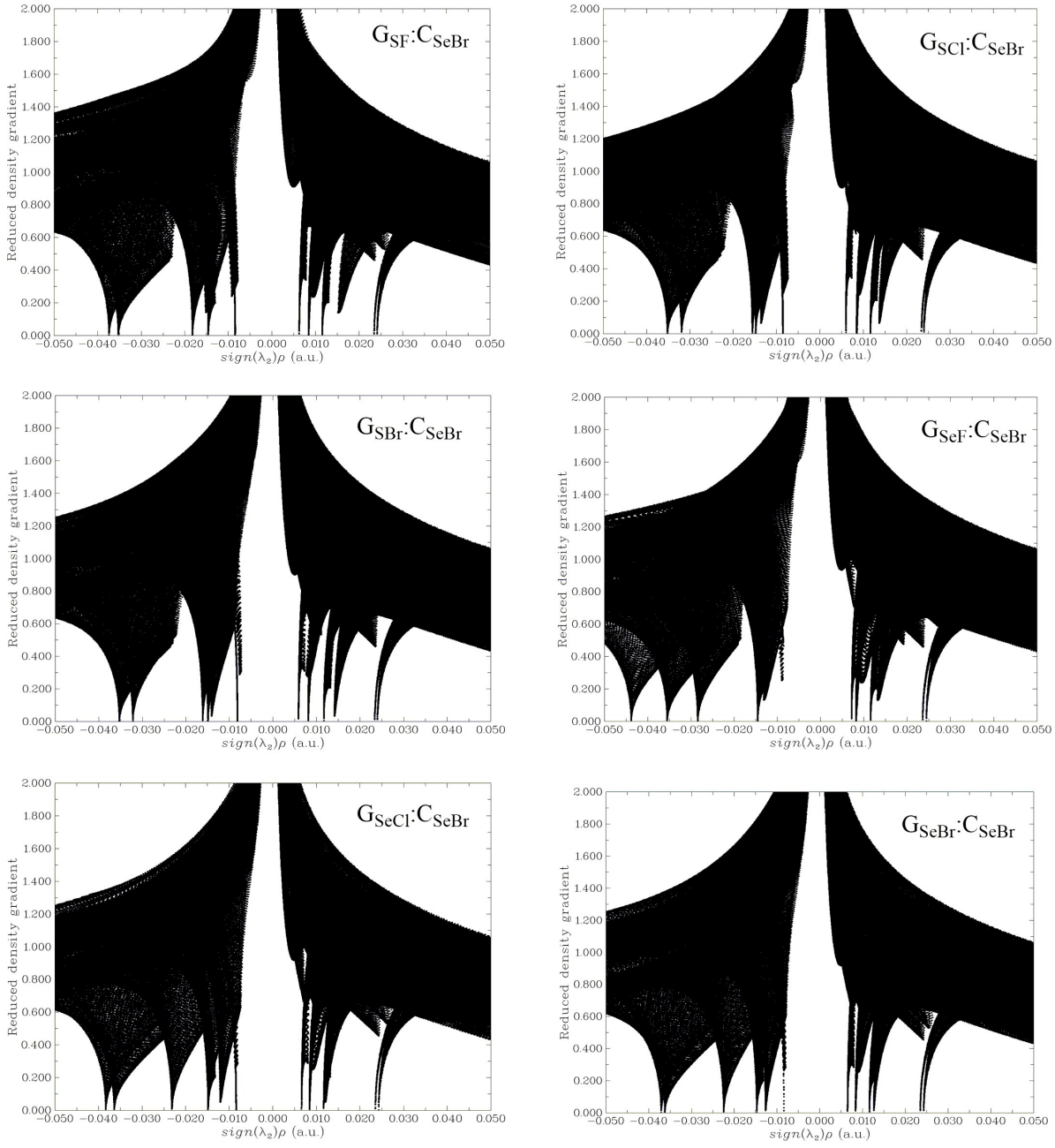


Figure S31. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C_{SeBr} pairs.

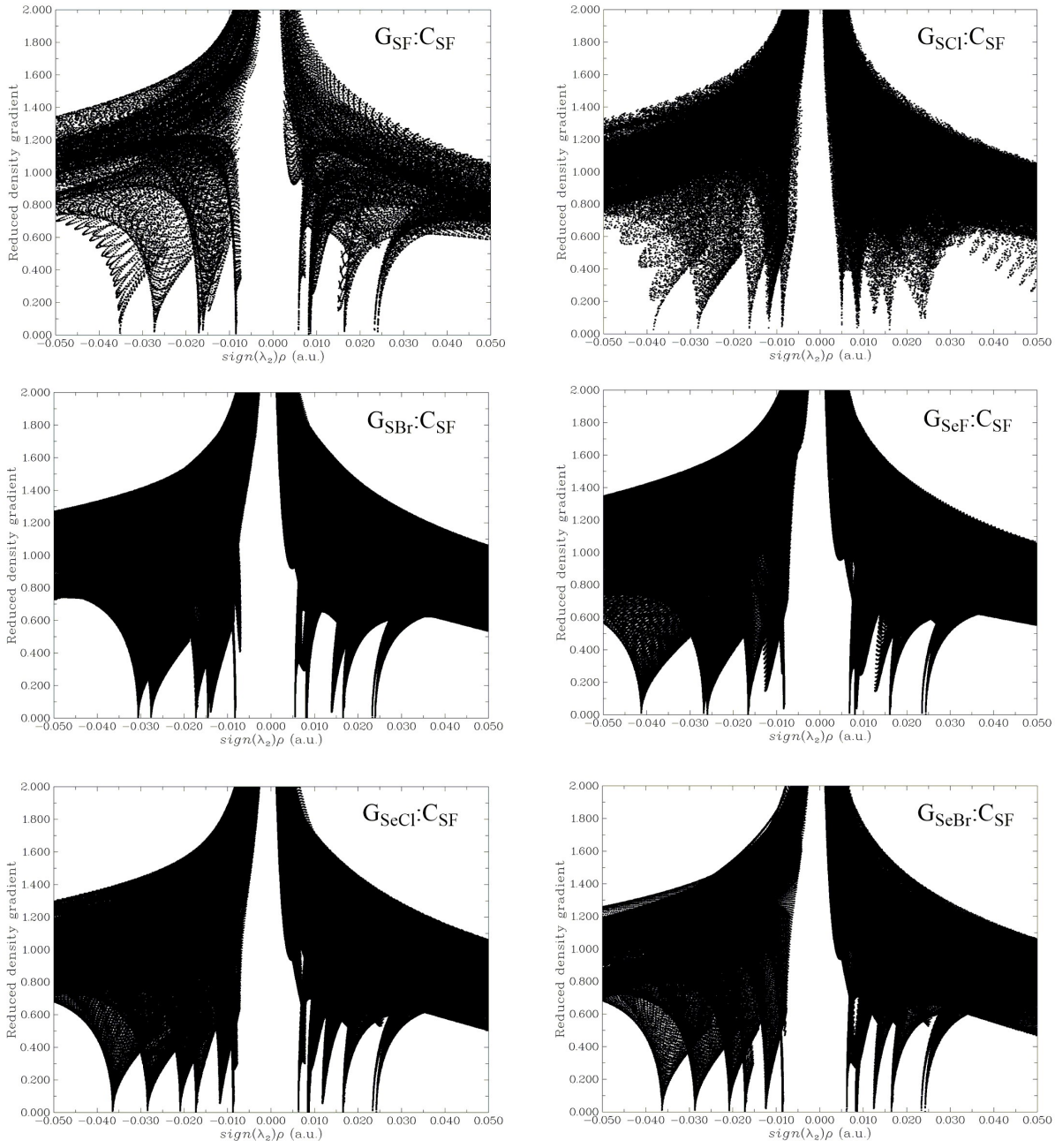


Figure S32. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C_{SF} pairs.

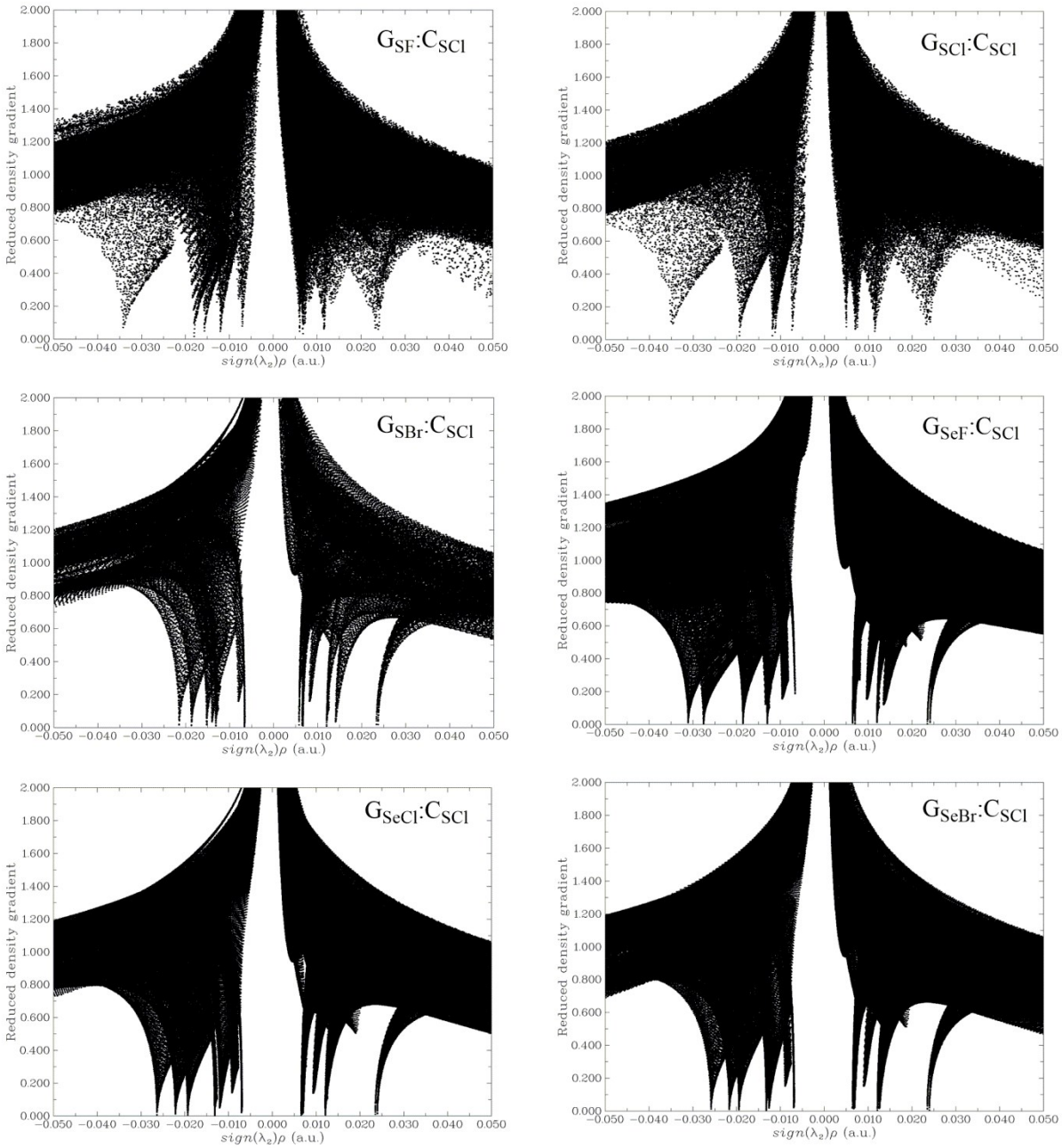


Figure S33. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C_{SCl} pairs.

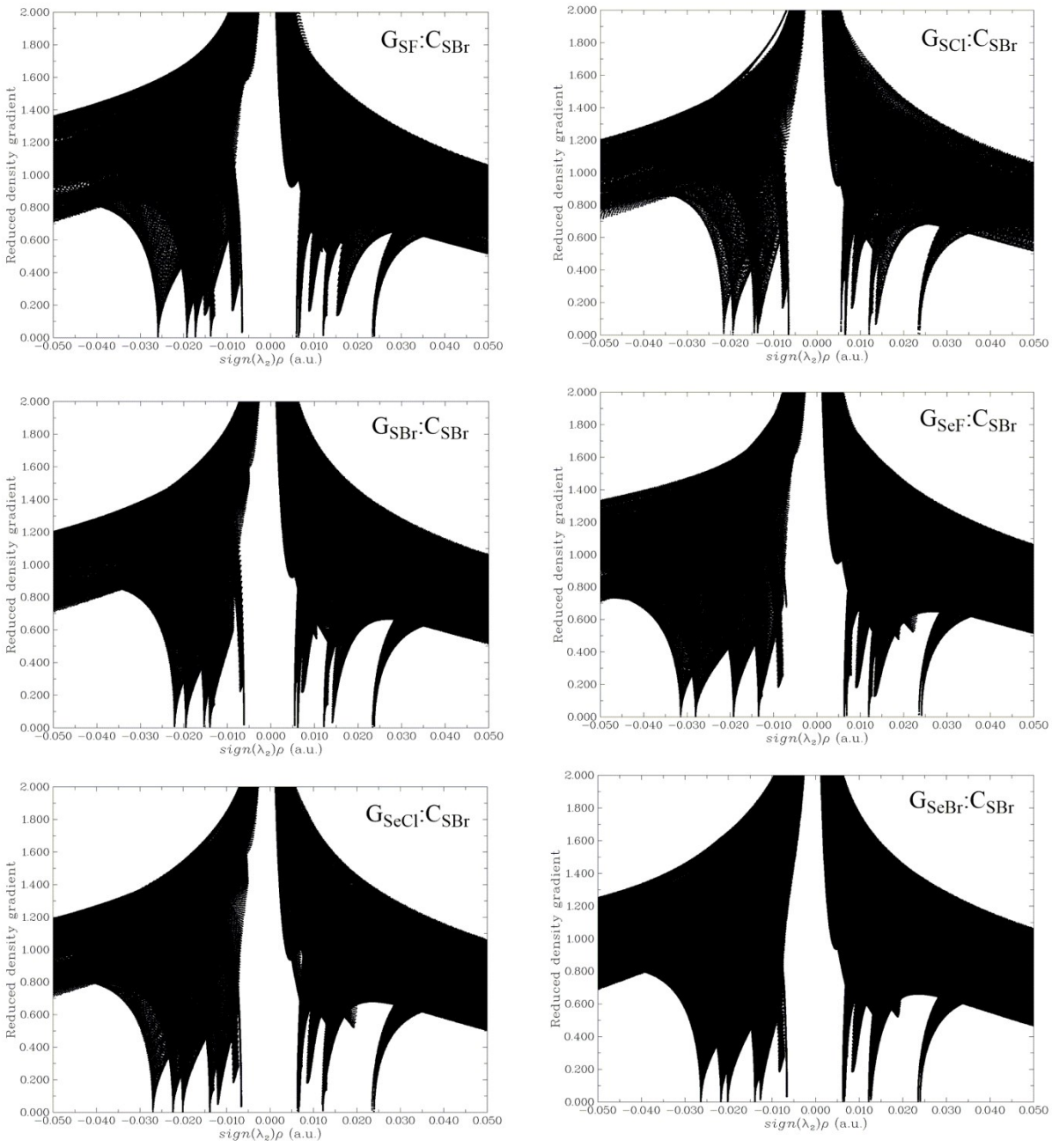


Figure S34. NCI plots of the reduced density gradient (s) against sign(λ_2)ρ(r) for G_{XY}:C_{SBr} pairs.

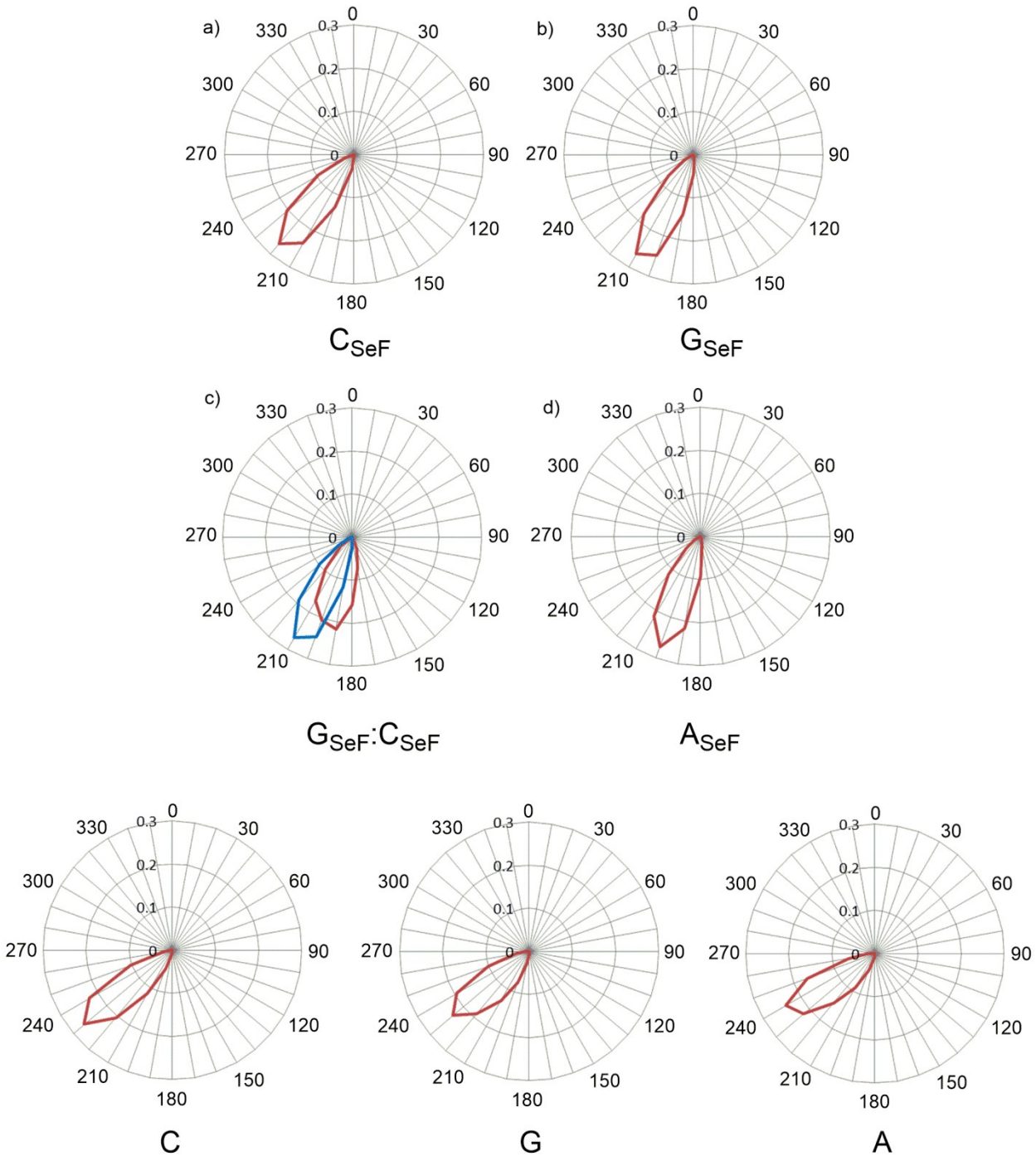


Figure S35. Radar plots for the glycosidic dihedral angle of modified bases (χ, ∠(O4′–C1′–N1–C2) for pyrimidines and ∠(O4′–C1′–N9–C4) for purines) obtained from the last 400 ns of MD simulations on the associated oligonucleotides. The blue and red line in plot c correspond to C_{SeF} and G_{SeF}, respectively.

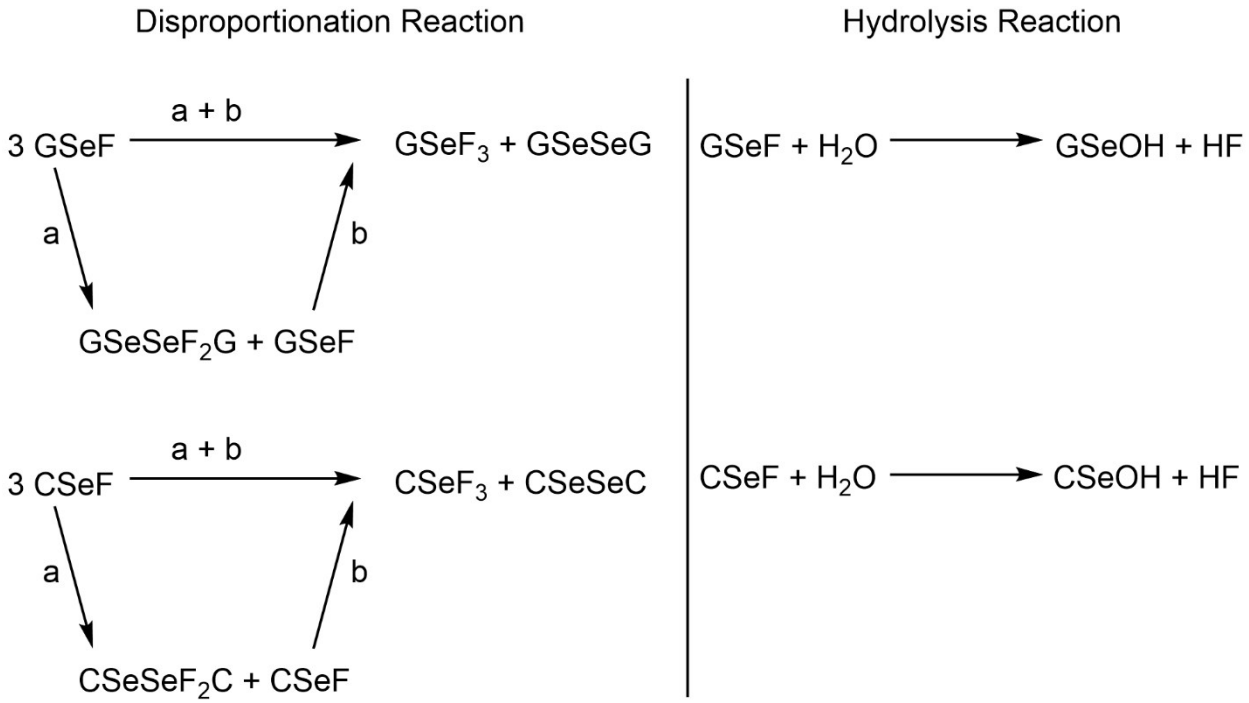


Figure S36. . Disproportionation (a + b) and associated partial (a and b) reactions (left) and hydrolysis reaction (right) of G_{SeF} and C_{SeF} analyzed in the present work.

Table S1. Combinations of modified base pairs analyzed in the present work.

Pairing type	No. of chalcogen bonds	Category	Base pairs
$G:C_{XY}$	One	-	$G:C_{SF}$, $G:C_{SCl}$, $G:C_{SBr}$, $G:C_{SeF}$, $G:C_{SeCl}$, $G:C_{SeBr}$
$G_{XY}:C$	One	-	$G_{SF}:C$, $G_{SCl}:C$, $G_{SBr}:C$, $G_{SeF}:C$, $G_{SeCl}:C$, $G_{SeBr}:C$
	One	-	$A_{SF}:T$, $A_{SCl}:T$, $A_{Br}:T$, $A_{SeF}:T$, $A_{SeCl}:T$, $A_{SeBr}:T$
$G_{XY}:C_{X'Y'}$	Two	$G_{XY}:C_{SeF}$	$G_{SeF}:C_{SeF}$, $G_{SeCl}:C_{SeF}$, $G_{SeBr}:C_{SeF}$, $G_{SF}:C_{SeF}$, $G_{SCl}:C_{SeF,}$ $G_{SBr}:C_{SeF}$
	Two	$G_{XY}:C_{SeCl}$	$G_{SeF}:C_{SeCl}$, $G_{SeCl}:C_{SeCl}$, $G_{SeBr}:C_{SeCl}$, $G_{SF}:C_{SeCl}$, $G_{SCl}:C_{SeCl,}$ $G_{SBr}:C_{SeCl}$
	Two	$G_{XY}:C_{SeBr}$	$G_{SeF}:C_{SeBr}$, $G_{SeCl}:C_{SeBr}$, $G_{SeBr}:C_{SeBr}$, $G_{SF}:C_{SeBr}$, $G_{SCl}:C_{SeBr}$, $G_{SBr}:C_{SeBr}$
	Two	$G_{XY}:C_{SF}$	$G_{SeF}:C_{SF}$, $G_{SeCl}:C_{SF}$, $G_{SeBr}:C_{SF}$, $G_{SF}:C_{SF}$, $G_{SCl}:C_{SF,}$ $G_{SBr}:C_{SF}$
	Two	$G_{XY}:C_{SCl}$	$G_{SeF}:C_{SCl}$, $G_{SeCl}:C_{SCl}$, $G_{SeBr}:C_{SCl}$, $G_{SF}:C_{SCl}$, $G_{SCl}:C_{SCl,}$ $G_{SBr}:C_{SCl}$
	Two	$G_{XY}:C_{SBr}$	$G_{SeF}:C_{SBr}$, $G_{SeCl}:C_{SBr}$, $G_{SeBr}:C_{SBr}$, $G_{SF}:C_{SBr}$, $G_{SCl}:C_{SBr,}$ $G_{SBr}:C_{SBr}$

Table S2: Significant donor–acceptor interactions in singly-substituted nucleobases along with $E^{(2)}$ values obtained from NBO analysis.

Base	Donor ⋯ Acceptor	$E^{(2)}$ (kJ mol^{-1})
A_{SF}:T	n[O4 (T)]⋯ σ*[S–F (A_{SF})]	3.9
A_{SCl}:T	n[O4 (T)]⋯ σ*[S–Cl (A_{SCl})]	2.8
A_{SBr}:T	n[O4 (T)]⋯ σ*[Se–Br (A_{SBr})]	3.9
A_{SeF}:T	n[O4 (T)]⋯ σ*[S–F (A_{SeF})]	31.9
A_{SeCl}:T	n[O4 (T)]⋯ σ*[Se–Cl (A_{SeCl})]	12.9
A_{SeBr}:T	n[O4 (T)]⋯ σ*[Se–Br (A_{SeBr})]	12.0
G:C_{SF}	n[O6 (G)]⋯ σ*[S–F (G_{SF})]	32.8
G:C_{SCl}	n[O6 (G)]⋯ σ*[S–Cl (G_{SCl})]	20.0
G:C_{SBr}	n[O6 (G)]⋯ σ*[S–Br (G_{SBr})]	19.8
G:C_{SeF}	n[O6 (G)]⋯ σ*[Se–F (G_{SeF})]	112.3
G:C_{SeCl}	n[O6 (G)]⋯ σ*[Se–Cl (G_{SeCl})]	82.9
G:C_{SeBr}	n[O6 (G)]⋯ σ*[Se–Br (G_{SeBr})]	76.4
G_{SF}:C	n[O2 (C)]⋯ σ*[S–F (C_{SF})]	13.0
G_{SCl}:C	n[O2 (C)]⋯ σ*[S–Cl (C_{SCl})]	10.8
G_{SBr}:C	n[O2 (C)]⋯ σ*[S–Br (C_{SBr})]	11.2
G_{SeF}:C	n[O2 (C)]⋯ σ*[Se–F (C_{SeF})]	40.8
G_{SeCl}:C	n[O2 (C)]⋯ σ*[Se–Cl (C_{SeCl})]	31.1

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Table S3: Donor–acceptor interactions associated with chalcogen bonds in doubly-substituted nucleobases along with $E^{(2)}$ values obtained from NBO analysis.

Nucleobase pairs	Donor ⋯ Acceptor	$E^{(2)}$ (kJ mol^{-1})
G_{SF}:C_{SBr}	n[O2 (C_{SBr})]⋯σ*[S–F (G_{SF})]	9.0
	n[O6 (G_{SF})]⋯σ*[S–Br (C_{SBr})]	14.6
G_{SCl}:C_{SBr}	n[O2 (C_{SBr})]⋯σ*[S–Cl (G_{SCl})]	7.3
	n[O6 (G_{SCl})]⋯σ*[S–Br (C_{SBr})]	13.3
G_{SBr}:C_{SBr}	n[O2 (C_{SBr})]⋯σ*[S–Br (G_{SBr})]	8.5
	n[O6 (G_{SBr})]⋯σ*[S–Br (C_{SBr})]	14.1
G_{SeF}:C_{SBr}	n[O2 (C_{SBr})]⋯σ*[Se–F (G_{SeF})]	28.3
	n[O6 (G_{SeF})]⋯σ*[S–Br (C_{SBr})]	16.5
G_{SeCl}:C_{SBr}	n[O2 (C_{SBr})]⋯σ*[Se–Cl (G_{SeCl})]	19.8
	n[O6 (G_{SeCl})]⋯σ*[S–Br (C_{SBr})]	16.2
G_{SeBr}:C_{SBr}	n[O2 (C_{SBr})]⋯σ*[Se–Br (G_{SeBr})]	19.5
	n[O6 (G_{SeBr})]⋯σ*[S–Br (C_{SBr})]	16.2
G_{SF}:C_{SCl}	n[O2 (C_{SCl})]⋯σ*[S–F (G_{SF})]	8.7
	n[O6 (G_{SF})]⋯σ*[S–Cl (C_{SCl})]	13.3
G_{SCl}:C_{SCl}	n[O2 (C_{SCl})]⋯σ*[S–Cl (G_{SCl})]	8.2t
	n[O6 (G_{SCl})]⋯σ*[S–Cl (C_{SCl})]	12.0
G_{SBr}:C_{SCl}	n[O2 (C_{SCl})]⋯σ*[S–Br (G_{SBr})]	5.9
	n[O6 (G_{SBr})]⋯σ*[S–Cl (C_{SCl})]	13.6
G_{SeF}:C_{SCl}	n[O2 (C_{SCl})]⋯σ*[Se–F (G_{SeF})]	26.8
	n[O6 (G_{SeF})]⋯σ*[S–Cl (C_{SCl})]	14.7

G_{SeCl}:C_{SCl}	n[O2 (C_{SCl})]···σ*[Se–Cl (G_{SeCl})]	19.0
	n[O6 (G_{SeCl})]···σ*[S–Cl (C_{SCl})]	14.1
G_{SeBr}:C_{SCl}	n[O2 (C_{SCl})]···σ*[Se–Br (G_{SeBr})]	18.9
	n[O6 (G_{SeBr})]···σ*[S–Cl (C_{SCl})]	14.2
G_{SF}:C_{SF}	n[O2 (C_{SF})]···σ*[S–F (G_{SF})]	8.9
	n[O6 (G_{SF})]···σ*[S–F (C_{SF})]	23.3
G_{SCl}:C_{SF}	n[O2 (C_{SF})]···σ*[S–Cl (G_{SCl})]	6.2
	n[O6 (G_{SCl})]···σ*[S–F (C_{SF})]	22.8
G_{SBr}:C_{SF}	n[O2 (C_{SF})]···σ*[S–Br (G_{SBr})]	8.6
	n[O6 (G_{SBr})]···σ*[S–F (C_{SF})]	22.4
G_{SeF}:C_{SF}	n[O2 (C_{SF})]···σ*[Se–F (G_{SeF})]	27.3
	n[O6 (G_{SeF})]···σ*[S–F (C_{SF})]	25.1
G_{SeCl}:C_{SF}	n[O2 (C_{SF})]···σ*[Se–Cl (G_{SeCl})]	19.5
	n[O6 (G_{SeCl})]···σ*[S–F (C_{SF})]	25.6
G_{SeBr}:C_{SF}	n[O2 (C_{SF})]···σ*[Se–Br (G_{SeBr})]	20.1
	n[O6 (G_{SeBr})]···σ*[S–F (C_{SF})]	26.2
Nucleobase pairs	Donor ··· Acceptor	$E^{(2)}$ (kJ mol-1)
G_{SF}:C_{SeBr}	n[O2 (C_{SeBr})]···σ*[S–F (G_{SF})]	10.8
	n[O6 (G_{SF})]···σ*[Se–Br (C_{SeBr})]	57.1
G_{SCl}:C_{SeBr}	n[O2 (C_{SeBr})]···σ*[S–Cl (G_{SCl})]	9.0
	n[O6 (G_{SCl})]···σ*[Se–Br (C_{SeBr})]	53.4
G_{SBr}:C_{SeBr}	n[O2 (C_{SeBr})]···σ*[S–Br (G_{SBr})]	10.1
	n[O6 (G_{SBr})]···σ*[Se–Br (C_{SeBr})]	54.9

G_{SeF}:C_{SeBr}	n[O2 (C_{SeBr})]···σ*[Se–F (G_{SeF})]	32.0
	n[O6 (G_{SeF})]···σ*[Se–Br (C_{SeBr})]	62.5
G_{SeCl}:C_{SeBr}	n[O2 (C_{SeBr})]···σ*[Se–Cl (G_{SeCl})]	23.3
	n[O6 (G_{SeCl})]···σ*[Se–Br (C_{SeBr})]	61.7
G_{SeBr}:C_{SeBr}	n[O2 (C_{SeBr})]···σ*[Se–Br (G_{SeBr})]	22.8
	n[O6 (G_{SeBr})]···σ*[S–Br (C_{SeBr})]	60.7
G_{SF}:C_{SeCl}	n[O2 (C_{SeCl})]···σ*[S–F (G_{SF})]	10.6
	n[O6 (G_{SF})]···σ*[Se–Cl (C_{SeCl})]	62.6
G_{SCl}:C_{SeCl}	n[O2 (C_{SeCl})]···σ*[S–Cl (G_{SCl})]	8.9
	n[O6 (G_{SCl})]···σ*[Se–Cl (C_{SeCl})]	58.5
G_{SBr}:C_{SeCl}	n[O2 (C_{SeCl})]···σ*[S–Br (G_{SBr})]	10.0
	n[O6 (G_{SBr})]···σ*[Se–Cl (C_{SeCl})]	59.8
G_{SeF}:C_{SeCl}	n[O2 (C_{SeCl})]···σ*[Se–F (G_{SeF})]	32.0
	n[O6 (G_{SeF})]···σ*[Se–Cl (C_{SeCl})]	68.2
G_{SeCl}:C_{SeCl}	n[O2 (C_{SeCl})]···σ*[Se–Cl (G_{SeCl})]	23.1
	n[O6 (G_{SeCl})]···σ*[Se–Cl (C_{SeCl})]	66.5
G_{SeBr}:C_{SeCl}	n[O2 (C_{SeCl})]···σ*[Se–Br (G_{SeBr})]	22.8
	n[O6 (G_{SeBr})]···σ*[Se–Cl (C_{SeCl})]	66.5
G_{SF}:C_{SeF}	n[O2 (C_{SeF})]···σ*[S–F (G_{SF})]	10.5
	n[O6 (G_{SF})]···σ*[Se–F (C_{SeF})]	92.4
G_{SCl}:C_{SeF}	n[O2 (C_{SeF})]···σ*[S–Cl (G_{SCl})]	9.2
	n[O6 (G_{SCl})]···σ*[Se–F (C_{SeF})]	89.0
G_{SBr}:C_{SeF}	n[O2 (C_{SeF})]···σ*[S–Br (G_{SBr})]	10.2

	n[O6 (G_{SBr})]···σ*[Se–F (C_{SeF})]	91.5
G_{SeF}:C_{SeF}	n[O2 (C_{SeF})]···σ*[Se–F (G_{SeF})]	31.4
	n[O6 (G_{SeF})]···σ*[Se–F (C_{SeF})]	96.9
G_{SeCl}:C_{SeF}	n[O2 (C_{SeF})]···σ*[Se–Cl (G_{SeCl})]	23.5
	n[O6 (G_{SeCl})]···σ*[Se–F (C_{SeF})]	96.9
G_{SeBr}:C_{SeF}	n[O2 (C_{SeF})]···σ*[Se–Br (G_{SeBr})]	23.4
	n[O6 (G_{SeBr})]···σ*[Se–F (C_{SeF})]	96.0

Table S4: Electron charge density ($\rho(r)$), Laplacian ($\nabla^2\rho(r)$), and sign(λ_2)$\rho(r)$ at the bond critical point (BCP) between the donor–acceptor chalcogen interactions for base pairs possessing one chalcogen bond.

Modified Base Pairs	X–Y(G_{XY})···O2(C)			H1-N1(G_{XY})···N3(C)			O6(G_{XY})···H4-N4(C)		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G_{SF}:C	0.019	0.063	-0.019	0.037	0.092	-0.037	0.038	0.126	-0.038
G_{SCl}:C	0.016	0.053	-0.016	0.032	0.084	-0.032	0.039	0.129	-0.039
G_{SBr}:C	0.016	0.053	-0.016	0.032	0.083	-0.032	0.040	0.130	-0.040
G_{SeF}:C	0.030	0.100	-0.030	0.043	0.102	-0.043	0.038	0.123	-0.038
G_{SeCl}:C	0.025	0.082	-0.025	0.038	0.094	-0.038	0.039	0.127	-0.039
G_{SeBr}:C	0.024	0.078	-0.024	0.037	0.093	-0.037	0.040	0.129	-0.040
Modified Base Pairs	N2–H2(G)···O2(C_{XY})			H1-N1(G)···N3(C_{XY})			O6(G)···X–Y(C_{XY})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G:C_{SF}	0.025	0.091	-0.025	0.036	0.098	-0.036	0.030	0.100	-0.030
G:C_{SCl}	0.025	0.092	-0.025	0.030	0.087	-0.030	0.021	0.069	-0.021
G:C_{SBr}	0.027	0.100	-0.027	0.025	0.077	-0.025	0.020	0.068	-0.020
G:C_{SeF}	0.026	0.094	-0.026	0.049	0.107	-0.049	0.052	0.153	-0.052
G:C_{SeCl}	0.027	0.099	-0.027	0.039	0.099	-0.039	0.042	0.128	-0.042
G:C_{SeBr}	0.028	0.101	-0.028	0.037	0.097	-0.037	0.039	0.120	-0.039
	C2–H2(A_{XY})··· O2(T)			N1(A_{XY})···H3-N3(T)			X–Y(A_{XY})···O4(T)		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
A_{SF}:T	0.009	0.030	-0.009	0.036	0.093	-0.036	0.009	0.032	-0.009
A_{SCl}:T	0.007	0.024	-0.007	0.031	0.085	-0.031	0.007	0.032	-0.007
A_{SBr}:T	0.011	0.036	-0.011	0.033	0.088	-0.033	0.009	0.030	-0.009
A_{SeF}:T	0.006	0.019	-0.006	0.049	0.102	-0.049	0.027	0.087	-0.027
A_{SeCl}:T	0.010	0.030	-0.010	0.039	0.096	-0.039	0.016	0.049	-0.016
A_{SeBr}:T	0.010	0.032	-0.010	0.039	0.095	-0.039	0.015	0.046	-0.015

Table S5: Electron charge density ($\rho(r)$), Laplacian ($\nabla^2\rho(r)$), and sign(λ_2)$\rho(r)$ at the bond critical point (BCP) between the donor–acceptor chalcogen interactions for base pairs possessing two chalcogen bonds.

Modified Base Pairs	O6(G_{XY})···S–F(C_{SF})			H1-N1(G_{XY})···N3(C_{SF})			X–Y(G_{XY})···O2(C_{SF})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G_{SF}:C_{SF}	0.027	0.094	-0.027	0.035	0.096	-0.035	0.016	0.055	-0.016
G_{SCl}:C_{SF}	0.028	0.002	-0.028	0.038	0.099	-0.038	0.012	0.039	-0.012
G_{SBr}:C_{SF}	0.028	0.096	-0.028	0.031	0.088	-0.031	0.015	0.049	-0.015
G_{SeF}:C_{SF}	0.027	0.090	-0.027	0.321	-0.321	-0.321	0.026	0.088	-0.026
G_{SeCl}:C_{SF}	0.028	0.097	-0.028	0.036	0.099	-0.036	0.021		-0.021
G_{SeBr}:C_{SF}	0.029	0.099	-0.029	0.036	0.098	-0.036	0.021	0.069	-0.021
Modified Base Pairs	O6(G_{XY})···S–Cl(C_{SCl})			H1-N1(G_{XY})···N3(C_{SCl})			X–Y(G_{XY})···O2(C_{SCl})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G_{SF}:C_{SCl}	0.016	0.052	-0.016	0.034	0.095	-0.034	0.018	0.059	-0.018
G_{SCl}:C_{SCl}	0.011	0.037	-0.011	0.035	0.095	-0.035	0.019	0.063	-0.019
G_{SBr}:C_{SCl}	0.019	0.066	-0.019	0.021	0.068	-0.021	0.015	0.053	-0.015
G_{SeF}:C_{SCl}	0.019	0.063	-0.019	0.031	0.031	-0.031	0.028	0.096	-0.028
G_{SeCl}:C_{SCl}	0.019	0.067	-0.019	0.026	0.081	-0.026	0.022	0.076	-0.022
G_{SeBr}:C_{SCl}	0.019	0.067	-0.019	0.026	0.080	-0.026	0.022	0.074	-0.022
Modified Base Pairs	O6(G_{XY})···S–Br(C_{SBr})			H1-N1(G_{XY})···N3(C_{SBr})			X–Y(G_{XY})···O2(C_{SBr})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G_{SF}:C_{SBr}	0.019	0.066	-0.019	0.026	0.079	-0.026	0.017	0.061	-0.017
G_{SCl}:C_{SBr}	0.019	0.068	-0.019	0.022	0.068	-0.022	0.014	0.050	-0.014
G_{SBr}:C_{SBr}	0.020	0.068	-0.020	0.022	0.069	-0.022	0.015	0.053	-0.015
G_{SeF}:C_{SBr}	0.019	0.065	-0.019	0.031	0.092	-0.031	0.028	0.097	-0.028
G_{SeCl}:C_{SBr}	0.020	0.069	-0.020	0.027	0.082	-0.027	0.022	0.076	-0.022
G_{SeBr}:C_{SBr}	0.019	0.067	-0.019	0.026	0.080	-0.026	0.022	0.074	-0.022
Modified Base Pairs	O6(G_{XY})···Se–F(C_{SeF})			H1-N1(G_{XY})···N3(C_{SeF})			X–Y(G_{XY})···O2(C_{SeF})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$

G_{SF}:C_{SeF}	0.048	0.150	-0.048	0.049	0.106	-0.049	0.017	0.056	-0.017
G_{SCl}:C_{SeF}	0.048	0.151	-0.048	0.043	0.101	-0.043	0.015	0.049	-0.015
G_{SBr}:C_{SeF}	0.049	0.152	-0.049	0.043	0.101	-0.043	0.015	0.050	-0.015
G_{SeF}:C_{SeF}	0.049	0.146	-0.049	0.057	0.111	-0.057	0.027	0.088	-0.027
G_{SeCl}:C_{SeF}	0.049	0.151	-0.049	0.050	0.107	-0.050	0.022	0.071	-0.022
G_{SeBr}:C_{SeF}	0.049	0.151	-0.049	0.049	0.107	-0.049	0.022	0.070	-0.022
Modified Base Pairs	O6(G_{XY})···Se–Cl(C_{SeCl})			H1-N1(G_{XY})···N3(C_{SeCl})			X–Y(G_{XY})···O2(C_{SeCl})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G_{SF}:C_{SeCl}	0.038	0.121	-0.038	0.039	0.100	-0.039	0.018	0.061	-0.018
G_{SCl}:C_{SeCl}	0.038	0.124	-0.038	0.012	0.055	-0.012	0.038	0.124	-0.038
G_{SBr}:C_{SeCl}	0.038	0.123	-0.038	0.034	0.092	-0.034	0.016	0.054	-0.016
G_{SeF}:C_{SeCl}	0.038	0.120	-0.038	0.046	0.108	-0.046	0.028	0.095	-0.028
G_{SeCl}:C_{SeCl}	0.039	0.124	-0.039	0.040	0.102	-0.040	0.023	0.076	-0.023
G_{SeBr}:C_{SeCl}	0.039	0.124	-0.039	0.039	0.100	-0.039	0.022	0.074	-0.022
Modified Base Pairs	O6(G_{XY})···Se–Br(C_{SeBr})			H1-N1(G_{XY})···N3(C_{SeBr})			X–Y(G_{XY})···O2(C_{SeBr})		
	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	sign(λ_2)$\rho(r)$
G_{SF}:C_{SeBr}	0.035	0.115	-0.035	0.037	0.098	-0.037	0.018	0.063	-0.018
G_{SCl}:C_{SeBr}	0.035	0.116	-0.035	0.032	0.089	-0.032	0.016	0.053	-0.016
G_{SBr}:C_{SeBr}	0.035	0.116	-0.035	0.032	0.089	-0.032	0.016	0.055	-0.016
G_{SeF}:C_{SeBr}	0.035	0.113	-0.035	0.044	0.107	-0.044	0.028	0.096	-0.028
G_{SeCl}:C_{SeBr}	0.036	0.117	-0.036	0.038	0.100	-0.038	0.023	0.077	-0.023
G_{SeBr}:C_{SeBr}	0.035	0.116	-0.035	0.032	0.089	-0.032	0.016	0.055	-0.016

Table S6. Average and standard deviation in the bond distance and angle of the chalcogen bond in the modified bases from the last 400 ns of MD simulations.

DNA Base pair Position 6:17	Chalcogen Bond	Average length of chalcogen bond (std. dev.) (Å)	Average bond angle (std. dev.) (deg.)
G_{SeF}:C	Se–F···O2	3.128 (0.177)	143.5 (10.2)
G:C_{SeF}	O6···Se–F	3.535 (0.181)	132.7 (10.5)
A_{SeF}:T	Se–F···O4	3.857 (0.563)	70.9 (50.6)
G_{SeF}:C_{SeF}	Se–F···O2	3.213 (0.227)	153.5 (15.9)
	O6···Se–F	4.016 (0.925)	134.5 (42.0)

Table S7. Occupancies (%) of the hydrogen bonds in the modified base pair, and the 3′ and 5' flanking base pairs over the last 400 ns of the MD simulations.[a]

Base pair 6-17	Base pairs	Hydrogen bond	Occupancy
Natural base pair, A:T	5′–A:T	(A5) N1···H3–N3 (T18) (T18) O4···H6–N6 (A5)	99.4 96.3
	A:T	(A6) N1···H3–N3 (T17) (T17) O4···H6–N6 (A6)	99.7 94.9
	3′–T:A	(A7) N1···H3–N3 (T16) (T16) O4···H6–N6 (A7)	99.8 95.2
Natural base pair, G:C	5′–A:T	(A5) N1···H3–N3 (T18) (T18) O4···H6–N6 (A5)	99.2 91.9
	G:C	(G6) O6···H4–N4 (C17) (C17) N3···H1-N1 (G6) (C17) O2···H2-N2 (G6)	97.6 99.9 99.9
	3′–T:A	(A7) N1···H3–N3 (T16) (T16) O4···H6–N6 (A7)	99.0 94.5
Modified base pair, G:C_{SeF}	5′–A:T	(A5) N1···H3–N3 (T18) (T18) O4···H6–N6 (A5)	99.6 96.7
	G:C_{SeF}	(C_{SeF}17)N3···H1-N1(G6) (C_{SeF}17) O2···H2-N2(G6)	85.0 98.9
	3′–T:A	(A7) N1···H3–N3 (T16) (T16) O4···H6–N6 (A7)	99.8 90.0
Modified base pair, G_{SeF}:C	5′–A:T	(A5) N1···H3–N3 (T18) (T18) O4···H6–N6 (A5)	99.1 94.9

	G_{SeF}:C	(G_{SeF}6)O6···H4–N4(C17) (C17) N3···H1-N1 (G_{SeF}6)	98.4 97.6
	3′–T:A	(A7) N1···H3–N3 (T16) (T16) O4···H6–N6 (A7)	99.5 97.9
Modified base pair, A_{SeF}:T	5′–A:T	(A5) N1···H3–N3 (T18) (T18) O4···H6–N6 (A5)	99.2 95.3
	A_{SeF}:T	(A_{SeF}6)N1···H3–N3 (T17)	70.8
	3′–T:A	(A7) N1···H3–N3 (T16) (T16) O4···H6–N6 (A7)	99.4 95.5
Modified base pair, G_{SeF}:C_{SeF}	5′–A:T	(A5) N1···H3–N3 (T18) (T18) O4···H6–N6 (A5)	99.5 96.6
	G_{SeF}:C_{SeF}	(C_{SeF}17)N3···H1-N1(G_{SeF}6)	73.9
	3′–T:A	(A7) N1···H3–N3 (T16) (T16) O4···H6–N6 (A7)	99.4 94.3

[a]Hydrogen-bonding interactions were determined using a cut off of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle. See Figure S2 for DNA sequence and base numbering.

Table S8. IEFPCM-B3LYP/6-311+G(2df,p)//IEFPCM-B3LYP/6-31G(d,p) electronic energies, zero-point vibrational energy corrections (ZPVE) and ZPVE-corrected electronic energies of the species involved in the disproportionation and hydrolysis reactions in Figure S36.

	Aqueous environment[a]			DNA environment[b]		
Species	Electronic energy (Hartrees)	ZPVE correction (Hartrees)	ZPVE corrected energy (Hartrees)	Electronic energy (Hartrees)	ZPVE correction (Hartrees)	ZPVE corrected energy (Hartrees)
G^{SeF}	–2988.187994	0.09165	-2988.096344	-2988.183065	0.09162	-2988.091445
$G^{SeSeF2}G$	-5976.419474	0.185558	-5976.233916	-5976.412431	0.18561	-5976.226821
G^{SeF3}	-3187.941802	0.097017	-3187.844785	-3187.93675	0.097034	-3187.839716
$G^{SeSe}G$	-5776.687993	0.181168	-5776.506825	-5776.681448	0.181168	-5776.50028
G^{SeOH}	-2964.170612	0.103811	-2964.066801	-2964.165607	0.103798	-2964.061809
C^{SeF}	-2840.517211	0.074039	-2840.443172	-2840.513769	0.074032	-2840.439737
$C^{SeSeF2}C$	-5681.057208	0.149579	-5680.907629	-5680.834983	0.149553	-5680.68543
C^{SeF3}	-3040.263692	0.078818	-3040.184874	-3040.257789	0.078847	-3040.178942
$C^{SeSe}C$	-5481.329985	0.145523	-5481.184462	-5481.323314	0.145468	-5481.177846
C^{SeOH}	-2816.497404	0.086195	-2816.411209	-2816.493191	0.086161	-2816.40703
HF	-100.489879	0.009233	-100.480646	-100.48884	0.009247	-100.479593
H_2O	-76.467785	0.021312	-76.446473	-76.466406	0.021336	-76.44507

[a]Aqueous environment was modeled using the dielectric constant of water. [b]The DNA environment was modeled using dielectric constant of THF (see Computational Details).

Table S9. IEFPCM-B3LYP/6-311+G(2df.p)//IEFPCM-B3LYP/6-31G(d.p) zero-point vibrational energy-corrected reaction energies (kcal mol^{-1}) for the total disproportionation reactions a + b: $3G^{SeF} \rightarrow G^{SeF3} + G^{Se\text{-}Se}G$ or $3C^{SeF} \rightarrow C^{SeF3} + C^{Se\text{-}Se}C$ and partial reactions a (dimerization) $2G^{SeF} \rightarrow G^{SeSeF2}G$ or $2C^{SeF} \rightarrow C^{SeSeF2}C$, b (disproportionation): $G^{SeSeF2}G + G^{SeF} \rightarrow G^{SeF3} + G^{Se\text{-}Se}G$ or $C^{SeSeF2}C + C^{SeF} \rightarrow C^{SeF3} + C^{Se\text{-}Se}C$.

Species	Aqueous environment[a]			DNA environment[b]		
	a	b	a + b	a	b	a + b
G^{SeF}	–25.9	–13.4	–39.3	–27.6	–13.4	–41.2
C^{SeF}	–107.2	+82.2	–25.0	–106.7	+83.1	–23.6

[a]Aqueous environment was modeled using the dielectric constant of water. [b]The DNA environment was modeled using the dielectric constant of THF (see Computational Details).

Table S10. IEFPCM-B3LYP/6-311+G(2df.p)//IEFPCM-B3LYP/6-31G(d,p) zero-point vibrational energy-corrected reaction energies (kcal mol^{-1}) for the hydrolysis reaction: $G^{SeF} + H_2O \rightarrow G^{SeOH} + G^{SeOH}$ or $C^{SeF} + H_2O \rightarrow C^{SeOH} + C^{SeOH}$.

Species	Aqueous environment[a]	DNA environment[b]
G^{SeF}	–2.9	–3.1
C^{SeF}	–1.2	–1.4

Table S11. Cartesian coordinates of A_{SF}:T
Energy (in hartrees) =-1363.887158093325

ATOM	X	Y	Z
N	-0.79142600	0.54239100	0.00046200
C	-1.18975100	1.83054900	0.00045300
N	-2.44801700	2.27549300	0.00020200
C	-3.33553600	1.27990300	-0.00003800
C	-3.07011800	-0.11110900	-0.00005700
C	-1.70478100	-0.44255000	0.00020400
N	-4.70466200	1.37488400	-0.00029700
C	-5.19099600	0.08059900	-0.00052000
N	-4.25362100	-0.83264100	-0.00036600
H	-0.38922400	2.56543100	0.00061500
H	-5.23474900	2.23458300	-0.00034700
H	-6.25338600	-0.12286600	-0.00076400
N	2.11470600	0.50595600	0.00009900
C	2.67542000	1.76367300	-0.00000100
N	4.06432400	1.75121000	-0.00016800
C	4.81592000	0.59221800	-0.00027300
C	4.25225800	-0.63888700	-0.00017700
C	2.78644200	-0.71959700	0.00003600
O	2.14821700	-1.77076000	0.00013900
O	2.02692700	2.80508300	0.00005600
C	5.03142100	-1.92135900	-0.00027100
H	1.08008300	0.46248300	0.00022200
H	4.50455900	2.66031700	-0.00029500
H	5.89107000	0.73824500	-0.00042200
H	4.78029900	-2.52609300	0.87754400
H	6.10866600	-1.73140500	-0.00038700
H	4.78011100	-2.52608300	-0.87804000
S	-0.98517200	-2.05158800	0.00024500
F	-2.35518300	-2.97838600	0.00008100

Table S12. Cartesian coordinates of A_{SCl}:T
Energy (in hartrees) =-1724.258192575887

ATOM	X	Y	Z
N	0.64616400	-0.73112500	-0.00005600
C	0.92619300	-2.04975900	-0.00013700
N	2.14099000	-2.60375600	-0.00023100
C	3.11159000	-1.69105400	-0.00030700
C	2.97090300	-0.28057500	-0.00028700
C	1.64098800	0.17105700	-0.00011700
N	4.46672600	-1.90941900	-0.00049100
C	5.06815900	-0.66543400	-0.00064700
N	4.21697200	0.32831600	-0.00053000
H	0.06366300	-2.70987500	-0.00004700
H	4.91593300	-2.81399800	-0.00056600
H	6.14450100	-0.55808900	-0.00083100
N	-2.30878600	-0.49976400	0.00020200
C	-2.89611300	-1.74604100	0.00073400
N	-4.28373400	-1.70755600	0.00079600
C	-5.01493500	-0.53542900	0.00021900

C	-4.42818700	0.68404100	-0.00040300
C	-2.96011300	0.74112100	-0.00047700
O	-2.30846700	1.78138100	-0.00109100
O	-2.27138500	-2.80230500	0.00111200
C	-5.18331400	1.98074800	-0.00103400
H	-1.27618900	-0.48361600	0.00015400
H	-4.73950200	-2.60891400	0.00112800
H	-6.09250800	-0.66225700	0.00030600
H	-4.92062900	2.58118600	0.87635400
H	-6.26394600	1.81085000	-0.00095700
H	-4.92061900	2.58034000	-0.87899700
S	0.97536600	1.81382100	-0.00021900
Cl	2.62134800	3.07186500	0.00139300

Table S13. Cartesian coordinates of ASBr:T

Energy (in hartrees) =-3838.179789180962

ATOM	**X**	**Y**	**Z**
N	-0.24072900	1.15483300	0.00042200
C	-0.38991500	2.49402100	0.00056000
N	-1.54502400	3.16447100	0.00046500
C	-2.60047200	2.35044700	0.00016700
C	-2.59605600	0.93349000	-0.00001400
C	-1.31789200	0.35246700	0.00008900
N	-3.92905600	2.69700200	-0.00005000
C	-4.64661100	1.51592500	-0.00048800
N	-3.89379000	0.44534500	-0.00029200
H	0.53379400	3.06540900	0.00073300
H	-4.29066200	3.64005400	0.00003100
H	-5.72827000	1.51145500	-0.00076800
N	2.63593100	0.52207800	-0.00030800
C	3.38282200	1.67960500	-0.00056300
N	4.75349500	1.45933700	-0.00036200
C	5.32304400	0.20098900	-0.00012000
C	4.57950500	-0.92958300	-0.00001300
C	3.11694300	-0.79403700	-0.00016100
O	2.33701300	-1.74178600	0.00033300
O	2.90160900	2.80857300	0.00003800
C	5.15941300	-2.31353600	0.00026100
H	1.61030800	0.65104600	-0.00012800
H	5.32399700	2.29282700	-0.00009800
H	6.40790300	0.18368500	0.00001800
H	4.82034700	-2.87434300	0.87766800
H	6.25295200	-2.28552900	0.00065900
H	4.82100600	-2.87443900	-0.87734500
S	-0.81113900	-1.34425600	-0.00013200
Br	-2.66321800	-2.55361600	0.00002700

Table S14. Cartesian coordinates of A_{SeF}:T

Energy (in hartrees) =-3367.225982936691

ATOM	**X**	**Y**	**Z**
N	0.63397400	0.92471300	0.00018800
C	1.06551400	2.20064600	0.00014100
N	2.33221800	2.61560400	0.00003400

C	3.18991400	1.59319000	-0.00007500
C	2.88245000	0.20940600	-0.00007400
C	1.50995100	-0.09604400	0.00008900
N	4.56012600	1.65268600	-0.00037500
C	5.01025200	0.34493900	-0.00037700
N	4.04856600	-0.54116700	-0.00030700
H	0.28479900	2.95761500	0.00017800
H	5.11336900	2.49754100	-0.00049700
H	6.06665500	0.11215100	-0.00057500
N	-2.15950600	0.80735300	0.00023600
C	-2.89789600	1.96997400	0.00013600
N	-4.27166800	1.74883900	-0.00007400
C	-4.84011200	0.49182200	-0.00021300
C	-4.09759100	-0.64258000	-0.00022700
C	-2.64338100	-0.48957100	-0.00000600
O	-1.84995200	-1.44117100	-0.00005000
O	-2.40715800	3.09194800	0.00035400
C	-4.67000500	-2.02968200	-0.00048200
H	-1.11668700	0.88921400	0.00035000
H	-4.84440900	2.58125600	0.00006700
H	-5.92494800	0.47347000	-0.00034400
H	-4.32981700	-2.58813200	-0.87885900
H	-5.76342600	-2.00747900	-0.00011300
H	-4.32921000	-2.58867800	0.87730300
Se	0.74099700	-1.84090200	0.00013500
F	2.29401400	-2.74570000	0.00045600

Table S15. Cartesian coordinates of A_{SeCl}:Tl

Energy (in hartrees) =-3727.598007069118

ATOM	**X**	**Y**	**Z**
N	0.48552600	1.02506900	0.00000700
C	0.75935800	2.34430800	0.00004000
N	1.97036900	2.90494700	0.00002800
C	2.94382000	1.99410200	-0.00004100
C	2.80429000	0.58332600	-0.00009800
C	1.48056300	0.12137400	-0.00004900
N	4.29790400	2.21568100	-0.00006900
C	4.90107600	0.97190600	-0.00017800
N	4.05105200	-0.02210000	-0.00020600
H	-0.10621900	3.00170900	0.00010700
H	4.74673200	3.12054900	-0.00004800
H	5.97757900	0.86621800	-0.00023000
N	-2.37369800	0.71261200	0.00004500
C	-3.08467200	1.89228400	0.00011800
N	-4.46191100	1.70808000	-0.00003300
C	-5.06440600	0.46569600	-0.00004600
C	-4.35270600	-0.68674200	-0.00008600
C	-2.89056900	-0.58177400	-0.00004900
O	-2.12605200	-1.54844200	-0.00011900
O	-2.56834300	3.00437600	0.00029700
C	-4.96547600	-2.05654200	-0.00016200
H	-1.33858200	0.79156700	0.00009700

H	-5.01141900	2.55577400	0.00024200
H	-6.14934800	0.47746300	-0.00007800
H	-4.64121100	-2.62512000	-0.87812600
H	-6.05790900	-2.00211400	-0.00026500
H	-4.64138300	-2.62515000	0.87784800
Se	0.79505100	-1.65533300	-0.00002200
Cl	2.63369600	-2.88380500	0.00027600

Table S16. Cartesian coordinates of A_{SeBr}:T

Energy (in hartrees) =-5841.520329610640

ATOM	X	Y	Z
N	0.05666100	1.31795300	-0.00061900
C	0.14395600	2.66222900	-0.00065300
N	1.26528700	3.38658400	-0.00031100
C	2.35597500	2.62036200	0.00016100
C	2.41333600	1.20407100	0.00027100
C	1.16765300	0.56093100	-0.00017100
N	3.66652600	3.02728100	0.00066100
C	4.43618900	1.87917800	0.00110700
N	3.73173800	0.77707100	0.00090200
H	-0.80462600	3.19254500	-0.00100300
H	3.98574400	3.98560600	0.00072800
H	5.51695500	1.92339000	0.00156400
N	-2.74207700	0.62227800	-0.00010900
C	-3.59080700	1.70706100	-0.00037300
N	-4.93573400	1.35816700	-0.00008400
C	-5.38478800	0.05232200	0.00030900
C	-4.53934000	-1.00552400	0.00047900
C	-3.09994000	-0.72575200	0.00026300
O	-2.22586500	-1.59320700	0.00031200
O	-3.21415200	2.87410600	-0.00068800
C	-4.98221600	-2.43923600	0.00088600
H	-1.72441400	0.82627300	-0.00033400
H	-5.58294200	2.13378800	-0.00019000
H	-6.46330300	-0.06630300	0.00046500
H	-4.59158300	-2.96468000	-0.87692600
H	-6.07323100	-2.51727600	0.00091400
H	-4.59157800	-2.96418900	0.87899100
Br	2.81351700	-2.35624900	-0.00034300
Se	0.72232700	-1.28961300	-0.00017500

Table S17. Cartesian coordinates of G:C_{SF}

Energy (in hartrees) =-1379.947840058597

ATOM	X	Y	Z
C	-4.96131800	-1.36220600	0.16479000
C	-3.63189900	0.40273500	-0.01101900
N	-3.76103500	-1.88117700	0.18198800
C	-2.90976700	-0.79507500	0.07269400
N	-3.17357900	1.66858500	-0.12232200
H	-5.88786800	-1.91553300	0.23061400
C	-1.48223100	-0.71114100	0.03689200
C	-1.85118800	1.72841000	-0.15919400
O	-0.64192900	-1.62439900	0.10317800

N	-1.04668100	0.61727600	-0.08908100
H	-0.02031600	0.70415200	-0.10146000
N	3.76674200	1.84481700	0.18126800
C	2.36901300	1.75698200	0.09140100
C	4.57342100	0.75002200	0.17032800
O	1.69741800	2.79211500	0.09909700
N	1.83283100	0.49973700	-0.00479700
C	4.03745600	-0.49884600	0.07492000
H	5.64024900	0.93051700	0.24334600
C	2.60707300	-0.57335900	-0.00840200
H	4.65882100	-1.38049800	0.06680300
H	4.14560500	2.78115800	0.24932000
N	-4.94764800	0.02136200	0.04949400
H	-5.74042000	0.64518000	0.01351200
N	-1.22318500	2.92169200	-0.29685500
H	-1.79914300	3.74535100	-0.22660200
H	-0.21755200	2.99749700	-0.15366500
S	1.81005200	-2.15327800	-0.11338000
F	3.24226800	-3.04758800	-0.22425800

Table S18. Cartesian coordinates of G:C_{SCl}

Energy (in hartrees) =-1740.315201575630

ATOM	**X**	**Y**	**Z**
C	-4.96131800	-1.36220600	0.16479000
C	-3.63189900	0.40273500	-0.01101900
N	-3.76103500	-1.88117700	0.18198800
C	-2.90976700	-0.79507500	0.07269400
N	-3.17357900	1.66858500	-0.12232200
H	-5.88786800	-1.91553300	0.23061400
C	-1.48223100	-0.71114100	0.03689200
C	-1.85118800	1.72841000	-0.15919400
O	-0.64192900	-1.62439900	0.10317800
N	-1.04668100	0.61727600	-0.08908100
H	-0.02031600	0.70415200	-0.10146000
N	3.76674200	1.84481700	0.18126800
C	2.36901300	1.75698200	0.09140100
C	4.57342100	0.75002200	0.17032800
O	1.69741800	2.79211500	0.09909700
N	1.83283100	0.49973700	-0.00479700
C	4.03745600	-0.49884600	0.07492000
H	5.64024900	0.93051700	0.24334600
C	2.60707300	-0.57335900	-0.00840200
H	4.65882100	-1.38049800	0.06680300
H	4.14560500	2.78115800	0.24932000
N	-4.94764800	0.02136200	0.04949400
H	-5.74042000	0.64518000	0.01351200
N	-1.22318500	2.92169200	-0.29685500
H	-1.79914300	3.74535100	-0.22660200
H	-0.21755200	2.99749700	-0.15366500
S	1.81005200	-2.15327800	-0.11338000
F	3.24226800	-3.04758800	-0.22425800

Table S19. Cartesian coordinates of G:C_{SBr}
Energy (in hartrees) =-3854.236572513111

ATOM	X	Y	Z
C	-5.25128400	-2.21103500	0.03829200
C	-4.34315600	-0.18950100	-0.00244700
N	-3.96568800	-2.45167400	0.03791800
C	-3.37517800	-1.19959000	0.01244800
N	-4.17679700	1.15143100	-0.02809200
H	-6.03259700	-2.95822100	0.05487700
C	-1.99582800	-0.80942600	0.00348200
C	-2.90116900	1.50645200	-0.04002400
O	-0.97982700	-1.51051400	0.01539300
N	-1.86617700	0.60001100	-0.02245900
H	-0.89515000	0.92819000	-0.02500100
N	2.51355700	3.24676400	0.03533200
C	1.20409900	2.73364100	0.02284400
C	3.61557100	2.45394500	0.03189000
O	0.25589000	3.52092200	0.02803700
N	1.07568100	1.36913500	0.00582900
C	3.48325400	1.09735100	0.01671800
H	4.57759300	2.95466200	0.04215500
C	2.14656100	0.59085000	0.00546100
H	4.34871400	0.45360400	0.01452800
H	2.58756000	4.25656700	0.04719800
N	-5.54318200	-0.85393400	0.01468000
H	-6.45388500	-0.41878300	0.00869800
N	-2.56578600	2.81653800	-0.08249500
H	-3.31887300	3.48378000	-0.04586600
H	-1.59801100	3.12905700	-0.03252400
S	1.73700800	-1.13787200	-0.00532600
Br	3.74244400	-2.13400500	-0.01666500

Table S20. Cartesian coordinates of G:C_{SeF}
Energy (in hartrees) =-3383.292949490667

ATOM	X	Y	Z
C	4.95274000	-1.49770000	0.00040700
C	3.78310300	0.38540100	0.00000400
N	3.71315000	-1.91212200	0.00010200
C	2.95918500	-0.75119100	-0.00000800
N	3.43341000	1.68686000	-0.00008600
H	5.82818400	-2.13222300	0.00068600
C	1.55367000	-0.53258800	-0.00021100
C	2.11818600	1.86080700	-0.00034700
O	0.64565900	-1.40069600	-0.00020900
N	1.22345600	0.81689200	-0.00040900
H	0.19609300	0.98188400	-0.00038900
N	-3.44196800	2.31938000	0.00091900
C	-2.04924700	2.18297400	0.00030100
C	-4.28111700	1.24595200	0.00023900
O	-1.33854200	3.19495800	0.00003000
N	-1.55275000	0.90728000	-0.00005100
C	-3.77954900	-0.01943500	-0.00032200

H	-5.34411900	1.46040500	0.00025900
C	-2.35210600	-0.15006200	-0.00018100
H	-4.42439300	-0.88449700	-0.00084300
H	-3.79406800	3.26832400	0.00108600
N	5.06004400	-0.11259600	0.00057200
H	5.90459500	0.44052400	0.00085100
N	1.58906100	3.10272100	-0.00064400
H	2.22676400	3.88182900	-0.00056800
H	0.57990300	3.25307400	-0.00031300
F	-3.26034800	-2.68291800	0.00005900
Se	-1.58490500	-1.89650000	-0.00005800

Table S21. Cartesian coordinates of G:C_{SeCl}

Energy (in hartrees) =-3743.659243142333

ATOM	X	Y	Z
C	5.02004600	-1.89560700	0.00123400
C	4.04023500	0.09263100	0.00048800
N	3.74540100	-2.18561000	0.00077400
C	3.10945400	-0.95606900	0.00037000
N	3.81994500	1.42311300	0.00014600
H	5.82875200	-2.61323600	0.00165900
C	1.72826000	-0.60532800	-0.00020500
C	2.52957900	1.72712200	-0.00049800
O	0.73986900	-1.37069300	-0.00043000
N	1.53367900	0.77736300	-0.00065500
H	0.53645300	1.04900800	-0.00118300
N	-2.95665900	2.87170200	0.00156800
C	-1.59878300	2.52565000	-0.00067500
C	-3.94764300	1.94054300	0.00288000
O	-0.74957000	3.42302700	-0.00216700
N	-1.29753400	1.18889500	-0.00114900
C	-3.63934100	0.61391200	0.00236400
H	-4.96661400	2.31168100	0.00436800
C	-2.25173300	0.26861100	0.00041800
H	-4.41756300	-0.13287700	0.00333900
H	-3.15915900	3.86363700	0.00171100
N	5.26258700	-0.52776500	0.00107300
H	6.15728700	-0.06021200	0.00129400
N	2.13149200	3.01725100	-0.00116900
H	2.84768700	3.72481700	-0.00051600
H	1.14434400	3.27191600	-0.00130200
Se	-1.65857700	-1.55588400	-0.00060300
Cl	-3.71263400	-2.53863500	-0.00061700

Table S22. Cartesian coordinates of G:C_{SeBr}

Energy (in hartrees) =-5857.580482403244

ATOM	X	Y	Z
C	5.09662400	-2.45237600	0.00042500
C	4.41473800	-0.34348400	0.00018800
N	3.79327800	-2.55459900	0.00014400
C	3.34207100	-1.24585400	0.00006000
N	4.39021300	1.00498500	0.00016100
H	5.79299900	-3.27945400	0.00059500

C	2.02477400	-0.69985300	-0.00018600
C	3.15785900	1.49350100	-0.00005200
O	0.93647000	-1.31066700	-0.00022700
N	2.03402100	0.69873000	-0.00024400
H	1.08901200	1.11483100	-0.00041900
N	-2.08243200	3.49512700	0.00066000
C	-0.79773200	2.93391200	-0.00033100
C	-3.21069000	2.73682300	0.00113000
O	0.18335400	3.68462600	-0.00109400
N	-0.71494500	1.56620700	-0.00059800
C	-3.11893300	1.37828300	0.00085200
H	-4.15673500	3.26705900	0.00178100
C	-1.80627500	0.81307700	0.00000600
H	-4.00663500	0.76592000	0.00123600
H	-2.12105600	4.50678600	0.00070600
N	5.53463800	-1.13416800	0.00046700
H	6.48747000	-0.80072100	0.00065000
N	2.95383400	2.82819100	-0.00014600
H	3.76703700	3.42173300	-0.00008300
H	2.01550300	3.22713700	-0.00042100
Br	-3.79443000	-1.81510400	-0.00004900
Se	-1.49988300	-1.07946500	-0.00021900

Table S23. Cartesian coordinates of G_{SF}:C

Energy (in hartrees) =-1379.948339385277

ATOM	**X**	**Y**	**Z**
C	-4.69880200	-1.70670800	0.00071400
C	-3.20911300	-0.07642200	0.00037000
N	-3.55028500	-2.33857900	0.00043500
C	-2.60286900	-1.33296000	0.00021800
N	-2.62023900	1.14024400	0.00025100
H	-5.67290200	-2.17587600	0.00094100
C	-1.17018200	-1.39009900	-0.00013600
C	-1.31520300	1.07391000	-0.00009200
O	-0.44959300	-2.39517600	-0.00040500
N	-0.59584000	-0.09288600	-0.00028100
H	0.44568400	-0.09866900	-0.00032200
N	4.30411400	0.86276400	0.00113000
C	2.89349700	0.84168000	0.00091800
C	5.05004000	-0.27700500	0.00039300
O	2.27978500	1.91245100	0.00157900
N	2.28535400	-0.37306300	0.00001700
C	4.44354900	-1.49251800	-0.00050000
H	6.12746000	-0.15371800	0.00058800
C	2.99895100	-1.50517100	-0.00060500
H	5.01970600	-2.40883800	-0.00106800
N	2.32148800	-2.65883600	-0.00135200
H	1.28965900	-2.63135700	-0.00109300
H	2.80605900	-3.54163900	-0.00180700
H	4.73196900	1.77907700	0.00178600
N	-4.55642200	-0.32986700	0.00068100
H	-5.28558000	0.36895900	0.00091600

S	-0.38867900	2.61406600	-0.00050600
F	-1.70456800	3.62468100	-0.00167600

Table S24. Cartesian coordinates of G_{SCl}:C

Energy (in hartrees) =-1740.319876308171

ATOM	X	Y	Z
C	4.41481200	-2.36533100	-0.00149400
C	3.09969100	-0.59235000	-0.00114800
N	3.20745600	-2.87616400	-0.00100000
C	2.36853000	-1.77874700	-0.00081200
N	2.63513500	0.67760700	-0.00104500
H	5.33573100	-2.93177700	-0.00181900
C	0.93702700	-1.69012800	-0.00009600
C	1.33183700	0.74813600	-0.00060100
O	0.12212600	-2.61824700	0.00056800
N	0.49494200	-0.34073400	-0.00019700
H	-0.54086300	-0.23788200	-0.00002800
N	-4.41082800	1.01180900	-0.00287400
C	-3.00071200	0.91034900	-0.00371700
C	-5.22472200	-0.07879100	0.00066200
O	-2.33467400	1.94617100	-0.00713300
N	-2.46202400	-0.34143900	-0.00099000
C	-4.69027600	-1.32707300	0.00340200
H	-6.29297900	0.10855500	0.00110900
C	-3.24848400	-1.42487200	0.00225200
H	-5.31811200	-2.20877900	0.00618600
N	-2.65332400	-2.62416300	0.00447200
H	-1.62382200	-2.67658100	0.00299800
H	-3.20113200	-3.46909600	0.00697500
H	-4.78101900	1.95279300	-0.00500100
N	4.41407200	-0.98109200	-0.00159400
H	5.21128100	-0.36101400	-0.00196600
S	0.50285900	2.34570400	-0.00026800
Cl	2.13890300	3.62242300	0.00472200

Table S25. Cartesian coordinates of G_{SBr}:C

Energy (in hartrees) =-3854.241959516558

ATOM	X	Y	Z
C	3.53326100	3.56074800	-0.00006300
C	2.60737500	1.55600500	0.00001000
N	2.24715200	3.81437900	0.00013200
C	1.64981800	2.56877900	0.00017200
N	2.41386400	0.21712000	-0.00001500
H	4.31928600	4.30311900	-0.00018600
C	0.26643800	2.19039400	0.00038300
C	1.15051600	-0.11646100	0.00013200
O	-0.72175700	2.93184000	0.00059900
N	0.10998200	0.78014500	0.00025100
H	-0.88105300	0.46161500	0.00033300
N	-4.42513000	-1.58631400	0.00039700
C	-3.06164500	-1.20897300	0.00052100
C	-5.43898100	-0.67967900	-0.00034100
O	-2.20770900	-2.09477300	0.00104100

N	-2.78135300	0.12614300	0.00010100
C	-5.16262800	0.64955000	-0.00084300
H	-6.44889500	-1.07521600	-0.00045600
C	-3.76876000	1.03077100	-0.00048200
H	-5.95222300	1.38985100	-0.00135700
N	-3.42737100	2.32548800	-0.00056600
H	-2.43077300	2.59057000	-0.00039100
H	-4.13587200	3.04115100	-0.00144900
H	-4.60096400	-2.58208100	0.00075600
N	3.81482900	2.20552000	-0.00018100
H	4.72190300	1.76150200	-0.00004400
S	0.65582400	-1.84292300	0.00022600
Br	2.62957000	-2.84527000	-0.00033500

Table S26. Cartesian coordinates of G_{SeF}:C

Energy (in hartrees) =-3383.290088829925

ATOM	X	Y	Z
C	-4.64980600	-2.02564100	-0.00077300
C	-3.14491000	-0.40926300	-0.00031100
N	-3.50761800	-2.66943300	-0.00057800
C	-2.55000500	-1.67332900	-0.00027700
N	-2.55006900	0.80327900	-0.00017200
H	-5.62826600	-2.48578900	-0.00106000
C	-1.11842700	-1.73618700	0.00053900
C	-1.24724000	0.73051200	0.00011300
O	-0.39366600	-2.74208800	0.00139600
N	-0.54478500	-0.44355200	0.00047700
H	0.49429700	-0.45508100	0.00097800
N	4.23318100	0.65609500	-0.00053600
C	2.83132000	0.56652700	0.00023700
C	5.02669600	-0.45266000	-0.00128600
O	2.16821300	1.61495000	0.00019100
N	2.27928000	-0.66563400	0.00102300
C	4.47579500	-1.69506500	-0.00098800
H	6.09733900	-0.28136000	-0.00194200
C	3.03381700	-1.77194400	0.00008100
H	5.09371800	-2.58369900	-0.00142700
N	2.39182500	-2.94336500	0.00092500
H	1.35677400	-2.94321900	0.00086800
H	2.90098100	-3.81257300	-0.00115700
H	4.62220800	1.58971500	-0.00096800
N	-4.49457200	-0.65096200	-0.00068200
H	-5.21667900	0.05516900	-0.00077200
F	-1.74604600	3.41180500	0.00018000
Se	-0.25871900	2.39485300	0.00011600

Table S27. Cartesian coordinates of G_{SeCl}:C

Energy (in hartrees) =-3743.661526450394

ATOM	X	Y	Z
C	4.25322800	2.77336000	0.00003300
C	2.97892600	0.97144300	-0.00006600
N	3.03482600	3.25791700	0.00029200
C	2.22016300	2.14200900	0.00027700

N	2.54973400	-0.30899700	-0.00014900
H	5.16101500	3.36074000	0.00001400
C	0.79291400	2.01234300	0.00043500
C	1.25104100	-0.41676300	0.00003400
O	-0.05354100	2.91568700	0.00055300
N	0.39332700	0.65325300	0.00037800
H	-0.63824400	0.52706800	0.00006700
N	-4.32628000	-0.95239000	0.00046500
C	-2.93452900	-0.73977400	0.00018500
C	-5.21786100	0.07714700	0.00016400
O	-2.18804200	-1.72671600	0.00045100
N	-2.49195600	0.54030300	-0.00036900
C	-4.78004500	1.36299300	-0.00033000
H	-6.26880200	-0.19008800	0.00041800
C	-3.35023000	1.56925500	-0.00053800
H	-5.47377200	2.19381700	-0.00047600
N	-2.82987200	2.80028700	-0.00101800
H	-1.80191100	2.90905900	-0.00053500
H	-3.42639200	3.61188600	-0.00087400
H	-4.62699400	-1.91796900	0.00065700
N	4.28417300	1.39021800	-0.00022400
H	5.09474700	0.78766300	-0.00049600
Cl	2.32154600	-3.35253600	-0.00052000
Se	0.43727700	-2.17579600	0.00015400

Table S28. Cartesian coordinates of G_{SeBr}:C

Energy (in hartrees) =-5857.583827672152

ATOM	X	Y	Z
C	3.12014000	4.00745800	0.00011700
C	2.34007800	1.94271600	0.00006000
N	1.81906800	4.16974400	0.00010700
C	1.31165300	2.88453300	0.00009900
N	2.24790800	0.59574500	-0.00002500
H	3.85095800	4.80432800	0.00012500
C	-0.03700900	2.39963800	0.00018100
C	1.01782100	0.16370000	-0.00006400
O	-1.08261200	3.06201800	0.00014900
N	-0.08204300	0.98360000	0.00012000
H	-1.04776200	0.59939100	-0.00005800
N	-4.27767500	-1.74871000	0.00018500
C	-2.97729900	-1.20638700	0.00012000
C	-5.39196100	-0.96616000	0.00022600
O	-2.01625600	-1.98400100	0.00022900
N	-2.85717600	0.14395800	-0.00016400
C	-5.27779200	0.38725600	0.00010600
H	-6.34705900	-1.47972200	0.00038500
C	-3.94015100	0.93306100	-0.00018400
H	-6.15156800	1.02602900	0.00017400
N	-3.73645100	2.25416500	-0.00054000
H	-2.76693300	2.61241400	-0.00054300
H	-4.51357100	2.89492700	-0.00011600
H	-4.33530200	-2.75834300	0.00024500

N	3.49822200	2.67660500	-0.00005400
H	4.43449900	2.29792400	-0.00024100
Br	2.90772000	-2.46500400	0.00005900
Se	0.66534200	-1.73960600	-0.00018900

Table S29. Cartesian coordinates of G_{SF}:C_{SBr}

Energy (in hartrees) =-4296.304809236699

ATOM	X	Y	Z
C	-4.31146500	-3.42722900	0.00036400
C	-3.89438400	-1.25878800	-0.00002100
N	-3.00189900	-3.36349100	0.00058300
C	-2.72042800	-2.01183400	0.00013200
N	-4.03402200	0.08879900	-0.00026900
H	-4.89573800	-4.33690400	0.00050300
C	-1.46354600	-1.31326000	-0.00005200
C	-2.88993800	0.71519300	-0.00025800
O	-0.32287900	-1.76963200	0.00044900
N	-1.66745600	0.09856000	-0.00013900
H	-0.78890600	0.62969800	-0.00002600
N	2.09042100	3.35281300	0.00039600
C	0.93690900	2.54737900	0.00051600
C	3.34598300	2.83465700	0.00013100
O	-0.17556400	3.07227700	0.00080700
N	1.13172900	1.19123000	0.00035600
C	3.53321000	1.48370800	-0.00003600
H	4.16610900	3.54440700	0.00009400
C	2.34935400	0.68254900	0.00003100
H	4.52396500	1.05737800	-0.00018200
H	1.92976600	4.35263300	0.00053200
N	-4.91003700	-2.17968400	-0.00003500
H	-5.89706300	-1.96561300	-0.00025700
S	-2.89521400	2.51110300	-0.00041300
F	-4.53874700	2.70616900	-0.00052600
S	2.34321000	-1.09413000	-0.00009500
Br	4.51585400	-1.61604800	-0.00025500

Table S30. Cartesian coordinates of G_{SCl}:C_{SBr}

Energy (in hartrees) =-4656.676788923849

ATOM	X	Y	Z
C	-3.72613000	-3.93521000	0.00076700
C	-3.55609100	-1.73432700	0.00033500
N	-2.43210200	-3.72362700	0.00072500
C	-2.30573200	-2.34901800	0.00048400
N	-3.84441300	-0.40999400	0.00006500
H	-4.20372900	-4.90513600	0.00096100
C	-1.13445600	-1.51392500	0.00033800
C	-2.78129500	0.34337200	-0.00008000
O	0.04755400	-1.84276100	0.00039400
N	-1.49491400	-0.13195200	0.00005700
H	-0.68327300	0.49605900	0.00000500
N	2.07605800	3.43967400	0.00137500
C	0.98008700	2.55412800	0.00148700
C	3.36520900	3.01417800	0.00083700

O	-0.16396100	3.00041900	0.00192900
N	1.27163300	1.21271300	0.00095000
C	3.64827200	1.68013400	0.00036500
H	4.13246700	3.78088100	0.00080800
C	2.52355800	0.79721100	0.00041700
H	4.66711100	1.32603600	-0.00006000
H	1.84315800	4.42507500	0.00173000
N	-4.46191200	-2.76332800	0.00058700
H	-5.46688100	-2.66308300	0.00058800
S	-2.92329900	2.13749800	-0.00042300
S	2.64902900	-0.97663500	-0.00015700
Br	4.85186800	-1.34351900	-0.00081600
Cl	-4.98033100	2.36615400	-0.00240100

Table S31. Cartesian coordinates of G_{SBr}:C_{SBr}

Energy (in hartrees) =-6770.598651556122

ATOM	X	Y	Z
C	2.83657900	4.48328600	-0.00002400
C	2.89516200	2.27601300	-0.00001500
N	1.57141600	4.13898200	0.00028600
C	1.58802000	2.75854300	0.00018900
N	3.32099800	0.98902300	-0.00007700
H	3.21145200	5.49735500	-0.00009400
C	0.50978900	1.80646000	0.00026900
C	2.33996200	0.12931800	0.00022900
O	-0.70057400	2.00954400	0.00055000
N	1.01136700	0.47041600	0.00032200
H	0.26937600	-0.23969700	0.00040500
N	-2.12706300	-3.51179400	0.00014600
C	-1.12946900	-2.51614500	0.00030800
C	-3.45355200	-3.22538900	-0.00001700
O	0.05343500	-2.84147000	0.00034100
N	-1.56115900	-1.21157700	0.00027200
C	-3.87548000	-1.92894400	-0.00001900
H	-4.13561600	-4.06882200	-0.00012600
C	-2.85067600	-0.93198900	0.00012800
H	-4.92581400	-1.68412300	-0.00015500
H	-1.79099200	-4.46692900	0.00014700
N	3.68950200	3.39373800	-0.00026500
H	4.69941700	3.39793800	-0.00051800
S	2.66164300	-1.63860900	0.00011300
S	-3.16957100	0.81816900	0.00000500
Br	-5.40080600	0.93783700	-0.00028600
Br	4.87162600	-1.67045700	-0.00027800

Table S32. Cartesian coordinates of G_{SeF}:C_{SBr}

Energy (in hartrees) =-6299.645691937028

ATOM	X	Y	Z
C	3.72471000	4.02948800	-0.00006600
C	3.46272300	1.83703400	0.00014600
N	2.42255500	3.87403800	-0.00026900
C	2.23718300	2.50581300	-0.00015900
N	3.70098100	0.50474700	0.00030300

H	4.24279800	4.97848300	-0.00009500
C	1.03823100	1.71385600	-0.00023700
C	2.60858400	-0.20457600	0.00009300
O	-0.13796700	2.07832900	-0.00053100
N	1.34883200	0.32633000	-0.00025200
H	0.50969100	-0.26375300	-0.00030600
N	-1.91572600	-3.31892800	-0.00010900
C	-0.87731000	-2.37605400	-0.00010900
C	-3.22576400	-2.95875000	-0.00015100
O	0.29423100	-2.76625000	-0.00030300
N	-1.23516700	-1.06029400	-0.00006000
C	-3.58034500	-1.64119300	-0.00018500
H	-3.95096100	-3.76508000	-0.00015400
C	-2.50628800	-0.69876200	-0.00016900
H	-4.61706100	-1.34259700	-0.00023500
H	-1.63275800	-4.29141900	-0.00017700
N	4.41008500	2.82818200	0.00019000
H	5.40982000	2.68451400	0.00037100
F	4.57951100	-2.09801400	0.00031600
S	-2.70351700	1.06347400	-0.00015600
Br	-4.92224500	1.32614100	0.00029100
Se	2.78518700	-2.12837700	0.00009300

Table S33. Cartesian coordinates of G_{SeCl}:C_{SBr}

Energy (in hartrees) =-6660.017568969830

ATOM	**X**	**Y**	**Z**
C	3.16536500	4.38152500	0.00005000
C	3.11908800	2.17531400	-0.00001900
N	1.88479100	4.09882600	0.00030400
C	1.83506200	2.71897600	0.00025100
N	3.48525400	0.87233900	-0.00011800
H	3.58757300	5.37688200	-0.00000700
C	0.71938400	1.81307800	0.00042300
C	2.47205300	0.05639100	0.00007300
O	-0.48388200	2.06706000	0.00076700
N	1.16301700	0.45978800	0.00032900
H	0.38597600	-0.21007300	0.00049700
N	-1.96284500	-3.39383000	0.00034800
C	-0.96686300	-2.40287400	0.00059500
C	-3.28786100	-3.09768900	0.00006700
O	0.21879300	-2.73802100	0.00063700
N	-1.38660100	-1.10189400	0.00037800
C	-3.70328600	-1.79861400	-0.00000100
H	-3.97446300	-3.93724700	-0.00008600
C	-2.67434600	-0.80650500	0.00015900
H	-4.75260600	-1.54894700	-0.00024000
H	-1.63281300	-4.35125100	0.00038500
N	3.96564700	3.25352400	-0.00017100
H	4.97467100	3.20924600	-0.00038300
S	-2.97188400	0.94422700	0.00003400
Br	-5.20301500	1.08207100	-0.00042200
Cl	4.98528400	-1.80376600	-0.00060200

Se	2.77417100	-1.85429100	-0.00011800

Table S34. Cartesian coordinates of G_{SeBr}:C_{SBr}

Energy (in hartrees) =-8773.939807236427

ATOM	X	Y	Z
C	2.38210800	4.73261000	-0.00000700
C	2.52208000	2.53017900	0.00000700
N	1.12998700	4.34271300	-0.00003400
C	1.19717400	2.96352300	-0.00001800
N	2.99792000	1.26359300	0.00002600
H	2.71892100	5.76000500	-0.00000400
C	0.16231200	1.96611000	-0.00002100
C	2.05768100	0.36360900	0.00001800
O	-1.05797000	2.11781700	-0.00006500
N	0.71906600	0.65523400	-0.00000500
H	0.00247400	-0.07899900	-0.00005600
N	-2.09639300	-3.44538200	-0.00000200
C	-1.18087200	-2.37900700	-0.00014100
C	-3.44041100	-3.25500700	0.00008800
O	0.02657900	-2.61969300	-0.00015400
N	-1.70247500	-1.11448900	-0.00016800
C	-3.95701800	-1.99279900	0.00004400
H	-4.05867400	-4.14613400	0.00018100
C	-3.00944100	-0.92260300	-0.00005400
H	-5.02254900	-1.82622900	0.00009900
H	-1.69199800	-4.37378800	0.00003800
N	3.27486000	3.67615200	0.00002000
H	4.28398600	3.71707100	0.00003800
S	-3.44639300	0.79910000	-0.00007900
Br	-5.68192300	0.75762900	0.00007000
Br	4.85140900	-1.27307700	0.00004300
Se	2.51667200	-1.51371400	0.00001100

Table S35. Cartesian coordinates of G_{SF}:C_{SCl}

Energy (in hartrees) =-2182.383633008154

ATOM	X	Y	Z
C	-4.42057500	-2.73995600	0.56699300
C	-3.57699400	-0.74443300	0.13915500
N	-3.12509700	-2.92877700	0.64503000
C	-2.57721900	-1.69017200	0.38091200
N	-3.44556000	0.57553400	-0.13802000
H	-5.17540700	-3.49896000	0.71889200
C	-1.20579600	-1.26143100	0.30723200
C	-2.19665000	0.94727100	-0.21700700
O	-0.17135100	-1.90849100	0.47356600
N	-1.12881600	0.11689400	-0.02856800
H	-0.15893100	0.45267900	-0.11469500
N	2.98887000	2.50733500	0.95391200
C	1.72936600	2.01898500	0.56300200
C	4.11677000	1.75106300	0.91118700
O	0.73615300	2.73773300	0.64399100
N	1.69555700	0.73029200	0.08907100
C	4.06623600	0.45926400	0.47427400

H	5.03298300	2.22438000	1.24686900
C	2.77987300	-0.01835300	0.07212700
H	4.95028400	-0.15926000	0.44902500
H	3.00660400	3.46449500	1.28445400
N	-4.75603000	-1.43331600	0.26247200
H	-5.67980100	-1.04103500	0.14915300
F	-3.24874800	3.03218000	-1.33393400
S	2.45676500	-1.69220000	-0.43469000
Cl	4.38455400	-2.36013800	-0.93448500
S	-1.81210100	2.65765800	-0.59387500

Table S36. Cartesian coordinates of G_{SCl}:C_{SCl}

Energy (in hartrees) =-2542.756134818470

ATOM	X	Y	Z
C	-3.93740100	-3.30069900	0.60960600
C	-3.30120500	-1.21956300	0.23705200
N	-2.63215300	-3.35050200	0.72694500
C	-2.21354700	-2.05565300	0.49877500
N	-3.30222300	0.11054300	-0.02474800
H	-4.61032000	-4.13872400	0.72704300
C	-0.89492900	-1.48125600	0.47213000
C	-2.10081600	0.61713500	-0.05092400
O	0.19782000	-2.01831200	0.65551000
N	-0.95554600	-0.09520800	0.16536200
H	-0.02161000	0.34235400	0.11073500
N	3.10778700	2.50729800	1.17486900
C	1.83311900	1.99968000	0.85593100
C	4.25509600	1.81365400	0.95807300
O	0.82814400	2.66097800	1.08983300
N	1.80633200	0.75490600	0.26603600
C	4.21306300	0.56735300	0.40430100
H	5.17991500	2.29639200	1.25467800
C	2.91371300	0.06793600	0.07712900
H	5.11330000	-0.00445900	0.23886500
H	3.11944300	3.43035000	1.59129000
N	-4.40239200	-2.03254500	0.31176900
H	-5.35938700	-1.74016900	0.17486900
S	-1.82742000	2.36895700	-0.34777400
S	2.62741700	-1.57349300	-0.55601400
Cl	4.50168400	-2.01935800	-1.40137500
Cl	-3.58310800	2.88009600	-1.32296000

Table S37. Cartesian coordinates of G_{SBr}:C_{SCl}

Energy (in hartrees) =-4656.677591663674

ATOM	X	Y	Z
C	2.68878900	4.36318700	0.00240100
C	2.58404500	2.15756600	0.00102700
N	1.40155300	4.11359700	0.00297300
C	1.31595400	2.73569200	0.00202200
N	2.91384500	0.84259700	0.00001200
H	3.13775600	5.34669800	0.00282500
C	0.17062400	1.86503800	0.00183600
C	1.87223300	0.05769700	0.00000900

O	-1.02219000	2.15624200	0.00291400
N	0.57288100	0.49637800	0.00088700
H	-0.21900900	-0.15582700	0.00064400
N	-2.87561300	-3.18687800	0.00450600
C	-1.81149900	-2.26365500	0.00258600
C	-4.17841500	-2.80818400	0.00406800
O	-0.65352700	-2.67034900	0.00324100
N	-2.15090600	-0.93278700	0.00054700
C	-4.51020300	-1.48501000	0.00180000
H	-4.91809200	-3.60146000	0.00557600
C	-3.41670500	-0.56241500	0.00023800
H	-5.54126800	-1.16769500	0.00140900
H	-2.60767800	-4.16336700	0.00614200
N	3.45860600	3.21348400	0.00127300
H	4.46604800	3.14307900	0.00073500
S	2.06003900	-1.72894400	-0.00062400
S	-3.60781500	1.20691900	-0.00227400
Cl	-5.69493500	1.43026200	-0.00540300
Br	4.26099400	-1.92671000	-0.00273300

Table S38. Cartesian coordinates of G_{SeF}:C_{SCl}

Energy (in hartrees) =-4185.724256535446

ATOM	X	Y	Z
C	3.85732300	3.60054800	0.00088300
C	3.26404200	1.47397700	0.00037500
N	2.54663700	3.64574800	0.00082600
C	2.15463700	2.32175400	0.00038100
N	3.29688900	0.12112100	0.00017200
H	4.51431100	4.45924400	0.00115700
C	0.84920800	1.72031300	-0.00001700
C	2.10958100	-0.41403300	0.00006000
O	-0.25894700	2.25890300	0.00021200
N	0.94564300	0.30234900	-0.00003400
H	0.02708300	-0.15253900	-0.00021500
N	-2.84235200	-2.77276300	-0.00005800
C	-1.67442600	-1.99654800	-0.00020000
C	-4.08315400	-2.22040400	0.00011000
O	-0.57478800	-2.55828800	-0.00035800
N	-1.83123600	-0.64199700	-0.00029200
C	-4.23743700	-0.86428900	0.00012100
H	-4.92129300	-2.90851700	0.00024100
C	-3.03304900	-0.09361300	-0.00010500
H	-5.21763900	-0.41340400	0.00026800
H	-2.70893300	-3.77678800	-0.00005500
N	4.35139900	2.30881600	0.00065900
H	5.31737600	2.01387600	0.00070700
F	3.77162800	-2.57538400	-0.00025200
S	-2.96738300	1.67989000	-0.00014900
Cl	-5.00487800	2.18756000	-0.00007600
Se	1.99312300	-2.34189000	-0.00039900

Table S39. Cartesian coordinates of G_{SeCl}:C_{SCl}

Energy (in hartrees) =-4546.096340929818

ATOM	X	Y	Z
C	3.17722000	4.14299700	-0.00033800
C	2.88829800	1.95522300	-0.00002500
N	1.87314400	4.00311200	-0.00049200
C	1.67189200	2.63728900	-0.00037700
N	3.10931000	0.61984000	0.00025600
H	3.70660000	5.08572000	-0.00038800
C	0.46336900	1.85889700	-0.00052800
C	2.01254000	-0.07970500	0.00020900
O	-0.70557400	2.24281800	-0.00073100
N	0.75622900	0.46583400	-0.00017000
H	-0.08922200	-0.11337800	-0.00021500
N	-2.78946700	-2.97997200	-0.00051600
C	-1.69369100	-2.10125200	-0.00029500
C	-4.07487500	-2.54439900	-0.00061200
O	-0.55046400	-2.56143300	-0.00026400
N	-1.97254500	-0.76332400	-0.00019100
C	-4.35101400	-1.20805000	-0.00052000
H	-4.84722800	-3.30572800	-0.00077600
C	-3.22066500	-0.33158300	-0.00032100
H	-5.36792800	-0.84788300	-0.00060100
H	-2.56396900	-3.96729100	-0.00059500
N	3.84828700	2.93365200	-0.00000200
H	4.84625600	2.77831400	0.00021100
S	-3.32721500	1.44169000	-0.00021300
Cl	-5.40374100	1.75546600	-0.00001300
Cl	4.30050500	-2.20790700	0.00122000
Se	2.09826700	-2.01137900	0.00052600

Table S40. Cartesian coordinates of G_{SeBr}:C_{SCl}

Energy (in hartrees) =-6660.018609136219

ATOM	X	Y	Z
C	2.21731600	4.65736700	-0.00042500
C	2.21673200	2.45047200	-0.00019600
N	0.94281200	4.34827000	-0.00058000
C	0.92188800	2.96759700	-0.00048100
N	2.61130400	1.15610500	-0.00001400
H	2.61897100	5.66119000	-0.00045400
C	-0.17405900	2.03730700	-0.00058800
C	1.61564000	0.31786700	-0.00005100
O	-1.38303100	2.26525300	-0.00070500
N	0.29862200	0.69451100	-0.00028800
H	-0.46303600	0.00851300	-0.00021500
N	-2.78691200	-3.18915700	-0.00061300
C	-1.80866900	-2.18044500	-0.00032600
C	-4.11658900	-2.91776000	-0.00080900
O	-0.61793600	-2.49413600	-0.00020800
N	-2.25289100	-0.88704200	-0.00010900
C	-4.55740300	-1.62647400	-0.00070800
H	-4.78778400	-3.76965100	-0.00104900
C	-3.54520200	-0.61564000	-0.00035700
H	-5.61141200	-1.39644600	-0.00087400

H	-2.43970000	-4.14048400	-0.00070800
N	3.04074100	3.54613900	-0.00016200
H	4.05041400	3.52291300	0.00000200
S	-3.87530600	1.13067000	-0.00019500
Cl	-5.97541300	1.17908000	0.00011700
Br	4.29500100	-1.50022900	0.00089500
Se	1.95025100	-1.58545700	0.00048300

Table S41. Cartesian coordinates of G_{SF}:C_{SF}

Energy (in hartrees) =-1822.015823749486

ATOM	X	Y	Z
C	-4.37692500	-2.54752700	-0.00529500
C	-3.41249500	-0.56082300	-0.00140900
N	-3.09604600	-2.82670800	-0.00630200
C	-2.47356600	-1.59458000	-0.00383100
N	-3.19666800	0.77610700	0.00112700
H	-5.17739600	-3.27425400	-0.00660100
C	-1.08286300	-1.23919900	-0.00311000
C	-1.92763900	1.08094200	0.00158400
O	-0.09693200	-1.98438600	-0.00525400
N	-0.91106000	0.16551000	-0.00026500
H	0.08476900	0.43543100	0.00024800
N	3.59307200	2.09166100	-0.00878200
C	2.23716800	1.72588100	-0.00662100
C	4.59784700	1.17522800	-0.00616900
O	1.36456800	2.59435100	-0.00894300
N	1.95814100	0.38426600	-0.00140200
C	4.31630300	-0.15852400	-0.00136200
H	5.61042200	1.56354000	-0.00822500
C	2.92637800	-0.51284800	0.00079100
H	5.09820200	-0.90166700	0.00064500
H	3.78276300	3.08619800	-0.01237200
N	-4.63144300	-1.18718000	-0.00225100
H	-5.52949500	-0.72492400	-0.00094600
S	-1.44608900	2.80877200	0.00494200
F	-2.97454300	3.44210000	0.01327200
S	2.43927100	-2.21534800	0.00636500
F	4.00360100	-2.84162500	0.01312400

Table S42. Cartesian coordinates of G_{SCl}:C_{SF}

Energy (in hartrees) =-2182.387905444364

ATOM	X	Y	Z
C	-3.88075500	-3.16664600	0.35838500
C	-3.14449800	-1.09412800	0.16490100
N	-2.57728500	-3.29583600	0.41610900
C	-2.09639800	-2.00771600	0.29839300
N	-3.07817800	0.25200500	0.02912600
H	-4.59471000	-3.97614200	0.42071900
C	-0.75447600	-1.49845300	0.27224100
C	-1.85188400	0.69654500	0.00772500
O	0.31117800	-2.11935000	0.35945300
N	-0.74123800	-0.09385700	0.11206700
H	0.22305100	0.28504700	0.08510600

N	3.60286700	2.17637800	0.67109300
C	2.26298600	1.75695000	0.57644400
C	4.65192000	1.36144000	0.38270100
O	1.35217100	2.53586000	0.84175700
N	2.05478000	0.46053900	0.16715500
C	4.43750700	0.07345500	-0.00904700
H	5.64345200	1.78787100	0.48916800
C	3.06814200	-0.34284000	-0.09228700
H	5.25422300	-0.59394600	-0.23618600
H	3.74276700	3.13526400	0.96435500
N	-4.28535300	-1.85230800	0.20521600
H	-5.22914700	-1.49908600	0.13678800
S	-1.48993500	2.45055000	-0.14036200
S	2.67869100	-2.01381000	-0.54357800
F	4.22358500	-2.40001500	-1.10423000
Cl	-3.31548200	3.17300600	-0.79709500

Table S43. Cartesian coordinates of G_{SBr}:C_{SF}

Energy (in hartrees) =-6299.651014458992

ATOM	X	Y	Z
C	2.57274700	4.27119900	-0.00008500
C	2.39034400	2.07041400	-0.00011000
N	1.27750000	4.06848400	-0.00029800
C	1.14283400	2.69467000	-0.00015900
N	2.67126300	0.74508700	-0.00009600
H	3.05673100	5.23795900	-0.00005000
C	-0.02667500	1.86161800	-0.00014900
C	1.59980800	-0.00013800	-0.00022900
O	-1.21244400	2.20405300	-0.00034200
N	0.31906900	0.48818600	-0.00024500
H	-0.50949200	-0.12603000	-0.00030000
N	-3.33887000	-2.88615900	-0.00035700
C	-2.17305000	-2.09842300	-0.00020200
C	-4.58760900	-2.35115500	-0.00025800
O	-1.07057000	-2.63948100	-0.00036100
N	-2.34683800	-0.73529800	0.00004400
C	-4.75677300	-0.99904800	-0.00004500
H	-5.41756300	-3.04938800	-0.00037700
C	-3.55820500	-0.21066900	0.00008200
H	-5.73831100	-0.55191200	0.00001400
H	-3.19117200	-3.88768800	-0.00053000
N	3.30137700	3.09459400	0.00001700
H	4.30578200	2.98867900	0.00013300
S	1.70897400	-1.79163600	0.00004000
S	-3.66822800	1.55918700	0.00031200
F	-5.35182100	1.63270200	0.00067700
Br	3.89907300	-2.08452600	0.00024200

Table S44. Cartesian coordinates of G_{SeF}:C_{SF}

Energy (in hartrees) =-3825.356588289052

ATOM	X	Y	Z
C	3.99159700	3.20334400	-0.00007800
C	3.16632400	1.15490400	-0.00001700

N	2.69451000	3.39499500	-0.00003000
C	2.15724200	2.12320900	-0.00001700
N	3.04813200	-0.19298400	0.00004700
H	4.74020400	3.98348000	-0.00010700
C	0.79769500	1.66548300	0.00000700
C	1.80616700	-0.58863400	0.00018500
O	-0.24772200	2.33050900	0.00006100
N	0.73394600	0.25635000	0.00021200
H	-0.23976500	-0.08174200	0.00032000
N	-3.44448100	-2.16489200	-0.00003200
C	-2.14916600	-1.63293400	0.00024500
C	-4.55355200	-1.37651900	-0.00020300
O	-1.17491800	-2.39321500	0.00027000
N	-2.03715000	-0.27399700	0.00014000
C	-4.43921700	-0.01761500	-0.00011300
H	-5.51035000	-1.88679300	-0.00037700
C	-3.10422100	0.50484400	0.00006000
H	-5.30689800	0.62367800	-0.00020000
H	-3.51210900	-3.17528300	-0.00007600
N	4.33893800	1.86442800	-0.00011200
H	5.26650400	1.46462400	-0.00016200
F	3.16835500	-2.95671900	0.00011600
S	-2.80904300	2.24695500	0.00015100
F	-4.43436300	2.69241900	-0.00026800
Se	1.43846500	-2.48243300	-0.00015000

Table S45. Cartesian coordinates of G_{SeCl}:C_{SF}

Energy (in hartrees) =-4185.728709345548

ATOM	**X**	**Y**	**Z**
C	3.21299600	3.93049600	-0.00020800
C	2.76891900	1.76859200	-0.00004600
N	1.90251400	3.88549900	-0.00011000
C	1.60339700	2.53773200	-0.00004200
N	2.89265700	0.42145200	-0.00008500
H	3.80893300	4.83263000	-0.00031000
C	0.34819900	1.84308800	0.00005000
C	1.74591200	-0.19497500	-0.00008200
O	-0.79417400	2.31869200	0.00002700
N	0.53538100	0.44271800	0.00008700
H	-0.36184000	-0.06439200	0.00029500
N	-3.33203100	-2.54248200	-0.00022500
C	-2.11310400	-1.84893900	-0.00011500
C	-4.53312600	-1.90546600	-0.00036600
O	-1.05303800	-2.47920500	0.00030900
N	-2.17467700	-0.48321500	-0.00003900
C	-4.59327800	-0.54370700	-0.00031500
H	-5.41665500	-2.53426900	-0.00048100
C	-3.33602100	0.14661100	-0.00009200
H	-5.53595300	-0.01937500	-0.00037300
H	-3.26725100	-3.55291700	-0.00017800
N	3.79579800	2.67597000	-0.00013200
H	4.78016300	2.44960900	-0.00018700

S	-3.28976700	1.91595100	0.00010200
F	-4.96270700	2.12688900	-0.00036300
Cl	3.84610800	-2.50425400	0.00047300
Se	1.66841900	-2.12506600	0.00008800

Table S46. Cartesian coordinates of G_{SeBr}:C_{SF}

Energy (in hartrees) =-4296.309924155852

ATOM	X	Y	Z
C	2.06841600	4.60193100	-0.00035000
C	2.02159200	2.39516100	-0.00010700
N	0.78762600	4.32124100	-0.00008000
C	0.73682600	2.94139200	0.00006100
N	2.38683900	1.09307600	-0.00005500
H	2.49187200	5.59676000	-0.00053400
C	-0.37178800	2.03099300	0.00032200
C	1.37033300	0.27833700	0.00021400
O	-1.58131600	2.29242700	0.00050400
N	0.06434600	0.68756300	0.00043600
H	-0.72759800	0.02688200	0.00073000
N	-3.20563200	-2.95957300	-0.00021800
C	-2.12788200	-2.06155600	0.00021000
C	-4.50050100	-2.54603300	-0.00072000
O	-0.97434100	-2.49511200	0.00066600
N	-2.43083800	-0.72714600	0.00015800
C	-4.80115800	-1.21651600	-0.00075200
H	-5.25834100	-3.32174400	-0.00104400
C	-3.68596900	-0.31415700	-0.00026600
H	-5.82190200	-0.86770400	-0.00110800
H	-2.96253000	-3.94242600	-0.00016900
N	2.86804900	3.47308200	-0.00037500
H	3.87707300	3.42857400	-0.00055100
S	-3.95525000	1.43597800	-0.00020200
F	-5.63960500	1.34844500	-0.00095900
Br	3.98678100	-1.62212000	0.00007600
Se	1.64111400	-1.63268600	0.00034600

Table S47. Cartesian coordinates of G_{SF}:C_{SeF}

Energy (in hartrees) =-3825.359557838628

ATOM	X	Y	Z
C	-4.16609500	-2.88421600	0.00017900
C	-3.49827500	-0.77919700	0.00027500
N	-2.85901100	-2.97846700	-0.00005200
C	-2.41997100	-1.66997300	0.00000800
N	-3.47229500	0.57222100	0.00040200
H	-4.85430000	-3.71806900	0.00021400
C	-1.10533700	-1.11197700	-0.00015700
C	-2.25703400	1.05333500	0.00026100
O	-0.02363600	-1.73556500	-0.00041200
N	-1.12291100	0.28780400	0.00000400
H	-0.15623700	0.68261100	-0.00013700
N	3.05148700	2.71866700	0.00043600
C	1.73615700	2.23692600	0.00034100
C	4.13110100	1.88773000	0.00022200

O	0.78583900	3.02246700	0.00049100
N	1.57694700	0.87680700	0.00000900
C	3.96227800	0.53608900	-0.00009600
H	5.10708800	2.36047000	0.00031800
C	2.61258500	0.05546500	-0.00019200
H	4.80281300	-0.14075800	-0.00027000
H	3.15612000	3.72553300	0.00066800
N	-4.61395000	-1.57401400	0.00038000
H	-5.56948400	-1.24620300	0.00057300
S	-2.01485900	2.82854200	0.00041800
F	-3.61684800	3.24450100	0.00064400
F	4.08053500	-2.20511800	-0.00073400
Se	2.28196000	-1.81871000	-0.00062200

Table S48. Cartesian coordinates of G_{SCl}:C_{SeF}

Energy (in hartrees) =-4185.731650259127

ATOM	X	Y	Z
C	-3.44579800	-3.64450200	-0.00014300
C	-3.14644700	-1.45743400	-0.00019100
N	-2.14166400	-3.51367800	0.00013300
C	-1.93320200	-2.14943800	0.00017100
N	-3.34827000	-0.12088900	-0.00035100
H	-3.98137200	-4.58367700	-0.00020800
C	-0.73182100	-1.37606200	0.00043000
C	-2.23661600	0.56394400	-0.00025200
O	0.43566700	-1.81221400	0.00045700
N	-0.98548200	0.00318400	0.00013600
H	-0.10285200	0.55803300	0.00020700
N	2.85678000	3.02765500	0.00001200
C	1.61622000	2.37262600	0.00015000
C	4.03912100	2.35357200	-0.00026600
O	0.57395300	3.02686800	0.00042700
N	1.63989800	0.99997200	0.00009600
C	4.05399500	0.99202100	-0.00029000
H	4.94225900	2.95403000	-0.00042300
C	2.78131500	0.33313100	-0.00005300
H	4.97867200	0.43587100	-0.00048400
H	2.82146900	4.03922800	0.00005300
N	-4.11091200	-2.43006900	-0.00035400
H	-5.10842500	-2.27054700	-0.00059800
S	-2.24790000	2.36025300	-0.00053100
F	4.56239600	-1.69433400	-0.00045500
Cl	-4.28527500	2.72793100	0.00038600
Se	2.72866900	-1.57148200	0.00015800

Table S49. Cartesian coordinates of G_{SBr}:C_{SeF}

Energy (in hartrees) =-6299.653535894677

ATOM	X	Y	Z
C	2.26802800	4.40350700	-0.00029000
C	2.38712200	2.19852800	0.00005100
N	1.01214100	4.02884100	-0.00021500
C	1.06511500	2.64971000	0.00004700
N	2.83939300	0.92419600	0.00018600

H	2.61679000	5.42687000	-0.00046700
C	0.03146300	1.66337200	0.00027700
C	1.87500800	0.04202600	0.00022600
O	-1.19807600	1.86904100	0.00005400
N	0.54069900	0.35839400	0.00027700
H	-0.22006200	-0.35530000	0.00035200
N	-2.64635700	-3.36403400	0.00003900
C	-1.55008300	-2.48805100	0.00024300
C	-3.93419300	-2.92521000	-0.00020400
O	-0.40505700	-2.93630300	0.00039000
N	-1.83272000	-1.14330900	0.00009400
C	-4.20575800	-1.59103400	-0.00028200
H	-4.70770100	-3.68546700	-0.00031700
C	-3.07988700	-0.70445700	-0.00014700
H	-5.21834600	-1.21834000	-0.00045400
H	-2.42098700	-4.35080100	0.00009500
N	3.15031100	3.33636600	-0.00009800
H	4.15994500	3.36818500	-0.00010500
S	2.21565500	-1.71840700	0.00033100
F	-5.21907600	0.94748200	-0.00050100
Br	4.42659700	-1.71871500	0.00003000
Se	-3.39351200	1.17651800	-0.00017700

Table S50. Cartesian coordinates of G_{SeF}:C_{SeF}
Energy (in hartrees) =-5828.700738422417

ATOM	**X**	**Y**	**Z**
C	-3.51928200	-3.69478800	-0.00006200
C	-3.11616900	-1.52343700	-0.00009400
N	-2.21025900	-3.62875800	-0.00001000
C	-1.93441500	-2.27615300	-0.00003000
N	-3.26211400	-0.18141000	-0.00012900
H	-4.09979000	-4.60696400	-0.00006300
C	-0.70426800	-1.55335300	0.00001500
C	-2.11940700	0.44997200	-0.00003500
O	0.45640300	-2.02522200	0.00012600
N	-0.90509800	-0.17293800	0.00007700
H	0.00235800	0.34313700	0.00019400
N	2.73677700	2.90840500	-0.00008700
C	1.53150400	2.20320900	0.00018900
C	3.94419400	2.27477600	-0.00033500
O	0.45505300	2.81591000	0.00021400
N	1.61132300	0.84361800	0.00026300
C	4.01444400	0.91385700	-0.00030300
H	4.82291700	2.91005600	-0.00055600
C	2.77007600	0.20482900	0.00001000
H	4.96076100	0.39481600	-0.00048800
H	2.66697900	3.91839800	-0.00015900
N	-4.12476300	-2.45039900	-0.00015400
H	-5.11323800	-2.24183500	-0.00022000
F	-3.91145700	2.49090100	0.00010300
F	4.58507700	-1.76839000	0.00003300
Se	2.74598200	-1.69463000	0.00005700

Se	-2.11996300	2.37790000	-0.00001400

Table S51. Cartesian coordinates of G_{SeCl}:C_{SeF}

Energy (in hartrees) =-6189.072585776366

ATOM	X	Y	Z
C	2.74898900	4.24214800	0.00001700
C	2.69123600	2.03573500	-0.00009000
N	1.46663200	3.97084100	-0.00013600
C	1.40782200	2.59172000	-0.00020200
N	3.04317800	0.73233600	0.00004600
H	3.17840800	5.23444300	0.00012600
C	0.30562100	1.68526300	-0.00030400
C	2.01811800	-0.07375700	0.00010000
O	-0.90952500	1.97939200	-0.00010100
N	0.71666700	0.34948200	-0.00016100
H	-0.09975400	-0.29917200	-0.00039100
N	-2.58550700	-3.17072500	-0.00023900
C	-1.46376800	-2.33494500	-0.00048300
C	-3.85600500	-2.67996300	0.00017500
O	-0.33051600	-2.82720200	-0.00089900
N	-1.69321500	-0.98847400	-0.00024900
C	-4.07758000	-1.33587500	0.00028600
H	-4.65765600	-3.41024600	0.00032500
C	-2.92010600	-0.49188300	0.00004200
H	-5.07571900	-0.92537500	0.00052200
H	-2.39982100	-4.16585900	-0.00038700
N	3.54288600	3.10855000	-0.00000700
H	4.55187600	3.05893900	0.00009700
F	-4.96933900	1.25417700	0.00067000
Cl	4.47794300	-1.98681200	0.00005700
Se	-3.13367700	1.39748800	-0.00005000
Se	2.26490000	-1.98768700	0.00030500

Table S52. Cartesian coordinates of G_{SeBr}:C_{SeF}

Energy (in hartrees) =-8302.994971424276

ATOM	X	Y	Z
C	1.75412600	4.68484600	0.00023700
C	1.99943800	2.49125100	0.00037600
N	0.52114000	4.23997600	0.00003000
C	0.65236700	2.86572700	0.00012700
N	2.52763700	1.24930000	0.00061700
H	2.04356600	5.72659900	0.00022500
C	-0.31534600	1.81645700	-0.00008500
C	1.62342500	0.30903300	0.00059200
O	-1.55906000	1.94188800	-0.00041900
N	0.27571200	0.54949900	0.00021600
H	-0.44182500	-0.20673400	-0.00009400
N	-2.52691200	-3.39433400	0.00008600
C	-1.52627800	-2.41600600	0.00002400
C	-3.85140100	-3.07826200	-0.00011100
O	-0.33875700	-2.75311600	0.00043500
N	-1.93336800	-1.11098500	-0.00013800
C	-4.24996000	-1.77595000	-0.00027700

H	-4.54854500	-3.90890900	-0.00007800
C	-3.21586400	-0.78447100	-0.00028300
H	-5.29384500	-1.50264700	-0.00039600
H	-2.20939700	-4.35550800	0.00026700
N	2.69613100	3.67084800	0.00044600
H	3.70237800	3.75983600	0.00063000
F	-5.48200000	0.66264200	-0.00057300
Br	4.45710900	-1.23878500	0.00027700
Se	-3.68454000	1.05927000	-0.00030000
Se	2.12936200	-1.55147700	-0.00021900

Table S53. Cartesian coordinates of G_{SF}:C_{SeCl}

Energy (in hartrees) =-4185.726551543925

ATOM	X	Y	Z
C	-4.11845900	-3.22970300	-0.00049400
C	-3.65125700	-1.07163500	0.00018400
N	-2.80812300	-3.19947500	-0.00044500
C	-2.49443300	-1.85525400	0.00008900
N	-3.75459500	0.27676800	0.00053100
H	-4.72477400	-4.12485000	-0.00081700
C	-1.23326700	-1.17892400	0.00042900
C	-2.59290300	0.87336700	0.00063300
O	-0.09944600	-1.68717900	-0.00002600
N	-1.38917600	0.22049500	0.00051200
H	-0.47938700	0.71444000	0.00056700
N	2.47530800	3.16702500	-0.00098500
C	1.25304900	2.47982400	-0.00032100
C	3.67226100	2.52149000	-0.00126100
O	0.19282700	3.10835300	-0.00025400
N	1.31036200	1.11149300	-0.00018000
C	3.71823600	1.15925500	-0.00095100
H	4.56129200	3.14254300	-0.00170200
C	2.46572700	0.47010700	-0.00044200
H	4.66257400	0.63776500	-0.00112600
H	2.41590100	4.17779100	-0.00121000
N	-4.68761600	-1.96780800	-0.00009200
H	-5.66958900	-1.73093300	-0.00005900
S	-2.53835200	2.66610600	0.00086100
F	-4.17570700	2.90843900	0.00210400
Cl	4.54475500	-1.90533100	-0.00062300
Se	2.33189000	-1.43823000	0.00005600

Table S54. Cartesian coordinates of G_{SCl}:C_{SeCl}

Energy (in hartrees) =-4546.098413079158

ATOM	X	Y	Z
C	-3.44206400	-3.84415900	-0.00124100
C	-3.29072600	-1.64211700	-0.00069500
N	-2.14976800	-3.62452500	-0.00092600
C	-2.03425200	-2.24924700	-0.00055300
N	-3.58463300	-0.32160700	-0.00047700
H	-3.91248700	-4.81759700	-0.00158000
C	-0.88221200	-1.39903100	-0.00006900
C	-2.52457900	0.43868000	-0.00020000

O	0.30902700	-1.74373600	-0.00010500
N	-1.23658800	-0.03404300	-0.00008500
H	-0.40967800	0.58602800	0.00009900
N	2.34466000	3.34166800	-0.00063100
C	1.19816200	2.53065900	-0.00040500
C	3.60243700	2.82707200	-0.00048800
O	0.08202300	3.04835300	-0.00079200
N	1.39715200	1.17256700	-0.00009100
C	3.79007200	1.47736600	-0.00012000
H	4.42153400	3.53795300	-0.00064100
C	2.61543700	0.66174700	-0.00003500
H	4.78387400	1.05797600	0.00004600
H	2.17821600	4.34030300	-0.00095700
N	-4.18763000	-2.67776700	-0.00109600
H	-5.19357700	-2.58605100	-0.00126100
S	-2.66829600	2.23042300	0.00005500
Cl	4.94610200	-1.47606000	0.00126800
Cl	-4.72719800	2.44837700	0.00096100
Se	2.69703200	-1.25210600	0.00054900

Table S55. Cartesian coordinates of G_{SBr}:C_{SeCl}

Energy (in hartrees) =-6660.020393250370

ATOM	X	Y	Z
C	2.43708500	4.45036100	0.00059400
C	2.59210300	2.24782600	0.00028300
N	1.18769400	4.05393100	0.00045000
C	1.26380200	2.67583200	0.00011300
N	3.06758900	0.98097300	0.00018100
H	2.76846000	5.47947500	0.00081300
C	0.24046800	1.67457600	-0.00028800
C	2.12102800	0.08124400	0.00006300
O	-0.98758000	1.84959400	-0.00023700
N	0.78010600	0.37276000	-0.00017000
H	0.04818400	-0.35799200	-0.00033000
N	-2.27434300	-3.50681000	0.00070000
C	-1.25116400	-2.54415700	0.00049000
C	-3.59139400	-3.17366300	0.00040900
O	-0.07539900	-2.90263600	0.00080300
N	-1.63844200	-1.22598300	0.00023700
C	-3.96587600	-1.86365600	-0.00000600
H	-4.30299900	-3.99217000	0.00056000
C	-2.91689200	-0.89205400	-0.00006200
H	-5.00833900	-1.58677100	-0.00019600
H	-1.96942000	-4.47219600	0.00100700
N	3.33676700	3.39822000	0.00050200
H	4.34569500	3.44642100	0.00062500
S	2.50405900	-1.67194600	-0.00029800
Cl	-5.53038600	0.89367400	-0.00016000
Br	4.71442300	-1.61956800	-0.00031100
Se	-3.27122000	0.99122400	-0.00033900

Table S56. Cartesian coordinates of G_{SeF}:C_{SeCl}

Energy (in hartrees) =-6189.067545865193

ATOM	X	Y	Z
C	-3.43827600	-3.95472900	-0.00045300
C	-3.21318000	-1.75793100	0.00003100
N	-2.13894600	-3.78103800	-0.00022000
C	-1.97509000	-2.41043100	0.00004600
N	-3.46896800	-0.43131800	0.00017500
H	-3.94186500	-4.91151000	-0.00069100
C	-0.80252100	-1.59264500	0.00034200
C	-2.38399500	0.29295200	0.00015600
O	0.38870400	-1.95910600	-0.00003400
N	-1.12030300	-0.22666700	0.00012500
H	-0.27075500	0.36418700	-0.00010100
N	2.18338000	3.24535700	-0.00028700
C	1.09128500	2.37305000	-0.00028600
C	3.46701400	2.79400600	-0.00009500
O	-0.05813400	2.83291100	-0.00063500
N	1.36169400	1.03768300	0.00000200
C	3.72854700	1.45569400	0.00003100
H	4.24652500	3.54777500	-0.00016100
C	2.60190800	0.57619300	0.00011000
H	4.74415100	1.09146900	0.00003400
H	1.96687000	4.23460000	-0.00047200
N	-4.14327000	-2.76408300	-0.00007900
H	-5.14542600	-2.63708600	-0.00004400
F	-4.35200000	2.17743900	0.00003800
Cl	5.01084200	-1.44796400	0.00026600
Se	2.75014600	-1.32790200	-0.00005500
Se	-2.55690100	2.21384500	0.00019100

Table S57. Cartesian coordinates of G_{SeCl}:C_{SeCl}

Energy (in hartrees) =-6549.439361866823

ATOM	X	Y	Z
C	2.80465700	4.35160100	0.00006200
C	2.83698000	2.14505400	0.00000600
N	1.53456800	4.02673900	0.00004000
C	1.53286200	2.64634900	0.00000000
N	3.24378300	0.85674800	0.00001800
H	3.19257100	5.36082700	0.00010300
C	0.46285300	1.69749300	-0.00001900
C	2.25583500	0.00751700	-0.00004200
O	-0.75868000	1.93217800	-0.00002100
N	0.93594900	0.37384900	-0.00016800
H	0.16247000	-0.31186700	-0.00042900
N	-2.14496900	-3.37676200	-0.00004800
C	-1.11483800	-2.42820400	-0.00033900
C	-3.45713500	-3.02127800	0.00031900
O	0.06057500	-2.80694200	-0.00065600
N	-1.47898900	-1.11133200	-0.00031200
C	-3.81265900	-1.70545500	0.00029600
H	-4.18072100	-3.82900100	0.00055300
C	-2.75121000	-0.74803600	-0.00010200
H	-4.85129800	-1.41384300	0.00052600

H	-1.85572300	-4.34711900	-0.00008600
N	3.64439300	3.25182500	0.00005400
H	4.65451500	3.24330700	0.00008000
Cl	-5.31955800	1.08336700	0.00043000
Cl	4.80958800	-1.78344300	0.00001700
Se	-3.05686800	1.13934300	-0.00025200
Se	2.59937700	-1.89289000	0.00022000

Table S58. Cartesian coordinates of G_{SeBr}:C_{SeCl}

Energy (in hartrees) =-8663.361566889636

ATOM	X	Y	Z
C	1.95870900	4.70784200	0.00040000
C	2.21307900	2.51563100	0.00060600
N	0.72787800	4.25653000	0.00018000
C	0.86556600	2.88287700	0.00038900
N	2.74801400	1.27560100	0.00084900
H	2.24308100	5.75098200	0.00037500
C	-0.10313100	1.83067100	0.00037000
C	1.85122500	0.32990800	0.00074200
O	-1.34200400	1.94257200	-0.00015900
N	0.50067400	0.56122600	0.00038200
H	-0.19854800	-0.20055300	0.00001300
N	-2.20581000	-3.48482600	0.00050100
C	-1.26978500	-2.44256900	0.00034700
C	-3.54563100	-3.25640600	0.00023400
O	-0.06480100	-2.70827500	0.00052900
N	-1.75785200	-1.16537600	-0.00005700
C	-4.02472000	-1.98048300	-0.00020000
H	-4.18910400	-4.12934900	0.00038000
C	-3.05916300	-0.92627500	-0.00035800
H	-5.08633700	-1.78925600	-0.00042700
H	-1.82541400	-4.42314900	0.00079600
N	2.90508500	3.69826100	0.00065500
H	3.91089200	3.79146900	0.00084500
Cl	-5.79511400	0.64745200	-0.00131800
Br	4.70694500	-1.18162500	0.00027300
Se	-3.54723200	0.92251000	-0.00086300
Se	2.38343500	-1.52490500	0.00013200

Table S59. Cartesian coordinates of G_{SF}:C_{SeBr}

Energy (in hartrees) =-6299.647894196165

ATOM	X	Y	Z
C	-4.13572200	-3.59672600	-0.00054700
C	-3.92951400	-1.39822800	-0.00019200
N	-2.83829100	-3.40991600	-0.00017900
C	-2.68770700	-2.03784400	0.00015000
N	-4.19365300	-0.07157200	-0.00015000
H	-4.63061600	-4.55797000	-0.00083800
C	-1.51495900	-1.21661100	0.00066000
C	-3.11182000	0.65979000	0.00010300
O	-0.32962300	-1.58177500	0.00055700
N	-1.83852500	0.15584300	0.00041500
H	-0.99576000	0.75477500	0.00057600

N	1.62806200	3.57319100	-0.00030400
C	0.50832500	2.72851200	0.00016500
C	2.90027700	3.09350900	-0.00054700
O	-0.62557300	3.21186400	0.00017500
N	0.74696000	1.37992300	0.00013800
C	3.12639900	1.74957500	-0.00037400
H	3.69873200	3.82743600	-0.00083400
C	1.97794000	0.89923900	-0.00010100
H	4.13193200	1.35901400	-0.00051600
H	1.43341100	4.56683100	-0.00042700
N	-4.85154600	-2.41193900	-0.00055200
H	-5.85478500	-2.29432900	-0.00081500
S	-3.27314800	2.44615600	-0.00003300
F	-4.92843700	2.49092900	0.00016900
Br	4.46635600	-1.24815200	-0.00015200
Se	2.08506300	-1.01070600	0.00028900

Table S60. Cartesian coordinates of G_{SCl}:C_{SeBr}

Energy (in hartrees) =-6660.019654043133

ATOM	X	Y	Z
C	-3.55642600	-4.04334700	0.00016900
C	-3.58544600	-1.83639400	0.00014000
N	-2.28637200	-3.71852100	-0.00013200
C	-2.28378600	-2.33830100	-0.00020400
N	-3.98696800	-0.54423300	0.00024000
H	-3.94558900	-5.05202900	0.00027300
C	-1.20362600	-1.39733700	-0.00049600
C	-2.99314400	0.30054900	0.00006000
O	0.01045500	-1.64021700	-0.00052000
N	-1.67063700	-0.06433700	-0.00029600
H	-0.89976900	0.62246100	-0.00041200
N	1.59857800	3.62757800	0.00000700
C	0.53593700	2.70869500	-0.00038700
C	2.90013200	3.23749100	0.00028200
O	-0.62456800	3.11739300	-0.00055200
N	0.86449200	1.37610500	-0.00045500
C	3.21581000	1.91210200	0.00017700
H	3.64702400	4.02393600	0.00061400
C	2.12670400	0.98655600	-0.00030400
H	4.24488400	1.58919800	0.00045800
H	1.33514400	4.60512300	0.00005800
N	-4.39485100	-2.94195000	0.00033300
H	-5.40490200	-2.93260900	0.00058400
S	-3.28655800	2.07468200	0.00031100
Br	4.76937300	-0.97760200	0.00045400
Cl	-5.35703200	2.11922100	0.00023200
Se	2.37811500	-0.91181400	-0.00036200

Table S61. Cartesian coordinates of G_{SBr}:C_{SeBr}

Energy (in hartrees) =-8773.941645451483

ATOM	X	Y	Z
C	2.71005700	4.50677800	0.00018600
C	2.94787300	2.31173800	0.00002700

N	1.47649500	4.06320800	-0.00002900
C	1.60468700	2.68886500	-0.00004700
N	3.47154500	1.06377900	0.00001800
H	3.00226300	5.54768900	0.00028700
C	0.61825600	1.65023200	-0.00014500
C	2.56027700	0.12855000	-0.00024800
O	-0.61383200	1.77628900	-0.00021800
N	1.20897600	0.36817800	-0.00031800
H	0.50796900	-0.39095000	-0.00053300
N	-1.66996900	-3.65832600	0.00012600
C	-0.69840200	-2.64298500	-0.00000600
C	-3.00241500	-3.39453100	0.00014600
O	0.49410300	-2.94076600	-0.00011100
N	-1.15301500	-1.34665700	0.00006800
C	-3.44323000	-2.10564200	0.00007700
H	-3.67083400	-4.24874000	0.00018200
C	-2.44726700	-1.08075100	0.00008200
H	-4.49838200	-1.88288800	0.00003500
H	-1.31436500	-4.60622100	0.00012800
N	3.64878100	3.48948000	0.00028700
H	4.65515800	3.57555200	0.00047100
S	3.01319100	-1.60827200	-0.00013200
Br	-5.27223000	0.61569300	0.00010300
Br	5.21998900	-1.46837300	0.00008500
Se	-2.88486100	0.78430600	-0.00011500

Table S62. Cartesian coordinates of G_{SeF}:C_{SeBr}

Energy (in hartrees) =-8302.988797205611

ATOM	**X**	**Y**	**Z**
C	3.49656400	4.18699300	0.00000800
C	3.46787600	1.97915700	-0.00025400
N	2.21786700	3.89793100	0.00018400
C	2.17689400	2.51798100	-0.00008400
N	3.84125700	0.68053500	-0.00055900
H	3.91281600	5.18487700	0.00007500
C	1.07998600	1.59981900	-0.00014500
C	2.82596500	-0.13807200	-0.00058700
O	-0.13709200	1.85756500	0.00040100
N	1.52022700	0.26532300	-0.00029300
H	0.73096100	-0.40171300	0.00003200
N	-1.43548400	-3.52220700	-0.00029300
C	-0.43931300	-2.54086800	0.00003300
C	-2.75887500	-3.20642000	-0.00054600
O	0.75085400	-2.88065000	0.00005900
N	-0.84499700	-1.24025300	0.00002700
C	-3.15537700	-1.90217500	-0.00049600
H	-3.45665600	-4.03647700	-0.00070200
C	-2.12659800	-0.91133700	-0.00038500
H	-4.20252000	-1.64280700	-0.00056800
H	-1.11681100	-4.48342200	-0.00033800
N	4.30486200	3.06408200	-0.00028800
H	5.31431900	3.02675800	-0.00047100

F	4.96160300	-1.83029200	-0.00008100
Br	-4.85305600	0.90697000	0.00020300
Se	-2.45769800	0.96883700	-0.00001000
Se	3.17774100	-2.03537200	0.00045700

Table S63. Cartesian coordinates of G_{SeCl}:C_{SeBr}

Energy (in hartrees) =-8663.360576011713

ATOM	X	Y	Z
C	2.98047000	4.46341700	-0.00000700
C	3.13793500	2.26239900	0.00024400
N	1.73084500	4.06656000	-0.00014300
C	1.80787200	2.68830100	0.00004000
N	3.61749700	0.99918300	0.00040300
H	3.31035600	5.49306800	-0.00009200
C	0.79190900	1.68081800	-0.00001200
C	2.67999600	0.09484500	0.00036200
O	-0.43929600	1.84457500	-0.00033800
N	1.34087200	0.38442200	0.00021300
H	0.60990400	-0.34553100	0.00029500
N	-1.49537800	-3.56828900	0.00047800
C	-0.53409500	-2.54945700	0.00062300
C	-2.82899500	-3.30569300	0.00001900
O	0.66444600	-2.84659000	0.00103500
N	-0.98824200	-1.26090300	0.00019400
C	-3.27400800	-2.01779300	-0.00023800
H	-3.49479800	-4.16174300	-0.00002600
C	-2.28309100	-0.98860300	-0.00017200
H	-4.33010100	-1.79863000	-0.00049400
H	-1.13825900	-4.51576800	0.00073600
N	3.88141800	3.41325200	0.00019700
H	4.89038100	3.46186200	0.00029400
Br	-5.09805400	0.70565200	-0.00096500
Cl	5.33676800	-1.54068800	0.00079100
Se	-2.70799800	0.87505200	-0.00030500
Se	3.13685400	-1.78188300	0.00029000

Table S64. Cartesian coordinates of G_{SeBr}:C_{SeBr}

Energy (in hartrees) =-10777.282884395440

ATOM	X	Y	Z
C	2.26972300	4.73642700	-0.00017900
C	2.57863100	2.55120400	-0.00017400
N	1.05057100	4.25418100	-0.00012900
C	1.22270100	2.88431000	-0.00027900
N	3.14518200	1.32498500	0.00000800
H	2.52784400	5.78636800	-0.00015400
C	0.27881700	1.80886000	-0.00043300
C	2.27295500	0.35691800	0.00026100
O	-0.96025600	1.88600100	0.00021500
N	0.91697500	0.55359000	0.00012700
H	0.23979000	-0.22577200	0.00036300
N	-1.66424400	-3.58751400	-0.00034100
C	-0.76967500	-2.50869900	-0.00012800
C	-3.01174800	-3.41225800	-0.00061400

O	0.44444300	-2.72850100	0.00016400
N	-1.30670200	-1.25133700	-0.00003500
C	-3.53931500	-2.15586900	-0.00061700
H	-3.62074000	-4.30964100	-0.00082800
C	-2.61662800	-1.06485500	-0.00026600
H	-4.60762800	-2.00608600	-0.00087800
H	-1.24652300	-4.50985200	-0.00031800
N	3.24099800	3.75090700	-0.00025400
H	4.24412100	3.86926900	-0.00026400
Br	-5.53482600	0.44847500	-0.00072500
Br	5.16899700	-1.07788100	0.00077000
Se	-3.16114800	0.76777400	-0.00023000
Se	2.85530700	-1.48321500	0.00071300

Table S65. Cartesian coordinates of A_{SF}:T (water phase).

ATOM	X	Y	Z
N	-0.80322900	-0.52549100	-0.00027300
C	-1.19225100	-1.81543400	-0.00013300
N	-2.44657300	-2.27078500	0.00009200
C	-3.34934900	-1.28670100	0.00017700
C	-3.08959300	0.10814000	0.00005600
C	-1.72961700	0.44464900	-0.00018800
N	-4.71385400	-1.38942800	0.00042400
C	-5.21103600	-0.10717900	0.00036700
N	-4.27872800	0.81961100	0.00023200
H	-0.38606300	-2.54313900	-0.00019800
H	-5.25193700	-2.24645500	0.00058400
H	-6.27553100	0.08153800	0.00052100
N	2.13576700	-0.49867700	-0.00017500
C	2.69416400	-1.75717800	-0.00015900
N	4.07323700	-1.75489700	0.00006500
C	4.83020400	-0.60387400	0.00025100
C	4.27287100	0.63354600	0.00023100
C	2.81576100	0.71934600	0.00002500
O	2.16987400	1.77552100	-0.00007000
O	2.02570900	-2.79430700	-0.00036600
C	5.07231000	1.90450700	0.00041400
H	1.10354400	-0.45030200	-0.00036800
H	4.52291500	-2.66126100	0.00007000
H	5.90270500	-0.75971000	0.00040700
H	4.83845400	2.51256100	-0.88025800
H	6.14446100	1.69257300	0.00056500
H	4.83818900	2.51247200	0.88107800
S	-1.00497000	2.05703800	-0.00038600
F	-2.37433600	2.99979400	-0.00017200

Table S66. Cartesian coordinates of A_{SCl}:T (water phase).

ATOM	X	Y	Z
N	-0.65685100	-0.71413400	0.00246000
C	-0.92436000	-2.03454600	0.00547800
N	-2.13262900	-2.60174900	0.00663200
C	-3.12010100	-1.70432100	0.00434000
C	-2.98877800	-0.28981100	0.00088400

C	-1.66590200	0.16958600	0.00009600
N	-4.46919200	-1.93280300	0.00467800
C	-5.08244200	-0.70231000	0.00150800
N	-4.24009400	0.30615700	-0.00084500
H	-0.05510500	-2.68489300	0.00672800
H	-4.92607400	-2.83570600	0.00682400
H	-6.15979300	-0.61220800	0.00112400
N	2.33418700	-0.49596100	0.00184700
C	2.92488600	-1.74079700	-0.00654000
N	4.30305500	-1.70545300	-0.01005800
C	5.03355000	-0.53748100	-0.00565000
C	4.44706000	0.68568200	0.00290000
C	2.98777900	0.73983000	0.00740600
O	2.32251000	1.78179700	0.01560100
O	2.28476100	-2.79555200	-0.01062900
C	5.21610800	1.97525700	0.00787700
H	1.30329900	-0.47807700	0.00350300
H	4.77318200	-2.60141900	-0.01629700
H	6.10931700	-0.66860900	-0.00944600
H	4.96504900	2.58260300	-0.86855100
H	6.29299900	1.78876500	0.00353000
H	4.97044100	2.57265400	0.89263300
S	-1.00488300	1.82037400	-0.00376700
Cl	-2.64644200	3.09188300	-0.00837200

Table S67. Cartesian coordinates of A_{SBr}:T (water phase).

ATOM	**X**	**Y**	**Z**
N	-0.24851500	1.14025500	-0.00000600
C	-0.38516900	2.48000300	0.00003200
N	-1.53236900	3.16296400	0.00015600
C	-2.60313800	2.36589400	0.00021100
C	-2.60899400	0.94586400	0.00016600
C	-1.33837600	0.35775100	0.00005200
N	-3.92424000	2.72276500	0.00031500
C	-4.65308100	1.55620200	0.00027500
N	-3.91096700	0.47161700	0.00024800
H	0.54397400	3.04140400	-0.00002700
H	-4.29258600	3.66523000	0.00037800
H	-5.73411400	1.56967200	0.00033300
N	2.66429100	0.51286400	-0.00014300
C	3.41213400	1.67000500	-0.00018400
N	4.77430200	1.45728600	0.00024500
C	5.34647800	0.20453100	0.00043500
C	4.60514600	-0.93125600	0.00030600
C	3.15126600	-0.79762700	0.00009700
O	2.36006000	-1.74718900	-0.00004000
O	2.91336800	2.79862900	-0.00012800
C	5.20354500	-2.30820600	0.00048400
H	1.63971800	0.63782700	-0.00031100
H	5.35660800	2.28459000	0.00039700
H	6.43034400	0.19411500	0.00069000
H	4.88006800	-2.87423800	0.88083400

H	6.29533400	-2.25996600	0.00069600
H	4.88041400	-2.87431500	-0.87994400
S	-0.84208000	-1.34804400	-0.00015800
Br	-2.69286500	-2.56458200	-0.00046100

Table S68. Cartesian coordinates of A_{SeF}:T (water phase).

ATOM	X	Y	Z
N	-0.64196100	0.95871800	-0.00004000
C	-1.09996600	2.22379300	-0.00021600
N	-2.37395200	2.61363200	-0.00031200
C	-3.21590800	1.57707100	-0.00020300
C	-2.87553200	0.19738700	-0.00000900
C	-1.49720400	-0.07679300	0.00007000
N	-4.58329200	1.60978500	-0.00032900
C	-5.01069200	0.30331900	0.00005000
N	-4.03091100	-0.57136700	-0.00002800
H	-0.33688000	2.99755000	-0.00029800
H	-5.16492500	2.43770500	-0.00052100
H	-6.06344100	0.05703600	0.00006800
N	2.15885400	0.85413200	-0.00006400
C	2.95154800	1.97969100	-0.00027100
N	4.30453300	1.70191300	-0.00013400
C	4.81740400	0.42553600	-0.00008300
C	4.02349900	-0.67814900	-0.00003500
C	2.58905200	-0.45532800	0.00017200
O	1.74289200	-1.37640800	-0.00002100
O	2.49658900	3.12426000	-0.00011500
C	4.54417800	-2.08606100	-0.00004200
H	1.12219500	0.97081700	-0.00000500
H	4.92645200	2.50039000	-0.00012400
H	5.89952100	0.36366000	-0.00009700
H	4.18975700	-2.63184900	0.88089500
H	5.63669100	-2.09882500	-0.00027700
H	4.18937100	-2.63199000	-0.88073500
Se	-0.68288400	-1.81778800	0.00021700
F	-2.25419000	-2.75255300	0.00050300

Table S69. Cartesian coordinates of A_{SeCl}:T (water phase).

ATOM	X	Y	Z
N	-0.49765900	1.03030900	0.00028100
C	-0.77759100	2.34708300	0.00015800
N	-1.99055000	2.90272600	-0.00003600
C	-2.96679000	1.99240600	-0.00012900
C	-2.81645200	0.57935100	-0.00000400
C	-1.49228800	0.12944700	0.00021800
N	-4.31813900	2.20515200	-0.00035800
C	-4.91590200	0.96693300	-0.00037600
N	-4.06085800	-0.03028600	-0.00021600
H	0.08507700	3.00754900	0.00021800
H	-4.78672200	3.10217600	-0.00048800
H	-5.99207100	0.86366100	-0.00055300
N	2.38309100	0.72868500	0.00021300
C	3.11139800	1.89687600	-0.00001400

N	4.47704600	1.70012200	-0.00039000
C	5.06369700	0.45420600	-0.00043500
C	4.33747400	-0.69290500	-0.00015100
C	2.88577600	-0.56781900	0.00011200
O	2.09509400	-1.52450200	0.00056400
O	2.59275700	3.01587500	0.00001100
C	4.94705900	-2.06486300	-0.00013700
H	1.35113200	0.81711900	0.00049100
H	5.05104200	2.53340700	-0.00059500
H	6.14757800	0.45685400	-0.00069600
H	4.62891200	-2.63300300	0.88072300
H	6.03832200	-2.00785700	-0.00036500
H	4.62855300	-2.63317700	-0.88075500
Se	-0.77998600	-1.64482400	0.00026200
Cl	-2.60846600	-2.91264400	-0.00019900

Table S70. Cartesian coordinates of A_{SeBr}:T (water phase).

ATOM	X	Y	Z
N	0.06888100	1.31664400	-0.00046400
C	0.15283000	2.65998900	-0.00063800
N	1.27159900	3.38778400	-0.00048600
C	2.37072600	2.63041200	-0.00011700
C	2.42802300	1.21085600	0.00010000
C	1.18489500	0.57083400	-0.00009600
N	3.67681300	3.03750400	0.00013800
C	4.44849800	1.89915100	0.00049500
N	3.74721700	0.78837500	0.00048300
H	-0.79732600	3.18647400	-0.00095300
H	4.00983200	3.99317300	0.00008200
H	5.52825000	1.95337400	0.00075100
N	-2.75705800	0.62699200	-0.00054500
C	-3.61271900	1.70550300	-0.00049400
N	-4.94762600	1.35685100	-0.00026200
C	-5.39151500	0.05294700	0.00002500
C	-4.54135500	-1.00502500	0.00004100
C	-3.11166600	-0.71947600	-0.00042600
O	-2.22032800	-1.58083600	-0.00019500
O	-3.22528500	2.87667900	-0.00076100
C	-4.99353700	-2.43660400	0.00042400
H	-1.74230500	0.83295500	-0.00072100
H	-5.61140100	2.12067300	-0.00026800
H	-6.46879100	-0.06526100	0.00026300
H	-4.61366900	-2.96569000	-0.88032700
H	-6.08440200	-2.50252600	0.00070000
H	-4.61324200	-2.96536000	0.88118900
Br	2.80805200	-2.38208600	0.00044700
Se	0.72506600	-1.28212100	0.00009900

Table S71. Cartesian coordinates of G:C_{SF} (water phase).

ATOM	X	Y	Z
C	5.06557900	-1.26508100	-0.15784100
C	3.66431500	0.43436000	0.06389600
N	3.88268000	-1.82738900	-0.25662900

C	2.98703800	-0.77713700	-0.11991800
N	3.14610700	1.67051000	0.22908800
H	6.01609800	-1.77613000	-0.21626600
C	1.55996600	-0.75101900	-0.13894500
C	1.81841100	1.68123100	0.21182200
O	0.76512900	-1.69969500	-0.28980700
N	1.06006100	0.54514200	0.04059200
H	0.02902200	0.60200900	0.03323100
N	-3.77921200	1.86114700	-0.20362000
C	-2.38932500	1.74685900	-0.15783600
C	-4.61111100	0.79481900	-0.14036200
O	-1.68795200	2.76795800	-0.21428900
N	-1.87038000	0.48305300	-0.04498800
C	-4.09973700	-0.46935200	-0.02956700
H	-5.67329900	1.00352500	-0.18505500
C	-2.68227700	-0.56167100	0.01172000
H	-4.74262800	-1.33432700	0.01780200
H	-4.15350500	2.80039500	-0.28168100
N	4.99297500	0.10039200	0.03634200
H	5.77222600	0.73651300	0.14049200
N	1.14156800	2.83706100	0.39763800
H	1.68216000	3.68915600	0.38121500
H	0.14402700	2.88695800	0.18121600
S	-1.88186900	-2.14375300	0.13571200
F	-3.27504000	-3.06018100	0.34929400

Table S72. Cartesian coordinates of G:C_{SCI} (water phase).

ATOM	X	Y	Z
C	5.27684500	-1.38737200	-0.12937000
C	3.87962300	0.28282800	0.26603600
N	4.11792300	-1.85040200	-0.53987700
C	3.22554000	-0.81600300	-0.30022700
N	3.35787700	1.47448100	0.63239900
H	6.21735300	-1.91904300	-0.15824700
C	1.81716500	-0.72278500	-0.53245800
C	2.05106900	1.55404800	0.41938100
O	1.04961100	-1.56853200	-1.01857800
N	1.31154000	0.52732400	-0.12431200
H	0.29120500	0.63311900	-0.20571500
N	-3.42432200	2.40333500	-0.30144800
C	-2.05656000	2.11991300	-0.31811300
C	-4.37596200	1.45383600	-0.15213700
O	-1.23815200	3.04224900	-0.44067300
N	-1.69558400	0.80440900	-0.18354100
C	-4.01941100	0.13857600	-0.01126700
H	-5.40519600	1.79199500	-0.15400600
C	-2.62813800	-0.12408300	-0.04006300
H	-4.76554600	-0.63247700	0.10373900
H	-3.68474500	3.37915900	-0.39771300
N	5.19102000	-0.10188900	0.36726100
H	5.95106900	0.45393300	0.73621400
N	1.37052500	2.67200000	0.77309400

H	1.93601900	3.46957400	1.02633900
H	0.45641500	2.85972100	0.35564400
S	-1.89925000	-1.74445600	0.07819700
Cl	-3.51318500	-2.96547000	0.56122800

Table S73. Cartesian coordinates of G:C_{SBr} (water phase).

ATOM	X	Y	Z
C	5.43184500	-2.08087000	-0.02837000
C	4.40902900	-0.11777500	0.00975600
N	4.15694400	-2.39660900	-0.03795100
C	3.49659600	-1.17665400	-0.01414300
N	4.15581900	1.20798300	0.03643900
H	6.25714800	-2.77856000	-0.04067300
C	2.10032700	-0.87203800	-0.01543600
C	2.85709800	1.48993000	0.03854500
O	1.13753600	-1.65358300	-0.03758400
N	1.87486900	0.52006300	0.01159400
H	0.88705900	0.80169400	0.01008300
N	-2.55424500	3.24613700	-0.02986400
C	-1.25851000	2.72364300	-0.02571300
C	-3.66469400	2.47421800	-0.02073900
O	-0.29343900	3.50197700	-0.03549200
N	-1.13496000	1.35914600	-0.01150000
C	-3.54814200	1.11058400	-0.00831000
H	-4.61719600	2.99060500	-0.02460400
C	-2.22496200	0.60453800	-0.00572200
H	-4.42247200	0.47890200	-0.00197700
H	-2.63150900	4.25743100	-0.04009300
N	5.64239500	-0.71596100	0.00022300
H	6.53687500	-0.24437200	0.01294800
N	2.44864300	2.77271100	0.07874800
H	3.15820500	3.48881700	0.05373700
H	1.46103300	3.03521400	0.02812800
S	-1.81061300	-1.12678300	0.00086900
Br	-3.77514000	-2.16217400	0.01886100

Table S74. Cartesian coordinates of G:C_{SeF} (water phase).

ATOM	X	Y	Z
C	4.97275600	-1.46907300	-0.00005700
C	3.78802500	0.40094600	-0.00003300
N	3.73184200	-1.89664400	0.00018000
C	2.96875000	-0.73886500	0.00024900
N	3.41927200	1.69681800	-0.00012500
H	5.85538200	-2.09275400	-0.00015900
C	1.56579100	-0.53229700	0.00050700
C	2.09934600	1.85971000	-0.00000100
O	0.67113200	-1.42504400	0.00060400
N	1.21400300	0.80473700	0.00028900
H	0.18168900	0.96164000	0.00041500
N	-3.45273700	2.31375600	-0.00007600
C	-2.06701800	2.18217500	0.00012700
C	-4.28884600	1.24674200	-0.00031300
O	-1.34800500	3.19425000	0.00046000

N	-1.56252800	0.90796500	0.00008000
C	-3.78402400	-0.02346800	-0.00036200
H	-5.35057500	1.46274100	-0.00044900
C	-2.36657100	-0.14406200	-0.00017300
H	-4.43536400	-0.88270800	-0.00051700
H	-3.82156900	3.25826600	-0.00001600
N	5.06613700	-0.09033300	-0.00018500
H	5.91785200	0.45522300	-0.00037600
N	1.55841500	3.09253100	-0.00021600
H	2.17894400	3.88707800	-0.00033400
H	0.54583100	3.22764300	-0.00010800
F	-3.25054200	-2.71842400	-0.00071400
Se	-1.57507100	-1.89581200	0.00000500

Table S75. Cartesian coordinates of G:C_{SeCl} (water phase).

ATOM	X	Y	Z
C	5.07351000	-1.85672500	0.00000800
C	4.06163700	0.11229700	0.00016200
N	3.79838800	-2.16915000	0.00002400
C	3.14356700	-0.94663700	-0.00004700
N	3.81219900	1.43733100	0.00027000
H	5.89614400	-2.55768200	-0.00000400
C	1.75979600	-0.62080900	-0.00022400
C	2.51347300	1.72125000	0.00016300
O	0.78803800	-1.41577900	-0.00018800
N	1.53288400	0.75189500	-0.00008500
H	0.52986500	1.01134000	-0.00013500
N	-2.96429600	2.87363300	0.00016700
C	-1.61520400	2.52364200	-0.00041100
C	-3.95910600	1.95607300	0.00064100
O	-0.75197300	3.41490100	-0.00091500
N	-1.31450800	1.18544500	-0.00044900
C	-3.65847400	0.62179900	0.00060800
H	-4.97356100	2.33602400	0.00106200
C	-2.28184800	0.28007900	0.00000500
H	-4.44618500	-0.11420500	0.00100600
H	-3.17686300	3.86548300	0.00017600
N	5.29080900	-0.49207600	0.00021300
H	6.18765000	-0.02464100	0.00033200
N	2.09342000	3.00004200	0.00032400
H	2.78901100	3.72979500	0.00050300
H	1.09860000	3.23276300	0.00007400
Se	-1.67711300	-1.55175300	-0.00010200
Cl	-3.71398300	-2.56281900	0.00003600

Table S76. Cartesian coordinates of G:C_{SeBr} (water phase).

C	5.20180400	-2.39415700	0.00010300
C	4.46023600	-0.30834300	0.00004400
N	3.89628200	-2.53389700	-0.00022500
C	3.40964400	-1.23484100	-0.00028200
N	4.39024400	1.03857200	0.00012600
H	5.92389700	-3.19832100	0.00022800
C	2.07829800	-0.73034400	-0.00059300

C	3.14125100	1.49390300	-0.00011900
O	1.00982400	-1.38177200	-0.00081800
N	2.03907800	0.66494500	-0.00047300
H	1.08389500	1.06073100	-0.00067800
N	-2.09899100	3.49519400	0.00019300
C	-0.82547200	2.92724800	-0.00038200
C	-3.23230900	2.75591700	0.00062700
O	0.17005400	3.66814000	-0.00079900
N	-0.74706700	1.55840200	-0.00046200
C	-3.15395900	1.39082800	0.00053200
H	-4.16989200	3.29872200	0.00107300
C	-1.85305100	0.82764900	-0.00007000
H	-4.05044200	0.79202600	0.00090600
H	-2.14312200	4.50854800	0.00024300
N	5.59864300	-1.07064700	0.00024100
H	6.54981500	-0.72679000	0.00047300
N	2.89944100	2.81807200	0.00002600
H	3.68920600	3.44469900	0.00008100
H	1.94628600	3.18747600	-0.00042700
Br	-3.80438700	-1.84032200	0.00057600
Se	-1.53874100	-1.07083500	-0.00012600

Table S77. Cartesian coordinates of G_{SF}:C (water phase).

ATOM	**X**	**Y**	**Z**
C	-4.71349600	-1.66242400	0.01275600
C	-3.20284500	-0.05737400	0.00651900
N	-3.56934100	-2.31348600	0.00763400
C	-2.60876000	-1.31908000	0.00367200
N	-2.58474400	1.14670000	0.00389400
H	-5.69517200	-2.11428500	0.01703900
C	-1.18090800	-1.39794900	-0.00329700
C	-1.28043400	1.05595800	-0.00197700
O	-0.48102500	-2.42458100	-0.00851200
N	-0.57976700	-0.11910100	-0.00476300
H	0.46747700	-0.14549400	-0.00707700
N	4.24273500	0.89084300	0.01901400
C	2.84974200	0.82315300	0.01468600
C	5.02368800	-0.22687900	0.00882900
O	2.18759700	1.88153300	0.02515100
N	2.26723000	-0.39829100	-0.00098900
C	4.45272900	-1.46052700	-0.00585100
H	6.09494500	-0.06705400	0.01332600
C	3.01602300	-1.51542100	-0.01002100
H	5.05421700	-2.35975900	-0.01379900
N	2.36685300	-2.68529500	-0.02286700
H	1.34271600	-2.68320000	-0.02154800
H	2.87284800	-3.55749300	-0.02906200
H	4.65944400	1.81339300	0.03010500
N	-4.55073200	-0.29507900	0.01229800
H	-5.28509100	0.40097700	0.01552000
S	-0.33753900	2.59625900	-0.00896700
F	-1.67148900	3.61070900	-0.02728800

Table S78. Cartesian coordinates of G_{SCl}:C (water phase).

ATOM	X	Y	Z
C	4.60245100	-1.98770900	-0.14306100
C	3.11611400	-0.36104100	-0.12603500
N	3.44842600	-2.62208800	-0.15155500
C	2.50258400	-1.61508800	-0.14432100
N	2.51627800	0.85354600	-0.11098800
H	5.57737800	-2.45389800	-0.14963400
C	1.07244800	-1.67359500	-0.12689800
C	1.21247700	0.77705800	-0.09859700
O	0.34705200	-2.68247400	-0.10409400
N	0.49668400	-0.38616000	-0.11508900
H	-0.55698200	-0.38270300	-0.12071700
N	-4.30042200	0.73543300	-0.49772100
C	-2.91866500	0.60640900	-0.66806900
C	-5.05136300	-0.21010100	0.13323500
O	-2.28700300	1.50039700	-1.25868700
N	-2.32351000	-0.50894200	-0.16814200
C	-4.46655500	-1.33625500	0.62245300
H	-6.11333200	-0.01032400	0.21018500
C	-3.04729700	-1.46516800	0.43822000
H	-5.04686800	-2.10309600	1.11808300
N	-2.38831400	-2.55006100	0.87090900
H	-1.40719100	-2.67377900	0.60759600
H	-2.88858300	-3.31891400	1.29043200
H	-4.73070800	1.57254000	-0.87043700
N	4.46012300	-0.61900200	-0.12600600
H	5.20456200	0.06631400	-0.11536900
S	0.20564900	2.27525600	-0.06772300
Cl	1.57017200	3.62530900	0.75201500

Table S79. Cartesian coordinates of G_{SBr}:C (water phase).

ATOM	X	Y	Z
C	-3.57556400	3.52880900	-0.00066500
C	-2.62989600	1.53840700	-0.00049500
N	-2.28662800	3.79722900	-0.00453300
C	-1.67832000	2.55602000	-0.00469300
N	-2.41023400	0.20218700	0.00076700
H	-4.37161100	4.25969200	0.00057600
C	-0.29465800	2.19540400	-0.00760200
C	-1.14260200	-0.11207500	-0.00222100
O	0.68126700	2.96271800	-0.01122800
N	-0.11105200	0.79405300	-0.00599200
H	0.88701400	0.48634700	-0.00560300
N	4.42114500	-1.56933100	-0.00950300
C	3.07281700	-1.18982400	-0.01091700
C	5.43850700	-0.66501800	0.00285900
O	2.20188600	-2.07589800	-0.02196300
N	2.78243900	0.13988600	-0.00070400
C	5.16402300	0.66517800	0.01390600
H	6.44462800	-1.06657600	0.00323900
C	3.77684900	1.04682500	0.01100400

H	5.95317100	1.40531800	0.02362900
N	3.43576600	2.34164400	0.02066000
H	2.44611600	2.60725700	0.01180200
H	4.14664700	3.05685400	0.02528500
H	4.61252900	-2.56323400	-0.01758200
N	-3.83989300	2.17746300	0.00186500
H	-4.75158400	1.73868600	0.00492400
S	-0.63285100	-1.83850800	-0.00328200
Br	-2.60097900	-2.86191600	0.00705100

Table S80. Cartesian coordinates of G_{SeF}:C (water phase).

ATOM	X	Y	Z
C	4.70531900	-1.90664900	0.00003300
C	3.14662500	-0.34706800	-0.00005400
N	3.58128600	-2.59237500	-0.00029000
C	2.59065000	-1.62756100	-0.00010600
N	2.49815400	0.83994000	0.00013400
H	5.70030400	-2.32858700	0.00007800
C	1.16560500	-1.74141500	-0.00005300
C	1.19709900	0.71662900	0.00027300
O	0.48290500	-2.78263600	-0.00014700
N	0.53972700	-0.47939700	0.00007600
H	-0.50698300	-0.53220100	-0.00009000
N	-4.14528900	0.65682300	0.00021800
C	-2.76539300	0.52222700	0.00009900
C	-4.97042500	-0.42965000	0.00032000
O	-2.06262500	1.56593000	-0.00005700
N	-2.23485700	-0.71138200	0.00002000
C	-4.45362400	-1.68772200	0.00025700
H	-6.03359300	-0.22333700	0.00042300
C	-3.02206700	-1.80414900	0.00009700
H	-5.09444600	-2.55912900	0.00031200
N	-2.40565300	-2.98910300	-0.00001700
H	-1.38092700	-3.01384100	-0.00013000
H	-2.93248400	-3.84942000	0.00003100
H	-4.52400200	1.59600400	0.00023300
N	4.50161800	-0.54546800	-0.00016700
H	5.21490700	0.17215900	-0.00018600
F	1.67023700	3.41331300	-0.00004500
Se	0.15456500	2.36267800	-0.00010700

Table S81. Cartesian coordinates of G_{SeCl}:C (water phase).

ATOM	X	Y	Z
C	4.31323800	-2.67634500	-0.00072800
C	2.98539600	-0.91837900	-0.00025100
N	3.10526500	-3.20011300	-0.00047600
C	2.25793300	-2.10779400	-0.00021100
N	2.50589000	0.34566500	0.00007300
H	5.24043300	-3.23154500	-0.00096200
C	0.83093000	-2.02295800	0.00012800
C	1.20312100	0.40866600	0.00037300
O	0.01699600	-2.96337600	0.00026700
N	0.38138200	-0.68567100	0.00027000

H	-0.66186300	-0.59631100	0.00037200
N	-4.23349200	0.94446700	-0.00098700
C	-2.86708500	0.68796200	-0.00062500
C	-5.15513900	-0.06026800	-0.00061800
O	-2.07723000	1.66230400	-0.00100000
N	-2.44846600	-0.59226900	0.00021000
C	-4.75333900	-1.35895900	0.00013200
H	-6.19535300	0.24131700	-0.00097100
C	-3.33708700	-1.60474100	0.00057600
H	-5.46972000	-2.16957700	0.00043200
N	-2.84201600	-2.84567600	0.00136400
H	-1.82462100	-2.97424000	0.00143100
H	-3.45407300	-3.64755700	0.00150200
H	-4.52230500	1.91497400	-0.00154400
N	4.30011100	-1.29979800	-0.00057700
H	5.10477600	-0.68633600	-0.00066100
Cl	2.25227300	3.37325200	0.00060700
Se	0.34492500	2.16068300	0.00012200

Table S82. Cartesian coordinates of G_{SeBr}:C (water phase).

ATOM	X	Y	Z
C	3.17300800	3.96449600	0.00008600
C	2.35549100	1.91857700	0.00009000
N	1.86961600	4.15162400	0.00017800
C	1.34061300	2.87398100	0.00026600
N	2.22671100	0.57297300	-0.00000100
H	3.92093700	4.74466600	0.00001400
C	-0.01357300	2.41633700	0.00045000
C	0.98645100	0.16850100	0.00010600
O	-1.04503200	3.11100800	0.00050600
N	-0.09605300	1.00761100	0.00037500
H	-1.07717100	0.64435500	0.00047700
N	-4.19736700	-1.73976100	0.00031500
C	-2.93019000	-1.16247100	0.00050200
C	-5.33451400	-0.98872800	0.00011300
O	-1.93088100	-1.91547700	0.00057300
N	-2.83361300	0.18400700	0.00031800
C	-5.25801500	0.36838400	0.00010500
H	-6.27101000	-1.53292500	0.00001400
C	-3.94268400	0.94815200	0.00017000
H	-6.14756100	0.98393200	-0.00001000
N	-3.76919200	2.27364100	0.00012000
H	-2.81602800	2.65093800	0.00029400
H	-4.56170000	2.89753600	0.00009800
H	-4.24395200	-2.75117500	0.00034000
N	3.52317400	2.63345900	0.00000300
H	4.46148900	2.25489900	-0.00011700
Br	2.87267600	-2.48328200	-0.00073200
Se	0.60812200	-1.74029000	-0.00013600

Table S83. Cartesian coordinates of G_{SF}:C_{SF} (water phase).

ATOM	X	Y	Z
C	-4.66882700	-2.15563900	-0.40397500

C	-3.46146600	-0.33366500	-0.11732000
N	-3.42804400	-2.59488200	-0.45350200
C	-2.65528500	-1.46434000	-0.27644200
N	-3.06780700	0.95103900	0.06489000
H	-5.55658800	-2.76312400	-0.50717300
C	-1.23254000	-1.29891200	-0.22239900
C	-1.76786300	1.07743300	0.12539400
O	-0.34273600	-2.15669700	-0.32544000
N	-0.88278000	0.04862200	0.00054400
H	0.14449900	0.20088700	0.03762100
N	3.50744400	1.91245700	-0.75796500
C	2.17104600	1.54586700	-0.60082600
C	4.53710400	1.06620700	-0.51076900
O	1.26195400	2.35219700	-0.84843100
N	1.92752500	0.27465000	-0.15966700
C	4.29469700	-0.21600800	-0.09447400
H	5.53457100	1.45831200	-0.66811500
C	2.92717600	-0.56257700	0.05666800
H	5.09760400	-0.91192300	0.09491500
H	3.68662800	2.86022500	-1.07218700
N	-4.74673500	-0.79699600	-0.20256000
H	-5.59167000	-0.24496200	-0.12964600
S	-1.06806700	2.71083900	0.41363900
F	-2.40376700	3.33809400	1.21083000
S	2.41805500	-2.19119100	0.52700200
F	3.92598300	-2.78167500	0.94560900

Table S84. Cartesian coordinates of G_{SCl}:C_{SF} (water phase).

ATOM	**X**	**Y**	**Z**
C	4.25142300	-2.80149700	-0.35738000
C	3.25974800	-0.84286600	-0.16392100
N	2.97175800	-3.08866700	-0.47868800
C	2.33319400	-1.86986100	-0.36192600
N	3.01332800	0.48193900	-0.01023400
H	5.06382200	-3.51284700	-0.40005000
C	0.94145000	-1.53281400	-0.39191600
C	1.73978900	0.76575800	-0.03836200
O	-0.03831400	-2.28169000	-0.53131300
N	0.74249600	-0.14873900	-0.21408300
H	-0.26444100	0.11973400	-0.22132100
N	-3.67293500	1.92786300	-0.83198800
C	-2.33338500	1.52807400	-0.85128700
C	-4.67151200	1.14835300	-0.35238100
O	-1.45851900	2.27629500	-1.29955100
N	-2.05660400	0.28496900	-0.33840300
C	-4.39782900	-0.10012300	0.13895500
H	-5.67166700	1.56329400	-0.39039600
C	-3.03129300	-0.48586600	0.11122400
H	-5.17834800	-0.74319700	0.51534600
H	-3.87492200	2.85145700	-1.19880600
N	4.48149800	-1.45856900	-0.16415700
H	5.38078500	-1.00944400	-0.04771200

S	1.15297500	2.46016200	0.12909300
S	-2.51588600	-2.09010100	0.67169800
F	-3.95701600	-2.52426400	1.41380700
Cl	2.76663800	3.33676700	1.10104500

Table S85. Cartesian coordinates of G_{SBr}:C_{SF} (water phase).

ATOM	X	Y	Z
C	-2.69888300	4.23653900	-0.00050400
C	-2.45498700	2.04603800	-0.00015000
N	-1.39275800	4.06961400	-0.00064100
C	-1.22258300	2.69850000	-0.00032600
N	-2.68755800	0.71044800	0.00005500
H	-3.21312300	5.18697700	-0.00062900
C	-0.03246000	1.90301600	-0.00019800
C	-1.59324200	-0.00081500	0.00012300
O	1.14517800	2.29112300	-0.00052100
N	-0.32642600	0.52261200	0.00000600
H	0.51977700	-0.07019300	0.00012000
N	3.34926800	-2.85615800	-0.00021000
C	2.19765800	-2.06462900	-0.00010200
C	4.60023900	-2.33868600	-0.00020700
O	1.08060500	-2.59433200	-0.00021700
N	2.37329600	-0.70378900	-0.00007200
C	4.78202300	-0.98308100	-0.00010700
H	5.42012600	-3.04704900	-0.00027700
C	3.59516000	-0.19841600	-0.00001300
H	5.76900300	-0.54819100	-0.00008900
H	3.20799700	-3.86007900	-0.00030700
N	-3.38958900	3.04558500	-0.00023600
H	-4.39485800	2.92968500	-0.00013400
S	-1.65769400	-1.79758500	0.00037100
S	3.69237900	1.57732000	0.00019200
F	5.37006200	1.68967500	0.00022000
Br	-3.84348300	-2.14735100	0.00036600

Table S86. Cartesian coordinates of G_{SeF}:C_{SF} (water phase).

ATOM	X	Y	Z
C	-4.20275500	3.02848500	-0.00032500
C	-3.24083400	1.04447800	-0.00009200
N	-2.91598500	3.30824100	-0.00041500
C	-2.29590100	2.07311400	-0.00023200
N	-3.01990800	-0.29180900	0.00011100
H	-5.00485400	3.75278400	-0.00039600
C	-0.91087600	1.71297000	-0.00018500
C	-1.75140500	-0.60075200	0.00013200
O	0.08421600	2.45649200	-0.00036000
N	-0.74097500	0.31458300	-0.00005900
H	0.25587000	0.03852900	-0.00012800
N	3.39286200	-2.11700900	-0.00019500
C	2.12598100	-1.54931900	-0.00021300
C	4.52382300	-1.37017500	-0.00009500
O	1.12244700	-2.29163400	-0.00029500
N	2.04150100	-0.19462900	-0.00011300

C	4.45059400	-0.00243600	-0.00001800
H	5.46094400	-1.91330400	-0.00008200
C	3.14092300	0.54411800	-0.00004000
H	5.33892500	0.61014800	0.00006300
H	3.44462100	-3.13038400	-0.00025500
N	-4.45551000	1.67570300	-0.00014600
H	-5.36386300	1.23015200	-0.00005800
F	-3.02623400	-3.01863800	0.00046800
S	2.85315200	2.28913000	0.00007900
F	4.45848500	2.76581300	0.00058600
Se	-1.27873000	-2.48252600	0.00022000

Table S87. Cartesian coordinates of G_{SeCl}:C_{SF} (water phase).

ATOM	X	Y	Z
C	-3.43010600	3.81248700	0.00011400
C	-2.85844400	1.68463200	-0.00011600
N	-2.11357700	3.84539100	0.00006600
C	-1.73748200	2.51568000	-0.00017000
N	-2.89070300	0.33101700	-0.00029100
H	-4.08167900	4.67466900	0.00024600
C	-0.44578300	1.90072800	-0.00038100
C	-1.70687800	-0.21373500	-0.00043900
O	0.66723800	2.45180300	-0.00026700
N	-0.53798500	0.49445100	-0.00038100
H	0.39145000	0.04017800	-0.00026600
N	3.30694300	-2.48031300	-0.00005600
C	2.10886200	-1.77246000	-0.00009600
C	4.51523900	-1.86854500	0.00008700
O	1.02952600	-2.39045800	-0.00019000
N	2.18031600	-0.41162100	0.00010200
C	4.59764700	-0.50234700	0.00022300
H	5.38530800	-2.51367600	0.00007500
C	3.35840200	0.19260400	0.00018800
H	5.55069300	0.00294000	0.00033700
H	3.24156600	-3.49257300	-0.00015700
N	-3.93325700	2.53166300	-0.00001400
H	-4.90957500	2.26562700	-0.00001800
S	3.30285700	1.96518100	0.00040200
F	4.96281300	2.21719400	0.00028200
Cl	-3.71524500	-2.62003300	0.00021500
Se	-1.52925400	-2.14686400	-0.00004800

Table S88. Cartesian coordinates of G_{SeBr}:C_{SF} (water phase).

ATOM	X	Y	Z
C	-2.23511100	4.56780000	-0.00010900
C	-2.10125000	2.36836500	-0.00005200
N	-0.93868500	4.33645400	-0.00002500
C	-0.83692800	2.95815500	-0.00011400
N	-2.40490300	1.04933500	-0.00003000
H	-2.70058500	5.54310700	-0.00012100
C	0.30493100	2.09637700	-0.00017900
C	-1.35453500	0.27746700	-0.00008700
O	1.50540400	2.41495100	-0.00020400

N	-0.06653700	0.73735200	-0.00018900
H	0.75204800	0.10555100	-0.00028900
N	3.17450500	-2.91748700	-0.00022200
C	2.12429200	-2.00287100	-0.00025800
C	4.47438100	-2.53741200	-0.00006300
O	0.95145300	-2.41112500	-0.00041400
N	2.44476700	-0.67618600	-0.00015000
C	4.80546600	-1.20948700	0.00004800
H	5.21130800	-3.33153600	-0.00003300
C	3.71368600	-0.29934500	-0.00001700
H	5.83495300	-0.88719100	0.00018900
H	2.92600300	-3.90106400	-0.00030700
N	-2.98471200	3.41374000	-0.00009700
H	-3.99450200	3.34929400	-0.00011600
S	3.98650000	1.45414000	0.00020900
F	5.66583000	1.39656200	0.00055100
Br	-3.92406900	-1.70255700	0.00023500
Se	-1.56055200	-1.64915700	-0.00002800

Table S89. Cartesian coordinates =of G_{SF}:C_{SBr} (water phase).

ATOM	X	Y	Z
C	-5.03091200	-2.65335400	-0.74746700
C	-4.05666500	-0.76399100	-0.17101300
N	-3.74619300	-2.95085300	-0.75313600
C	-3.11905300	-1.77596300	-0.39553400
N	-3.82198800	0.52504200	0.17938200
H	-5.83528900	-3.33524100	-0.98381900
C	-1.72516600	-1.47610000	-0.21563900
C	-2.55080600	0.78102600	0.34874800
O	-0.74548100	-2.21550900	-0.35945800
N	-1.55058900	-0.13160900	0.17825600
H	-0.56829500	0.18575400	0.21625000
N	1.80927000	2.95924600	-1.31469400
C	0.74300900	2.18221200	-0.86501500
C	3.09844400	2.54813200	-1.25355800
O	-0.42116700	2.61046400	-0.95552300
N	1.04999600	0.96240000	-0.33580800
C	3.40757700	1.31622300	-0.73815200
H	3.84410100	3.23556500	-1.63444600
C	2.30492700	0.54291400	-0.30611100
H	4.42818300	0.96792900	-0.69408600
H	1.57865000	3.86808600	-1.70244300
N	-5.27453200	-1.34611200	-0.40308100
H	-6.17878600	-0.89693100	-0.33576800
S	-2.07799100	2.41959400	0.92399600
F	-3.18356500	2.44133300	2.21876700
S	2.37098700	-1.13540100	0.26401600
Br	4.52396900	-1.54392200	0.56808800

Table S90. Cartesian coordinates of G_{SCl}:C_{SBr} (water phase).

ATOM	X	Y	Z
C	4.85643000	-1.91684500	-0.91798300
C	3.47559900	-0.43039900	-0.05760500

N	3.91860000	-1.79583800	-1.83451700
C	3.04230600	-0.86542800	-1.31129800
N	2.87826500	0.47059300	0.76687600
H	5.71943300	-2.56426300	-0.97965300
C	1.82568400	-0.32498900	-1.84823100
C	1.77514600	0.94884600	0.26888100
O	1.26182900	-0.57850600	-2.91559700
N	1.25806000	0.61778400	-0.95377500
H	0.31645600	0.95960700	-1.19934600
N	-3.62698500	2.17029500	-1.36003200
C	-2.22421300	2.22622200	-1.37336300
C	-4.32916600	1.13151400	-0.85396400
O	-1.64278700	3.20082200	-1.85011300
N	-1.57494000	1.14119800	-0.83005800
C	-3.67692200	0.05558100	-0.30983200
H	-5.40910900	1.20508600	-0.90304400
C	-2.26515900	0.12984800	-0.32931800
H	-4.22026600	-0.78138400	0.10047200
H	-4.11049100	2.96698800	-1.76028000
N	4.63736800	-1.11264600	0.17732900
H	5.22153100	-1.03937500	1.00034300
S	-1.16912100	-1.10823600	0.33145300
Br	-2.47585300	-2.71865300	1.07369200
S	0.76973100	2.15146700	1.14896600
Cl	1.83908100	2.38648000	2.89628200

Table S91. Cartesian coordinates of G_{SBr}:C_{SBr} (water phase).

ATOM	X	Y	Z
C	2.97807400	4.46422700	-0.00050900
C	2.97455300	2.26037100	-0.00039600
N	1.69820400	4.15425400	-0.00063300
C	1.67928600	2.77248800	-0.00069000
N	3.35268100	0.95814100	-0.00023200
H	3.38453400	5.46549900	-0.00048000
C	0.57750900	1.85557300	-0.00095300
C	2.34536500	0.12917200	-0.00026400
O	-0.62992300	2.10983900	-0.00082500
N	1.02610300	0.50773100	-0.00051800
H	0.26444500	-0.18388000	-0.00038300
N	-2.12436500	-3.48529900	-0.00052500
C	-1.15184200	-2.47927100	-0.00053700
C	-3.45268900	-3.22815500	-0.00035600
O	0.04721100	-2.77858000	-0.00070800
N	-1.59643700	-1.18209500	-0.00035900
C	-3.90015100	-1.93507100	-0.00016900
H	-4.11501300	-4.08551200	-0.00037300
C	-2.89547500	-0.93433300	-0.00016600
H	-4.95566500	-1.71338200	-0.00003300
H	-1.78543000	-4.44099100	-0.00065900
N	3.79472500	3.35614000	-0.00035100
H	4.80662100	3.35082000	-0.00020100
S	2.62351700	-1.64897800	0.00012900

S	-3.22593800	0.81755800	0.00007100
Br	-5.44465500	0.95602200	0.00080200
Br	4.83656300	-1.73693600	0.00073400

Table S92. Cartesian coordinates of G_{SeF}:C_{SBr} (water phase).

ATOM	X	Y	Z
C	-3.95186000	3.92441700	-0.00007500
C	-3.55797800	1.75523700	-0.00007400
N	-2.63722600	3.84705900	-0.00014700
C	-2.37285800	2.49030400	-0.00012900
N	-3.70194100	0.40879600	-0.00001300
H	-4.52934700	4.83789200	-0.00006400
C	-1.13113000	1.77649700	-0.00018600
C	-2.56511300	-0.23205500	0.00001500
O	0.01914200	2.23091400	-0.00019800
N	-1.34134200	0.37554700	-0.00006600
H	-0.46452500	-0.16613800	-0.00004600
N	1.87268300	-3.26398200	0.00010900
C	0.87008600	-2.30172100	0.00008200
C	3.18787100	-2.94264500	0.00010500
O	-0.32203100	-2.67094600	0.00008900
N	1.24462500	-0.99734000	0.00011800
C	3.57722600	-1.62949200	0.00005200
H	3.88790800	-3.76927400	0.00011700
C	2.53152100	-0.67540800	0.00006300
H	4.62236500	-1.36174800	0.00002100
H	1.57956800	-4.23562600	0.00012600
N	-4.55924000	2.68949300	-0.00010500
H	-5.55413500	2.50572400	-0.00010000
F	-4.47736900	-2.18584600	0.00011300
S	2.75392200	1.08585800	-0.00005100
Br	4.95667300	1.35543900	0.00002500
Se	-2.64818300	-2.17176100	0.00004000

Table S93. Cartesian coordinates of G_{SeCl}:C_{SBr} (water phase).

ATOM	X	Y	Z
C	3.36945800	4.32218200	-0.00003200
C	3.21306000	2.12463000	0.00005000
N	2.07088800	4.10252900	-0.00003600
C	1.95582800	2.72529900	0.00012500
N	3.50151200	0.80161400	-0.00001600
H	3.84399800	5.29310800	-0.00008500
C	0.79894800	1.88062700	0.00034300
C	2.44562600	0.03901500	-0.00017300
O	-0.39181400	2.21095000	0.00004800
N	1.15957300	0.50884900	-0.00002600
H	0.34756200	-0.12346000	-0.00004700
N	-1.90971100	-3.33806400	0.00007300
C	-0.95390800	-2.32488000	-0.00004500
C	-3.23953200	-3.08780500	0.00011700
O	0.25278100	-2.62732000	-0.00002000
N	-1.39857300	-1.03828200	0.00007900
C	-3.69614900	-1.79695700	0.00009500

H	-3.89579400	-3.94959000	0.00016500
C	-2.70041200	-0.78938400	0.00009900
H	-4.75335800	-1.58279500	0.00009700
H	-1.56375200	-4.29154600	0.00009700
N	4.10767100	3.16088400	0.00006000
H	5.11679300	3.08653300	0.00006200
S	-3.02711100	0.95854100	-0.00005600
Br	-5.24428900	1.09602800	-0.00006800
Cl	4.90700000	-1.90707200	-0.00008800
Se	2.66778500	-1.89169900	-0.00000500

Table S94. Cartesian coordinates of G_{SeBr}:C_{SBr} (water phase).

ATOM	X	Y	Z
C	-2.57178400	4.71209300	-0.00001500
C	-2.61524500	2.50933600	-0.00002600
N	-1.29855700	4.37528200	0.00012100
C	-1.30890300	2.99315500	0.00012600
N	-3.02426200	1.21920500	-0.00005400
H	-2.95614700	5.72211700	-0.00005400
C	-0.23393600	2.04619600	0.00023700
C	-2.04300400	0.36232400	0.00009300
O	0.98181700	2.26742200	0.00035200
N	-0.71844400	0.71296200	0.00021200
H	0.03116900	0.00794000	0.00027200
N	2.04582800	-3.39142700	-0.00007900
C	1.17048400	-2.30666700	0.00006800
C	3.39081600	-3.24643200	-0.00015200
O	-0.05443800	-2.51270900	0.00011400
N	1.71568300	-1.05737700	0.00012600
C	3.94682400	-1.99528300	-0.00008000
H	3.97735600	-4.15731800	-0.00026000
C	3.03263600	-0.91262000	0.00005400
H	5.01726600	-1.86369800	-0.00013300
H	1.62660800	-4.31487600	-0.00013100
N	-3.41236900	3.62253300	-0.00011100
H	-4.42407200	3.63912400	-0.00021800
S	3.49898600	0.80447100	0.00015700
Br	5.72099800	0.76040500	0.00019400
Br	-4.79591600	-1.36027500	-0.00029000
Se	-2.43574500	-1.53788000	-0.00016700

Table S95. Cartesian coordinates of G_{SF}:C_{SCl} (water phase).

ATOM	X	Y	Z
C	5.06019600	-2.03514500	-0.69630300
C	3.74163000	-0.37256700	-0.10355800
N	3.84862200	-2.54226800	-0.81040500
C	3.00804300	-1.51272700	-0.44179700
N	3.26605200	0.83923000	0.27772900
H	5.98323300	-2.55767800	-0.90338100
C	1.57382600	-1.46003000	-0.36480300
C	1.96239800	0.86487300	0.37398300
O	0.74827500	-2.34001700	-0.63006300
N	1.14740100	-0.19724600	0.10380800

H	0.12973800	-0.07277100	0.19440200
N	-2.44804500	2.03269000	-1.80261700
C	-1.40555300	1.62028800	-0.97561100
C	-3.67301900	1.45788300	-1.78717500
O	-0.29994100	2.18713700	-1.04800600
N	-1.66139000	0.58388500	-0.12470100
C	-3.93869200	0.42029100	-0.93086600
H	-4.40683000	1.86206000	-2.47395100
C	-2.85993600	0.02206400	-0.10857500
H	-4.91089600	-0.04775100	-0.90130700
H	-2.25015800	2.80116900	-2.43499200
N	5.05332400	-0.72759900	-0.27386500
H	5.86148500	-0.13868900	-0.11869700
F	2.20870800	2.58903200	2.27900900
S	-2.89622700	-1.28074600	1.09361400
Cl	-4.79590700	-2.08178000	0.91704400
S	1.17145800	2.37544900	0.94265100

Table S96. Cartesian coordinates of G_{SCl}:C_{SCl} (water phase).

ATOM	X	Y	Z
C	4.84914400	-2.49160800	-0.54459600
C	3.62236900	-0.69177500	-0.21574900
N	3.61207900	-2.94551800	-0.58719800
C	2.82822500	-1.82933000	-0.38240000
N	3.21268500	0.58552600	-0.01669000
H	5.74255700	-3.08721000	-0.66668700
C	1.39935200	-1.69021400	-0.31900900
C	1.91365600	0.69385800	0.06547200
O	0.52737100	-2.55498000	-0.45106500
N	1.04057400	-0.34920700	-0.04971600
H	0.02802300	-0.15857800	-0.00175500
N	-2.68258000	1.62189000	-2.20273800
C	-1.55605300	1.29083300	-1.44552800
C	-3.91920400	1.13905000	-1.94186600
O	-0.44818200	1.76243900	-1.73712400
N	-1.75366000	0.43229100	-0.39612500
C	-4.11948900	0.28228500	-0.89014800
H	-4.71612300	1.46646200	-2.59872600
C	-2.96276600	-0.03766000	-0.14203500
H	-5.09884100	-0.11176800	-0.66530000
H	-2.53418800	2.25592800	-2.98071300
N	4.91286700	-1.13696200	-0.32332100
H	5.75170400	-0.57534000	-0.25228200
S	1.16025500	2.30681000	0.34495600
S	-2.90561200	-1.11232700	1.26949700
Cl	-4.85516200	-1.77486400	1.48548500
Cl	2.34892100	2.95076800	1.97130300

Table S97. Cartesian coordinates of G_{SBr}:C_{SCl} (water phase).

ATOM	X	Y	Z
C	-2.84514400	4.32934300	-0.04375700
C	-2.67207400	2.13232900	-0.01954800
N	-1.54525300	4.11897000	-0.05940700

C	-1.42001300	2.74289900	-0.04455900
N	-2.94922400	0.80479300	-0.00003900
H	-3.32762000	5.29626700	-0.04889400
C	-0.25080300	1.91306400	-0.04945000
C	-1.88096300	0.05606300	-0.00591400
O	0.93438800	2.25740500	-0.06963100
N	-0.59564600	0.53571800	-0.02754200
H	0.21490800	-0.09505100	-0.02348500
N	2.87558200	-3.14766300	-0.09441500
C	1.83991300	-2.20826600	-0.05875700
C	4.18395000	-2.80381900	-0.08481300
O	0.66209200	-2.58343300	-0.07171000
N	2.19959300	-0.88637500	-0.01042900
C	4.54818400	-1.48484700	-0.03755500
H	4.90071800	-3.61572800	-0.11578900
C	3.47830700	-0.55392700	-0.00215500
H	5.58732200	-1.19490200	-0.03015200
H	2.60204300	-4.12390500	-0.12807800
N	-3.57395400	3.16189500	-0.01943100
H	-4.58232800	3.07920300	-0.00470800
S	-2.01652300	-1.73777300	0.00923600
S	3.68465300	1.21695000	0.05381200
Cl	5.75684900	1.45432300	0.11200500
Br	-4.21397800	-1.99932500	0.06076800

Table S98. Cartesian coordinates of G_{SeF}:C_{SCl} (water phase).

ATOM	**X**	**Y**	**Z**
C	4.10224500	3.44324900	0.00062200
C	3.36281500	1.36658800	0.00017100
N	2.79240300	3.57988500	0.00070200
C	2.31197800	2.28364200	0.00038400
N	3.28764800	0.01469300	-0.00012600
H	4.82005200	4.25117700	0.00081200
C	0.97088700	1.77926800	0.00021800
C	2.06245800	-0.43471200	-0.00016200
O	-0.09248200	2.41163600	0.00053400
N	0.95296000	0.36278900	0.00004100
H	0.00144300	-0.02887800	0.00008400
N	-2.79544600	-2.71144200	-0.00062000
C	-1.66361100	-1.90555800	-0.00035500
C	-4.05011600	-2.20530900	-0.00052900
O	-0.53943700	-2.44729700	-0.00058600
N	-1.84463300	-0.56068800	-0.00005000
C	-4.24605000	-0.84885800	-0.00012200
H	-4.86215300	-2.92232200	-0.00075400
C	-3.07159100	-0.05765800	0.00008300
H	-5.24040800	-0.43008300	-0.00001700
H	-2.64366700	-3.71453300	-0.00091200
N	4.50200600	2.12641400	0.00033500
H	5.45422400	1.78420700	0.00025600
F	3.63475300	-2.67055900	-0.00018300
S	-3.03370700	1.71829500	0.00057400

Cl	-5.05087600	2.23352700	0.00025500
Se	1.83172500	-2.36139400	-0.00043400

Table S99. Cartesian coordinates of G_{SeCl}:C_{SCl} (water phase).

ATOM	X	Y	Z
C	4.60827000	2.94844600	-0.50723600
C	3.44492300	1.08956000	-0.30277100
N	3.36087100	3.36850900	-0.43010600
C	2.61618300	2.21415800	-0.30249500
N	3.08412100	-0.21471400	-0.20453100
H	5.47898600	3.57940500	-0.61514100
C	1.19900200	2.02276500	-0.16178100
C	1.79863100	-0.37460800	-0.06168000
O	0.29690200	2.86659900	-0.13722300
N	0.89671900	0.65047100	-0.02360100
H	-0.09833500	0.42045200	0.08942200
N	-2.56467200	-1.35606400	-2.32809100
C	-1.53476300	-1.11368100	-1.42890600
C	-3.82528000	-0.89986700	-2.13877400
O	-0.39802100	-1.58318400	-1.66006400
N	-1.82215900	-0.36148900	-0.33302200
C	-4.13010500	-0.15319000	-1.02952600
H	-4.55164900	-1.15521400	-2.90057400
C	-3.05415800	0.08902300	-0.14651500
H	-5.12965100	0.21804800	-0.86116800
H	-2.33781100	-1.91445200	-3.14486400
N	4.71593000	1.58054700	-0.43872500
H	5.57065000	1.03997600	-0.47514200
S	-3.12947000	1.03135600	1.35137400
Cl	-5.08552100	1.69706900	1.43338400
Cl	2.46478300	-2.68404900	1.91735200
Se	1.06085100	-2.14073600	0.19076200

Table S100. Cartesian coordinates of G_{SeBr}:C_{SCl} (water phase).

ATOM	X	Y	Z
C	-2.43628900	4.61859200	0.00035100
C	-2.32785200	2.41802000	0.00003700
N	-1.14268400	4.37072100	0.00047600
C	-1.05784500	2.99105000	0.00025700
N	-2.64765600	1.10260100	-0.00015000
H	-2.88972700	5.59954700	0.00046100
C	0.08009100	2.12006200	0.00021000
C	-1.60955200	0.31549700	-0.00007000
O	1.27848100	2.42231400	0.00039100
N	-0.31274600	0.75712200	0.00007500
H	0.48087700	0.10537000	0.00003200
N	2.73965600	-3.12359500	0.00046000
C	1.80822100	-2.08666700	0.00022800
C	4.07494900	-2.90924800	0.00067900
O	0.59605100	-2.35688000	0.00015300
N	2.28799300	-0.81091900	0.00011000
C	4.56671400	-1.63051500	0.00063100
H	4.70825400	-3.78808800	0.00087300

C	3.59467000	-0.59882400	0.00029600
H	5.62914900	-1.44270300	0.00081000
H	2.36867000	-4.06751000	0.00050600
N	-3.19948000	3.47373700	0.00008000
H	-4.20992800	3.42108500	-0.00004000
S	3.95993200	1.14337200	0.00016300
Cl	6.04417600	1.19190500	0.00009900
Br	-4.22951800	-1.60231400	-0.00063200
Se	-1.86454500	-1.60711700	-0.00035900

Table S101. Cartesian coordinates of G_{SF}:C_{SeF} (water phase).

ATOM	X	Y	Z
C	-4.20506100	-2.84330200	-0.00051500
C	-3.50577700	-0.75326900	0.00010800
N	-2.89412500	-2.95890300	-0.00039800
C	-2.43700600	-1.65564800	0.00013300
N	-3.44692200	0.59883100	0.00036200
H	-4.90936900	-3.66296200	-0.00084500
C	-1.11839800	-1.11970900	0.00054400
C	-2.22170100	1.05498000	0.00046000
O	-0.04653500	-1.77466100	0.00005500
N	-1.10219800	0.27310800	0.00043800
H	-0.12236400	0.65110500	0.00041700
N	3.03958600	2.71003100	-0.00004500
C	1.73468300	2.22678500	0.00019900
C	4.11923000	1.88893500	-0.00035000
O	0.77012800	3.00703500	0.00048900
N	1.57374300	0.86899000	0.00000300
C	3.95504800	0.53104800	-0.00049800
H	5.09097100	2.36811900	-0.00045700
C	2.61517800	0.05437200	-0.00040100
H	4.80375900	-0.13454000	-0.00069000
H	3.15673900	3.71721800	0.00005900
N	-4.62906100	-1.53275000	-0.00014200
H	-5.58769600	-1.20807700	-0.00015300
S	-1.95115200	2.83183700	0.00054200
F	-3.56123100	3.26376500	0.00058000
F	4.07217100	-2.24127400	-0.00061500
Se	2.26455400	-1.82711600	-0.00031300

Table S102. Cartesian coordinates of G_{SCl}:C_{SeF} (water phase).

ATOM	X	Y	Z
C	3.47716800	-3.62323500	0.00038300
C	3.15874700	-1.44365700	0.00006300
N	2.16626500	-3.50430900	0.00032400
C	1.94813800	-2.14073900	0.00007300
N	3.33717800	-0.10240100	-0.00009100
H	4.02494000	-4.55476000	0.00054400
C	0.74418300	-1.38067700	-0.00013200
C	2.21659000	0.56666500	-0.00019300
O	-0.42122900	-1.84455900	0.00004500
N	0.97127700	-0.00427900	-0.00017100
H	0.07889000	0.54217000	-0.00017600

N	-2.86754100	3.01808300	0.00023200
C	-1.63112200	2.37374800	0.00001200
C	-4.04293100	2.34327400	0.00024700
O	-0.58203100	3.03049300	0.00023200
N	-1.64052000	1.00178900	-0.00007300
C	-4.05112000	0.97661300	0.00007900
H	-4.94617000	2.94152900	0.00041700
C	-2.78173900	0.33376000	-0.00009600
H	-4.97725800	0.42433200	0.00013600
H	-2.85420700	4.03205200	0.00039900
N	4.12679000	-2.40861600	0.00020500
H	5.12759000	-2.25810300	0.00021000
S	2.20876500	2.36658400	-0.00029000
F	-4.55089500	-1.73572700	-0.00013800
Cl	4.24654200	2.75777300	-0.00017300
Se	-2.70243400	-1.58167600	-0.00001500

Table S103. Cartesian coordinates of G_{SBr}:C_{SeF} (water phase).

ATOM	X	Y	Z
C	-2.28525600	4.40140600	0.00013200
C	-2.39625100	2.20084100	0.00002000
N	-1.02244300	4.03021000	0.00019600
C	-1.07344600	2.65017400	0.00012000
N	-2.83319500	0.92007500	-0.00007200
H	-2.64136700	5.42167700	0.00015900
C	-0.04025200	1.67106400	0.00011400
C	-1.86222700	0.04618300	-0.00004600
O	1.19362400	1.89918200	0.00013100
N	-0.52937800	0.36611200	0.00001100
H	0.23796100	-0.34555800	0.00000200
N	2.65538500	-3.36506100	0.00004300
C	1.56115500	-2.50010400	-0.00002500
C	3.93668300	-2.92541500	0.00016200
O	0.40948500	-2.95001500	-0.00007300
N	1.82965700	-1.15311000	0.00001300
C	4.20281400	-1.58488900	0.00020800
H	4.71055600	-3.68381200	0.00023500
C	3.07742400	-0.71410700	0.00009300
H	5.21624200	-1.21656800	0.00033800
H	2.45016200	-4.35795900	0.00002300
N	-3.15829200	3.33603100	0.00001100
H	-4.16928000	3.38232800	-0.00006000
S	-2.19573800	-1.71845500	-0.00028600
F	5.21611900	0.98051600	0.00060400
Br	-4.40888000	-1.73512400	-0.00056700
Se	3.36918800	1.18223000	0.00034600

Table S104. Cartesian coordinates of G_{SeF}:C_{SeF} (water phase).

ATOM	X	Y	Z
C	-3.61702200	3.63005700	0.00030300
C	-3.14618500	1.47618300	0.00022900
N	-2.30106600	3.60506800	0.00016100
C	-1.98507600	2.26031500	0.00014000

N	-3.24068500	0.12721800	0.00025200
H	-4.22905600	4.52073900	0.00036100
C	-0.73653700	1.57750500	-0.00002600
C	-2.07505200	-0.46385000	0.00020800
O	0.41233500	2.09260700	-0.00025600
N	-0.88560800	0.19656300	0.00000100
H	0.04522300	-0.29265200	-0.00024400
N	2.69566100	-2.88401300	0.00027100
C	1.50924300	-2.16869600	0.00010100
C	3.90568500	-2.26852700	0.00030400
O	0.41395900	-2.76986300	0.00006500
N	1.59650100	-0.81430100	-0.00004900
C	3.99247000	-0.90245500	0.00014900
H	4.77468100	-2.91494200	0.00044600
C	2.76382100	-0.19005400	-0.00006500
H	4.94916800	-0.40405900	0.00017500
H	2.63033700	-3.89636400	0.00037600
N	-4.17871200	2.37314600	0.00033200
H	-5.16627300	2.15247100	0.00041600
F	-3.83407900	-2.53793300	-0.00035300
F	4.57453500	1.81574700	-0.00021400
Se	2.72695500	1.71936200	-0.00018700
Se	-2.01369800	-2.40101200	-0.00009900

Table S105. Cartesian coordinates of G_{SeCl}:C_{SeF} (water phase).

ATOM	X	Y	Z
C	-2.80054600	4.22488100	-0.00017600
C	-2.70852700	2.02372700	-0.00009000
N	-1.50857600	3.97266000	-0.00024700
C	-1.43114400	2.59365300	-0.00018000
N	-3.03081300	0.71071900	-0.00000500
H	-3.24898800	5.20815400	-0.00019200
C	-0.31882500	1.70679400	-0.00016800
C	-1.98934700	-0.07486800	0.00000200
O	0.89590500	2.03175700	-0.00016600
N	-0.69758400	0.36823900	-0.00005100
H	0.13575500	-0.26865200	0.00002000
N	2.54462500	-3.16062200	-0.00010900
C	1.44093400	-2.31775600	-0.00009400
C	3.81592700	-2.68875400	-0.00013300
O	0.29133100	-2.79366400	-0.00004700
N	1.67761000	-0.97551300	-0.00003300
C	4.05382000	-1.34151500	-0.00011800
H	4.60628900	-3.42977700	-0.00017900
C	2.91128900	-0.49558800	-0.00002000
H	5.05950100	-0.95164400	-0.00016400
H	2.36296300	-4.15832200	-0.00012000
N	-3.57148500	3.08430300	-0.00009400
H	-4.58245400	3.03861800	-0.00003800
F	4.96904500	1.27564500	-0.00014000
Cl	-4.43651600	-2.02127800	0.00057100
Se	3.11845300	1.40544300	-0.00011400

Se	-2.20285100	-2.00085900	0.00021800

Table S106. Cartesian coordinates of G_{SeBr}:C_{SeF} (water phase).

ATOM	X	Y	Z
C	1.77356100	4.68972800	-0.00011900
C	2.00502900	2.49897900	-0.00006300
N	0.53261100	4.25063300	-0.00026900
C	0.65842700	2.87507700	-0.00026400
N	2.51633100	1.24820000	0.00007300
H	2.07312000	5.72807900	-0.00008800
C	-0.31205700	1.83478200	-0.00039300
C	1.60207400	0.31730500	0.00005200
O	-1.56089800	1.98168700	-0.00036400
N	0.25770600	0.56558600	-0.00012700
H	-0.47094800	-0.18815800	-0.00015200
N	-2.48676500	-3.39400400	-0.00064500
C	-1.50183300	-2.41246200	-0.00048200
C	-3.80867700	-3.09392800	-0.00064700
O	-0.30173800	-2.73279800	-0.00042500
N	-1.91429800	-1.11077800	-0.00035100
C	-4.22175200	-1.79044200	-0.00049100
H	-4.49534100	-3.93177700	-0.00079300
C	-3.20100900	-0.80076400	-0.00037900
H	-5.27007100	-1.53745200	-0.00050500
H	-2.17607000	-4.35952300	-0.00076900
N	2.70366600	3.67468300	-0.00005600
H	3.71053000	3.77645000	0.00003900
F	-5.48426600	0.66481700	-0.00020200
Br	4.43638400	-1.25306800	0.00101000
Se	-3.66998600	1.05487900	-0.00027200
Se	2.09314800	-1.55354400	0.00031300

Table S107. Cartesian coordinates of G_{SF}:C_{SeCl} (water phase).

ATOM	X	Y	Z
C	4.19715600	-3.18180100	0.00408100
C	3.67646900	-1.04030600	0.00143200
N	2.88082300	-3.18434700	0.00358800
C	2.53602800	-1.84662000	0.00191500
N	3.73497900	0.31235400	-0.00006600
H	4.82872800	-4.05867700	0.00535600
C	1.26133600	-1.20479000	0.00058500
C	2.55601100	0.87555700	-0.00125800
O	0.13946500	-1.75151200	0.00053500
N	1.37106600	0.19398800	-0.00085500
H	0.44458200	0.66523500	-0.00171500
N	-2.45117100	3.15838000	0.00539200
C	-1.24586600	2.46064100	0.00416300
C	-3.65279700	2.53332400	0.00430800
O	-0.16727700	3.07424000	0.00525900
N	-1.31161300	1.09513200	0.00167300
C	-3.71674900	1.16631400	0.00204800
H	-4.53090200	3.16760000	0.00534400

C	-2.47911600	0.47382400	0.00097200
H	-4.67077000	0.66360000	0.00125400
H	-2.39524300	4.17120400	0.00711900
N	4.73036000	-1.91218000	0.00283700
H	5.71265500	-1.66892500	0.00296300
S	2.46430600	2.67299100	-0.00392300
F	4.11248700	2.93458000	-0.00896200
Cl	-4.55205800	-1.92541000	-0.00376300
Se	-2.34408200	-1.44203300	-0.00166900

Table S108. Cartesian coordinates of G_{SCl}:C_{SeCl} (water phase).

ATOM	X	Y	Z
C	3.50697400	-3.82002500	-0.00016600
C	3.31949300	-1.62521000	-0.00013300
N	2.20557800	-3.62113400	-0.00005800
C	2.07024500	-2.24665700	-0.00006200
N	3.58102800	-0.29653800	-0.00012000
H	3.99680200	-4.78326700	-0.00020700
C	0.90735000	-1.41889100	-0.00000300
C	2.50566600	0.44164700	0.00000200
O	-0.28087000	-1.79562800	0.00015800
N	1.22644900	-0.05129000	0.00001400
H	0.38574700	0.55482300	0.00006600
N	-2.34390200	3.33257000	-0.00022900
C	-1.20782100	2.52287500	-0.00016900
C	-3.60051400	2.82947600	-0.00014600
O	-0.07993300	3.03322200	-0.00021400
N	-1.40376000	1.16584200	-0.00004400
C	-3.79489500	1.47532800	-0.00003000
H	-4.41291300	3.54644000	-0.00018400
C	-2.62816600	0.66694600	-0.00003700
H	-4.79267000	1.06662200	0.00003900
H	-2.18819300	4.33449300	-0.00031600
N	4.22833100	-2.64703700	-0.00021100
H	5.23636200	-2.55726700	-0.00028000
S	2.62093500	2.23949600	0.00001900
Cl	-4.94581400	-1.50746200	0.00011400
Cl	4.68274700	2.48852900	0.00031000
Se	-2.69787000	-1.25595600	0.00008300

Table S109. Cartesian coordinates of G_{SBr}:C_{SeCl} (water phase).

ATOM	X	Y	Z
C	2.48789100	4.44777400	0.00055800
C	2.61873800	2.24822300	0.00013800
N	1.22877400	4.06326600	0.00039300
C	1.29314300	2.68361800	0.00018000
N	3.07017500	0.97132600	-0.00006400
H	2.83368500	5.47158500	0.00076900
C	0.26164300	1.69722600	-0.00000100
C	2.11083600	0.08603700	-0.00019900
O	-0.96881600	1.89999600	0.00013000
N	0.77312100	0.39087300	-0.00014300
H	0.03119700	-0.33317300	-0.00017800

N	-2.28004600	-3.50470700	0.00064100
C	-1.26323600	-2.54778800	0.00016400
C	-3.59302000	-3.17734800	0.00078800
O	-0.07834300	-2.90086600	0.00035400
N	-1.64324400	-1.22849700	0.00010500
C	-3.97047100	-1.86291900	0.00051300
H	-4.30036700	-3.99806900	0.00106600
C	-2.92516600	-0.90319900	0.00032000
H	-5.01476300	-1.59468700	0.00055600
H	-1.99043800	-4.47677500	0.00085300
N	3.37072200	3.39087500	0.00036000
H	4.38114600	3.44664800	0.00039500
S	2.47511900	-1.67422800	-0.00004400
Cl	-5.52949700	0.92417200	-0.00085900
Br	4.68932300	-1.65022800	-0.00023800
Se	-3.26613500	0.99160100	-0.00022100

Table S110. Cartesian coordinates of G_{SeF}:C_{SeCl} (water phase).

ATOM	X	Y	Z
C	-3.59349700	3.88312500	-0.00005500
C	-3.27409600	1.70160300	0.00019100
N	-2.28240300	3.76427200	-0.00018900
C	-2.06271400	2.40026100	0.00001100
N	-3.46278100	0.36146500	0.00034500
H	-4.14115600	4.81480800	-0.00011200
C	-0.85722300	1.63713700	0.00003600
C	-2.34399300	-0.31271100	0.00020200
O	0.31842700	2.06080500	-0.00035300
N	-1.10713600	0.26025000	-0.00000300
H	-0.22908200	-0.29644300	-0.00022100
N	2.14530500	-3.21020600	0.00013700
C	1.07942900	-2.32365200	-0.00003900
C	3.43265600	-2.78835700	0.00015500
O	-0.08852300	-2.76674700	-0.00001400
N	1.36231500	-0.99588000	-0.00005800
C	3.72057600	-1.44919100	0.00001000
H	4.19400500	-3.55887700	0.00023600
C	2.61483100	-0.56346600	-0.00000700
H	4.74474400	-1.11057400	-0.00005000
H	1.92521900	-4.20081700	0.00022100
N	-4.24213700	2.66886900	0.00027900
H	-5.24279000	2.51871700	0.00047300
F	-4.27055200	-2.24502700	0.00036700
Cl	5.01396200	1.49032400	0.00000100
Se	2.76389500	1.34594500	-0.00035400
Se	-2.44273300	-2.24887000	0.00013300

Table S111. Cartesian coordinates of G_{SeCl}:C_{SeCl} (water phase).

ATOM	X	Y	Z
C	2.91414800	4.32399300	-0.00122800
C	2.88066700	2.12123400	-0.00089800
N	1.62952500	4.03551500	-0.00095700
C	1.58980600	2.65456200	-0.00073600

N	3.23991500	0.81699100	-0.00075300
H	3.33531900	5.31925300	-0.00145900
C	0.49456100	1.74090900	-0.00038200
C	2.22355100	0.00063600	-0.00036000
O	-0.72306600	2.02016000	-0.00009000
N	0.91760000	0.40554100	-0.00016300
H	0.11940200	-0.25875000	0.00026900
N	-2.10379900	-3.35342300	0.00004500
C	-1.09633300	-2.39578700	-0.00003600
C	-3.41652300	-3.02215100	0.00019700
O	0.09500900	-2.75529600	-0.00006600
N	-1.47050500	-1.08538500	0.00009500
C	-3.79436600	-1.70660300	0.00030400
H	-4.12405700	-3.84248700	0.00025000
C	-2.75097200	-0.74688700	0.00024500
H	-4.83904600	-1.43893700	0.00043700
H	-1.81581300	-4.32635800	-0.00000200
N	3.71547100	3.20479700	-0.00125200
H	4.72724700	3.18587900	-0.00145000
Cl	-5.32027000	1.10568400	0.00124100
Cl	4.75174800	-1.84444700	0.00033100
Se	-3.05934800	1.14745200	0.00041800
Se	2.51586600	-1.91763600	0.00001600

Table S112. Cartesian coordinates of G_{SeBr}:C_{SeCl} (water phase).

ATOM	**X**	**Y**	**Z**
C	2.03555400	4.71012000	0.00060700
C	2.24649200	2.51740500	0.00029800
N	0.79084700	4.28087000	0.00034500
C	0.90491900	2.90394300	0.00016300
N	2.74849800	1.26197900	0.00023100
H	2.34378900	5.74592500	0.00078300
C	-0.08214000	1.87420800	-0.00013900
C	1.82994900	0.33658900	0.00014800
O	-1.32299400	2.01891500	-0.00013100
N	0.48576700	0.59363000	0.00003800
H	-0.23256300	-0.15566900	-0.00000100
N	-2.15823500	-3.46674300	0.00067600
C	-1.24722500	-2.41550500	0.00048500
C	-3.49681900	-3.26742500	0.00048900
O	-0.02848800	-2.65781900	0.00082900
N	-1.74829300	-1.14626800	0.00006400
C	-4.00089800	-1.99491400	0.00015100
H	-4.12067500	-4.15305200	0.00074400
C	-3.05595500	-0.93745800	-0.00012400
H	-5.06644700	-1.82943200	0.00016100
H	-1.77361800	-4.40507500	0.00101300
N	2.95641900	3.68699000	0.00044700
H	3.96408300	3.77952000	0.00052000
Cl	-5.80049800	0.64974900	-0.00062800
Br	4.67426600	-1.22186500	-0.00054700
Se	-3.55384600	0.91714700	-0.00017000

Se	2.32967500	-1.53439500	0.00005100

Table S113. Cartesian coordinates of G_{SF}:C_{SeBr} (water phase).

ATOM	X	Y	Z
C	4.25677600	-3.54744900	0.00025400
C	3.97961800	-1.36094100	0.00012500
N	2.94841200	-3.40176200	0.00034000
C	2.75644400	-2.03363200	0.00028100
N	4.19004500	-0.02297600	0.00000500
H	4.78589600	-4.48971400	0.00027500
C	1.55908000	-1.25461100	0.00034700
C	3.08232200	0.66986100	0.00002800
O	0.38473100	-1.66575200	0.00044100
N	1.82791800	0.12632200	0.00019700
H	0.96381700	0.69951600	0.00018500
N	-1.60350400	3.55589700	0.00019900
C	-0.50666600	2.69723300	0.00023200
C	-2.88056800	3.10535900	0.00008800
O	0.64556800	3.15917800	0.00028800
N	-0.75932300	1.35410700	0.00015300
C	-3.13222400	1.76035500	0.00002400
H	-3.66162200	3.85623900	0.00005400
C	-2.00311100	0.90297200	0.00009200
H	-4.14644800	1.39373500	-0.00007200
H	-1.40594000	4.55068800	0.00024300
N	4.92939400	-2.34579700	0.00012400
H	5.93279900	-2.21475900	0.00003600
S	3.19725000	2.46647000	-0.00016000
F	4.86583100	2.53783900	-0.00057300
Br	-4.48685200	-1.26155100	-0.00044700
Se	-2.11824100	-1.01142100	0.00002500

Table S114. Cartesian coordinates of G_{SCl}:C_{SeBr} (water phase).

ATOM	X	Y	Z
C	-3.65193700	-4.02104100	-0.00007400
C	-3.63175100	-1.81827700	-0.00000600
N	-2.36942200	-3.72301500	-0.00004900
C	-2.33926800	-2.34192500	-0.00001400
N	-3.99482100	-0.51337400	0.00003400
H	-4.06677800	-5.01888600	-0.00010700
C	-1.24035700	-1.42900200	0.00001700
C	-2.98007100	0.30575600	0.00007100
O	-0.02904300	-1.70842600	0.00003200
N	-1.66643400	-0.08660600	0.00005200
H	-0.87882500	0.58424300	0.00007400
N	1.59905400	3.61840500	0.00008100
C	0.55016600	2.69742200	0.00009600
C	2.89998500	3.24406100	0.00003000
O	-0.62307400	3.09309800	0.00015400
N	0.88036600	1.36687500	0.00004900
C	3.22816800	1.91644300	-0.00001200
H	3.63643700	4.03882800	0.00003200
C	2.14954300	0.99528000	-0.00002100

H	4.26154600	1.60862600	-0.00004200
H	1.34393100	4.60011800	0.00011800
N	-4.46028500	-2.90641400	-0.00004500
H	-5.47218200	-2.89328000	-0.00005200
S	-3.23934400	2.08970000	0.00012300
Br	4.77951200	-1.00080500	-0.00014100
Cl	-5.31578900	2.17357500	0.00011500
Se	2.39652200	-0.90994700	-0.00005600

Table S115. Cartesian coordinates of G_{SBr}:C_{SeBr} (water phase).

ATOM	X	Y	Z
C	2.79330200	4.50467500	0.00014500
C	2.99368400	2.31041000	0.00008100
N	1.54704600	4.07994300	0.00011100
C	1.65541200	2.70274000	0.00013300
N	3.48701100	1.04869400	0.00002100
H	3.10636800	5.53896600	0.00016600
C	0.65267000	1.68512100	0.00013700
C	2.55726600	0.13238800	0.00006600
O	-0.58086200	1.84239400	0.00003900
N	1.21030100	0.39287800	0.00009800
H	0.49660600	-0.35633800	0.00000500
N	-1.67118900	-3.65038400	0.00035000
C	-0.71337400	-2.63390500	0.00036200
C	-3.00150300	-3.40329700	0.00027100
O	0.49027700	-2.91809500	0.00030800
N	-1.16955700	-1.33996600	0.00035000
C	-3.45489600	-2.11330300	0.00022400
H	-3.65881300	-4.26452500	0.00022200
C	-2.46911200	-1.09354600	0.00037100
H	-4.51273600	-1.90539200	0.00010300
H	-1.32132400	-4.60203700	0.00035600
N	3.70918600	3.47660800	0.00008700
H	4.71732200	3.56403800	0.00006100
S	2.98495500	-1.61430200	0.00004300
Br	-5.28431300	0.63537100	-0.00034400
Br	5.19761700	-1.51024500	-0.00037300
Se	-2.90288100	0.77877000	0.00008500

Table S116. Cartesian coordinates of G_{SeF}:C_{SeBr} (water phase).

ATOM	X	Y	Z
C	-3.69156800	4.12277800	-0.00007700
C	-3.55247300	1.92254500	-0.00002600
N	-2.39469700	3.89587600	-0.00007200
C	-2.28833400	2.51815500	-0.00004400
N	-3.85104000	0.60231400	0.00000000
H	-4.16018000	5.09659900	-0.00009800
C	-1.14679900	1.66022400	-0.00004600
C	-2.79248300	-0.16275400	0.00001000
O	0.05663400	1.98396200	-0.00009100
N	-1.51129200	0.30470400	-0.00001900
H	-0.68728500	-0.32587100	-0.00002400
N	1.40042800	-3.48088200	0.00015500

C	0.43463100	-2.48502100	0.00013100
C	2.72532600	-3.19913200	0.00014500
O	-0.77269800	-2.80604500	0.00011100
N	0.85417500	-1.19433100	0.00003000
C	3.15152100	-1.89820300	0.00010100
H	3.40120000	-4.04550000	0.00019900
C	2.14710600	-0.90072500	-0.00000800
H	4.20514700	-1.66780600	0.00012600
H	1.07488200	-4.44192800	0.00019400
N	-4.43790900	2.96628100	-0.00002900
H	-5.44756300	2.89936100	-0.00001000
F	-4.88317800	-1.92557000	-0.00005100
Br	4.86759800	0.93701300	-0.00007900
Se	2.48946000	0.98038200	-0.00005000
Se	-3.06046700	-2.08416100	0.00008300

Table S117. Cartesian coordinates of G_{SeCl}:C_{SeBr} (water phase).

ATOM	X	Y	Z
C	3.14090400	4.43473600	0.00031500
C	3.20878800	2.23293300	-0.00000200
N	1.87098000	4.08663100	0.00029500
C	1.89531600	2.70521400	0.00005600
N	3.62831100	0.94660300	-0.00024100
H	3.51549600	5.44842800	0.00045700
C	0.84010500	1.74348000	-0.00008000
C	2.65191600	0.08315200	-0.00041200
O	-0.38625700	1.96175500	0.00013400
N	1.32778300	0.42564200	-0.00025100
H	0.56548900	-0.27658200	-0.00014500
N	-1.45207700	-3.53195400	0.00024200
C	-0.52137900	-2.49928100	0.00000400
C	-2.78640400	-3.30475200	0.00032900
O	0.69343800	-2.77173000	0.00007800
N	-0.99211500	-1.22144100	-0.00004200
C	-3.26198700	-2.02154700	0.00020400
H	-3.42868800	-4.17702700	0.00050200
C	-2.29600000	-0.98502700	0.00000500
H	-4.32348800	-1.83191600	0.00028800
H	-1.08623200	-4.47787800	0.00035400
N	3.99320200	3.35392300	0.00014700
H	5.00474300	3.38120100	0.00012700
Br	-5.11070400	0.72045400	-0.00007400
Cl	5.27652500	-1.62716100	-0.00008200
Se	-2.73307300	0.88033200	-0.00008500
Se	3.04509600	-1.81826900	0.00000100

Table S118. Cartesian coordinates of G_{SeBr}:C_{SeBr} (water phase).

ATOM	X	Y	Z
C	-2.38361200	4.74020000	-0.00001600
C	-2.63191800	2.55124300	-0.00008300
N	-1.14660100	4.28900600	0.00015900
C	-1.28454700	2.91410400	0.00011100
N	-3.15605100	1.30449100	-0.00015300

H	-2.67374300	5.78123300	-0.00003700
C	-0.31250100	1.86854800	0.00022100
C	-2.25438900	0.36269800	-0.00006700
O	0.92758700	1.98733000	0.00028000
N	-0.90556300	0.59523500	0.00004000
H	-0.20404000	-0.16732200	-0.00005300
N	1.61912400	-3.55949000	0.00022000
C	0.75275200	-2.47049700	0.00027300
C	2.96468700	-3.41656300	0.00026700
O	-0.47489400	-2.66530200	-0.00001200
N	1.30431500	-1.22282800	0.00029900
C	3.51991200	-2.16598200	0.00034200
H	3.55097900	-4.32761100	0.00024100
C	2.62033200	-1.07066100	0.00035600
H	4.59131400	-2.04385300	0.00036000
H	1.19577700	-4.48102400	0.00012900
N	-3.32183500	3.73312100	-0.00016000
H	-4.32769300	3.84321300	-0.00029300
Br	5.54426900	0.44895500	0.00051600
Br	-5.13265500	-1.13618300	-0.00071200
Se	3.18024300	0.76340200	0.00030500
Se	-2.79373300	-1.49820100	-0.00050800

Table S119. Cartesian coordinates of G^{SeF} (THF phase).

ATOM	X	Y	Z
N	2.29313600	-1.88919600	-0.00191500
C	3.53778900	-1.29996200	-0.00012100
H	4.44139800	-1.89292800	0.00019900
N	3.48326900	0.01333400	0.00114400
C	2.13337100	0.29840700	0.00008900
C	1.45662500	1.56871100	0.00124600
O	1.90716600	2.70565600	0.00346700
N	0.03949300	1.36042900	0.00075700
H	-0.49886700	2.22088300	0.00411900
C	-0.58441100	0.14381000	-0.00160300
N	0.02219400	-1.00419300	-0.00347200
C	1.37655000	-0.87448000	-0.00181300
H	2.08707400	-2.87854900	-0.00283700
Se	-2.50429200	0.19147500	-0.00264500
F	-2.72524500	-1.55403600	0.01092400

Table S120. Cartesian coordinates of G^{SeF3} (water phase).

N	-2.85806200	-1.77746500	-0.06692100
C	-4.02395100	-1.06495700	0.04713300
H	-4.98519200	-1.55804100	0.07431100
N	-3.82832300	0.23794900	0.11679300
C	-2.46378900	0.38071300	0.04527100
C	-1.65857600	1.57909500	0.06276100
O	-2.00095800	2.74984100	0.14959600
N	-0.28141000	1.23042500	-0.04497100
H	0.39823300	1.98900800	-0.06504800
C	0.19384800	-0.03501300	-0.14093000
N	-0.50900300	-1.12090700	-0.16795300

C	-1.83980000	-0.86451500	-0.07064800
H	-2.76473700	-2.78226200	-0.13506800
Se	2.15769900	-0.21444300	-0.28284400
F	2.00861300	-1.96077700	0.15021600
F	2.22772500	1.64461300	-0.42675000
F	2.55130400	0.05857300	1.39048700

Table S121. Cartesian coordinates of G^{SeF3} (THF phase).

N	-2.85905900	-1.77563700	-0.07953000
C	-4.02503800	-1.06232200	0.04140300
H	-4.98730500	-1.55360300	0.06683800
N	-3.82815400	0.23893000	0.11967200
C	-2.46404500	0.38190900	0.04789100
C	-1.65778000	1.58119500	0.07258500
O	-1.99535400	2.75057800	0.16565900
N	-0.27839700	1.22881200	-0.03795400
H	0.40105700	1.98742000	-0.05722300
C	0.19448700	-0.03664400	-0.14246800
N	-0.51008100	-1.12123900	-0.17751000
C	-1.84033600	-0.86234200	-0.07765900
H	-2.76344200	-2.77956200	-0.15224400
Se	2.15673100	-0.22246600	-0.28043400
F	2.00548300	-1.95673700	0.19286100
F	2.22690300	1.63068000	-0.47362700
F	2.55314700	0.09251600	1.38397300

Table S122. Cartesian coordinates of $G^{SeSeF2}G$ (water phase).

N	-5.26593000	0.05212000	-0.52906300
C	-5.70105600	1.31398300	-0.20693400
H	-6.74652800	1.58111400	-0.26713200
N	-4.72514000	2.11581300	0.16797800
C	-3.59380300	1.33559500	0.08817500
C	-2.21757400	1.65236900	0.36716000
O	-1.71499200	2.71534100	0.74257800
N	-1.40315600	0.52349300	0.13894300
H	-0.41441800	0.65127700	0.40855300
C	-1.82372800	-0.68835100	-0.30266800
N	-3.06659200	-1.00338700	-0.54982900
C	-3.90999000	0.04321700	-0.34759400
H	-5.83361300	-0.72297000	-0.84428100
Se	-0.52979200	-1.99651100	-0.88364700
N	1.39346200	3.18833000	0.30162100
C	2.34131100	4.00610100	-0.26652000
H	2.17747200	5.06871700	-0.37414000
N	3.42709000	3.35780200	-0.64483500
C	3.17351700	2.04316000	-0.31950100
C	3.94036100	0.84522400	-0.57555600
O	5.03567600	0.71191600	-1.09753200
N	3.20414900	-0.31238100	-0.14072700
H	3.58801000	-1.22416700	-0.38017300
C	1.98558200	-0.27650700	0.43410100
N	1.30922400	0.79553100	0.69509100
C	1.91706100	1.93134100	0.27021100

H	0.43809900	3.40579200	0.58220400
Se	1.11113300	-1.99844200	0.86287100
F	2.22704700	-2.74461500	-0.48373200
F	-0.04059200	-1.10065700	1.98389800

Table S123. Cartesian coordinates of $G^{SeSeF2}G$ (THF phase).

N	-5.22410000	0.03322000	-0.64766900
C	-5.67116300	1.29125700	-0.31956100
H	-6.71028400	1.56667600	-0.43149500
N	-4.71516300	2.07688600	0.12882200
C	-3.58457100	1.29191700	0.09552000
C	-2.22370500	1.59474200	0.45439600
O	-1.73394200	2.64779300	0.86904900
N	-1.40372700	0.46076100	0.25621100
H	-0.42611000	0.58525100	0.56521100
C	-1.80311400	-0.73175900	-0.24935100
N	-3.03107200	-1.03200100	-0.57598900
C	-3.88069900	0.01254900	-0.38931000
H	-5.77400000	-0.73167700	-1.01407500
Se	-0.50656300	-2.03741200	-0.83389500
N	1.28323600	3.19627500	0.39547600
C	2.16601600	4.05631600	-0.21456400
H	1.95883200	5.11387900	-0.29466100
N	3.24945800	3.45476100	-0.66804600
C	3.06300400	2.12710900	-0.35286000
C	3.85128900	0.96049800	-0.68491200
O	4.91274400	0.87069100	-1.27692400
N	3.17699200	-0.23158800	-0.23237800
H	3.56789500	-1.12552600	-0.52282600
C	1.99667100	-0.24657200	0.41795100
N	1.30661500	0.79650000	0.74870900
C	1.84932500	1.96026000	0.30970700
H	0.33125000	3.36663900	0.72028400
Se	1.19672300	-2.00254200	0.85259000
F	2.29006500	-2.69703600	-0.53900000
F	0.05244300	-1.16366500	2.02420900

Table S124. Cartesian coordinates of $G^{SeSe}G$ (water phase).

N	5.23124500	0.26384500	0.32880700
C	5.55864300	1.55966200	0.00876800
H	6.58315700	1.90305100	0.03343800
N	4.51226700	2.28917500	-0.31681700
C	3.44516800	1.42277600	-0.20846400
C	2.03788600	1.64070800	-0.41369600
O	1.43609900	2.67675300	-0.71510600
N	1.32427700	0.44354000	-0.19744900
H	0.29773400	0.51752200	-0.34553900
C	1.84936900	-0.73338200	0.22612600
N	3.12100200	-0.95578400	0.42783700
C	3.87378100	0.15373900	0.19802700
H	5.86636800	-0.46952200	0.61314900
Se	0.63172000	-2.13386500	0.79367200
N	-1.72908500	2.88593500	-0.05338400

C	-2.81647700	3.62362300	0.35376500
H	-2.75408100	4.69439000	0.48493400
N	-3.89499000	2.89041500	0.55290700
C	-3.49326500	1.60245900	0.26475100
C	-4.20976500	0.35136300	0.32153700
O	-5.37224400	0.12535900	0.62578500
N	-3.33625300	-0.73523600	-0.03093800
H	-3.75383300	-1.65790400	0.03205800
C	-2.03273800	-0.62288400	-0.39743500
N	-1.40987200	0.52071100	-0.47255600
C	-2.15344400	1.59237100	-0.11121900
H	-0.77772300	3.18926700	-0.25475200
Se	-1.01576600	-2.20009100	-0.88104100

Table S125. Cartesian coordinates of $G^{SeSe}G$ (THF phase).

N	5.21952700	0.26372600	0.34385300
C	5.54495600	1.56280200	0.02983600
H	6.56781800	1.91063300	0.06287500
N	4.49940800	2.28919800	-0.30095100
C	3.43438000	1.41948100	-0.20451000
C	2.02736300	1.63320100	-0.41940100
O	1.42160900	2.66685000	-0.71724100
N	1.31778500	0.42965700	-0.21604200
H	0.29237600	0.49959300	-0.37651700
C	1.84315100	-0.74485600	0.21202200
N	3.11342700	-0.96276200	0.42509400
C	3.86315900	0.15011200	0.20131100
H	5.85237500	-0.47004700	0.63110600
Se	0.62680300	-2.14729400	0.78227100
N	-1.68606200	2.88483200	-0.08827100
C	-2.75584300	3.63938000	0.33607600
H	-2.67691400	4.70981800	0.46153500
N	-3.84068900	2.92311300	0.55858500
C	-3.46360200	1.62851100	0.26981800
C	-4.19550600	0.38618600	0.35001500
O	-5.35236100	0.17201400	0.67563000
N	-3.33730800	-0.71562600	-0.00867200
H	-3.76440100	-1.63211100	0.07448100
C	-2.03925600	-0.62169100	-0.39881500
N	-1.40699400	0.51435300	-0.49803900
C	-2.13123200	1.59775800	-0.13112300
H	-0.73014100	3.16799300	-0.30273700
Se	-1.03898400	-2.21116300	-0.87633400

Table S126. Cartesian coordinates of C^{SeF} (THF phase).

C	-0.36312600	1.46065600	-0.00059300
C	-0.06205500	0.07492900	0.00026300
N	-0.92318900	-0.91152200	0.00077200
C	-2.27501100	-0.62401000	0.00019100
N	-2.60820100	0.75138800	0.00038000
C	-1.69745100	1.75404100	-0.00025000
H	0.40418700	2.21997700	-0.00128400
H	-2.08591900	2.76600200	-0.00056700

H	-3.59933600	0.95931500	0.00046400
O	-3.16514200	-1.46346700	-0.00036300
Se	1.73438900	-0.54472900	-0.00023300
F	2.52650900	1.04560800	0.00072000

Table S127. Cartesian coordinates of C^{SeF3} (water phase).

C	0.89885100	1.56693700	0.32987300
C	0.39596600	0.26305600	0.14386100
N	1.06332600	-0.81997800	-0.08581700
C	2.44903000	-0.74022700	-0.18296100
N	2.99618200	0.54187700	0.03887400
C	2.26725800	1.65223300	0.28071900
H	0.26629300	2.42681600	0.48435300
H	2.81503100	2.57586100	0.42483800
H	4.00799500	0.59774400	0.00046300
O	3.17605200	-1.68968000	-0.42984400
Se	-1.58064600	0.02931800	0.24992600
F	-1.69089600	1.58281800	-0.74691400
F	-1.33125900	-1.61156000	0.99803900
F	-1.78217400	-0.81404400	-1.25876200

Table S128. Cartesian coordinates of C^{SeF3} (THF phase).

C	0.88958600	1.57139300	0.28670900
C	0.40229800	0.25408400	0.14040200
N	1.08392100	-0.82431600	-0.05655700
C	2.46945100	-0.73245800	-0.16058800
N	3.00010500	0.56568000	0.01947900
C	2.25565900	1.67301000	0.22881600
H	0.24463400	2.42574900	0.41491000
H	2.79085300	2.60862300	0.34033400
H	4.01075400	0.63184300	-0.02531300
O	3.20905400	-1.67656900	-0.37864900
Se	-1.57836600	-0.00473300	0.26365000
F	-1.73580300	1.63669400	-0.57680800
F	-1.31567900	-1.70215400	0.84900600
F	-1.80900400	-0.69881400	-1.31412300

Table S129. Cartesian coordinates of $C^{SeSeF2}C$ (water phase).

C	1.66570500	0.42635100	-1.61038400
C	1.79839700	0.26735200	-0.21541000
N	2.17876600	1.14742000	0.65274500
C	2.50532200	2.42524600	0.20571200
N	2.35429800	2.63660000	-1.17933900
C	1.95599600	1.68877100	-2.05710800
H	1.34443700	-0.37233900	-2.25890600
H	1.88334600	1.98667400	-3.09638600
H	2.57134600	3.57180700	-1.50515500
O	2.88927300	3.32683000	0.93462400
Se	1.33184600	-1.51834100	0.54740200
C	-1.35232800	0.94990600	0.96259400
C	-1.82848400	-0.10249500	0.14588500
N	-2.98850600	-0.14642100	-0.45713900
C	-3.87109200	0.91043300	-0.32526000
N	-3.41018400	1.98829000	0.45809500

C	-2.21100500	2.00895600	1.08298800
H	-0.40645500	0.91418000	1.47586000
H	-1.98484400	2.89162300	1.66975800
H	-4.04701600	2.77122100	0.54725100
O	-4.98107100	0.95443200	-0.84038700
Se	-0.87697300	-1.71585800	-0.31455300
F	1.80695400	-2.29359100	-1.11268500
F	0.74773400	-0.69294400	2.11737100

Table S130. Cartesian coordinates of $C^{SeSeF2}C$ (THF phase).

C	1.93656900	0.33469200	-1.57990000
C	1.84844900	0.27322100	-0.17164100
N	2.04826900	1.22626800	0.67739600
C	2.38724100	2.49003500	0.19835100
N	2.46981300	2.59846300	-1.20608200
C	2.25696700	1.57450100	-2.06431000
H	1.75730900	-0.52134800	-2.20953400
H	2.35187000	1.79650600	-3.12083800
H	2.70880600	3.51825200	-1.55823700
O	2.59646600	3.45951200	0.90840100
Se	1.32841500	-1.48544800	0.63222900
C	-1.43155000	0.95303400	0.94108200
C	-1.84768400	-0.11110400	0.10448700
N	-2.99072300	-0.19680200	-0.52371400
C	-3.92205600	0.81969300	-0.40175500
N	-3.52575400	1.90413300	0.41130600
C	-2.33957800	1.96928000	1.05958500
H	-0.49156400	0.95506600	1.46676800
H	-2.16356500	2.85224500	1.66329600
H	-4.20145200	2.65355500	0.49992600
O	-5.01842700	0.82759200	-0.94291600
Se	-0.82264000	-1.67532500	-0.36780000
F	1.86728000	-2.34187300	-0.97213800
F	0.67455600	-0.61694400	2.14063200

Table S131. Cartesian coordinates of $C^{SeSe}C$ (water phase).

C	1.63143700	0.70733200	-1.19824600
C	2.02844300	-0.05052800	-0.06883800
N	3.14221800	0.09992900	0.60281300
C	4.04600600	1.07211300	0.21187600
N	3.67339600	1.84189300	-0.90962500
C	2.51687700	1.67154500	-1.59148700
H	0.69839900	0.53355800	-1.71346600
H	2.34883400	2.32758800	-2.43759900
H	4.33419500	2.55515700	-1.19429400
O	5.11338700	1.28768900	0.77424600
Se	0.93779000	-1.46228300	0.69002000
C	-1.63103000	0.70818800	1.19764100
C	-2.02843400	-0.05040500	0.06886500
N	-3.14249500	0.09954100	-0.60242000
C	-4.04621900	1.07187700	-0.21169700
N	-3.67317000	1.84244200	0.90910800
C	-2.51637300	1.67259000	1.59062600

H	-0.69780100	0.53476900	1.71262900
H	-2.34802000	2.32921100	2.43622900
H	-4.33385400	2.55591100	1.19352700
O	-5.11366400	1.28728100	-0.77401200
Se	-0.93789100	-1.46238900	-0.68974000

Table S132. Cartesian coordinates of $C^{SeSe}C$ (THF phase).

C	1.63540000	0.70019900	-1.20531700
C	2.02845300	-0.05011400	-0.06730500
N	3.13637500	0.10689100	0.60955000
C	4.04371700	1.07667000	0.21748700
N	3.67539800	1.83773100	-0.91476800
C	2.52215500	1.66102000	-1.60151500
H	0.70501000	0.52019100	-1.72336500
H	2.35799800	2.30962500	-2.45445000
H	4.33981100	2.54677200	-1.20059800
O	5.10601800	1.29981300	0.78188100
Se	0.93732800	-1.46228700	0.69098800
C	-1.63506200	0.70095200	1.20481400
C	-2.02843400	-0.04999700	0.06732900
N	-3.13661400	0.10653400	-0.60920700
C	-4.04388900	1.07647700	-0.21737900
N	-3.67524900	1.83816900	0.91433600
C	-2.52175800	1.66191400	1.60079000
H	-0.70451500	0.52125700	1.72268400
H	-2.35736600	2.31099400	2.45331900
H	-4.33957700	2.54737100	1.19996100
O	-5.10626700	1.29941500	-0.78170800
Se	-0.93739400	-1.46236100	-0.69074500

Table S133. Cartesian coordinates of G^{SeOH} (water phase).

N	2.29204400	-1.89590800	-0.02704900
C	3.53902600	-1.31367800	-0.01209000
H	4.43897800	-1.91211200	-0.01603400
N	3.49098500	0.00043600	0.00606300
C	2.14113900	0.29200600	0.00267000
C	1.46951700	1.56312600	0.02499400
O	1.93225500	2.69834200	0.05033800
N	0.05651500	1.36362300	0.02574600
H	-0.48252200	2.22210600	0.07644200
C	-0.58081000	0.15341300	-0.00791100
N	0.02523700	-0.99879600	-0.03469600
C	1.37895900	-0.87745400	-0.01735200
H	2.08423100	-2.88497700	-0.04154100
Se	-2.50408100	0.20958300	-0.05325100
O	-2.80327400	-1.54116300	0.27815300
H	-2.67422400	-1.99823500	-0.56856100

Table S134. Cartesian coordinates of G^{SeOH} (THF phase).

N	2.28894500	-1.89619900	-0.03552800
C	3.53748600	-1.31494100	-0.01481200
H	4.43725400	-1.91382600	-0.01921300
N	3.49083500	-0.00183700	0.00900700
C	2.14207200	0.29218300	0.00384600

C	1.47198600	1.56560100	0.03216900
O	1.93026500	2.70005500	0.06497200
N	0.05589300	1.36420600	0.03128800
H	-0.48204800	2.22243700	0.09530900
C	-0.58144900	0.15495100	-0.01172200
N	0.02367900	-0.99718700	-0.04651800
C	1.37767700	-0.87570500	-0.02318100
H	2.07719700	-2.88407100	-0.05312600
Se	-2.50407700	0.20696700	-0.06659800
O	-2.80094900	-1.53202100	0.32410900
H	-2.63042300	-2.02112200	-0.49682100

Table S135. Cartesian coordinates of C^{SeOH} (water phase).

C	-0.37113500	1.45223400	0.02434300
C	-0.07283200	0.06555900	0.00711800
N	-0.94990600	-0.91147100	-0.00869600
C	-2.29668600	-0.60875300	-0.01176400
N	-2.62189700	0.76463200	-0.00083900
C	-1.70214600	1.75932000	0.01832200
H	0.40117100	2.20664700	0.04596100
H	-2.08262700	2.77408600	0.02914200
H	-3.61085600	0.98300100	-0.00583400
O	-3.19450400	-1.44501500	-0.02522100
Se	1.73216400	-0.55816700	0.01350300
O	2.60641100	1.03962600	0.04894900
H	2.76289800	1.27475800	-0.87955600

Table S136. Cartesian coordinates of C^{SeOH} (THF phase).

C	-0.37111900	1.45334700	0.02700200
C	-0.07332500	0.06496000	0.00737200
N	-0.94862800	-0.91124700	-0.01099500
C	-2.29689100	-0.61119300	-0.01357000
N	-2.62162400	0.76527800	-0.00088600
C	-1.70153200	1.76014200	0.02123800
H	0.40252200	2.20630100	0.05349600
H	-2.08185500	2.77524800	0.03487000
H	-3.61096700	0.98069100	-0.00516900
O	-3.19487300	-1.44409300	-0.02861800
Se	1.73186400	-0.55838800	0.01647400
O	2.60582800	1.04134600	0.03855200
H	2.76823800	1.26315100	-0.89185000

Table S137. Cartesian coordinates of HF (water phase).

F	0.00000000	0.00000000	0.09278700
H	0.00000000	0.00000000	-0.83508300

Table S138. Cartesian coordinates of HF (THF phase).

F	0.00000000	0.00000000	0.09274400
H	0.00000000	0.00000000	-0.83469700

Table S139. Cartesian coordinates of H_2O (water phase).

O	0.00000000	0.00000000	0.12019800
H	0.00000000	0.75677100	-0.48079100
H	0.00000000	-0.75677100	-0.48079100

Table S140. Cartesian coordinates of H_2O (THF phase).

O	0.00000000	0.00000000	0.11992400

H	0.00000000	0.75717300	-0.47969600
H	0.00000000	-0.75717300	-0.47969600