Electronic Supplementary Material (ESI) for RSC Advances.


# Comparison of $^{\pm}\sigma$-hole and $^{\pm}R^{\bullet}$-hole interactions formed by tetrel-containing complexes: A computational study

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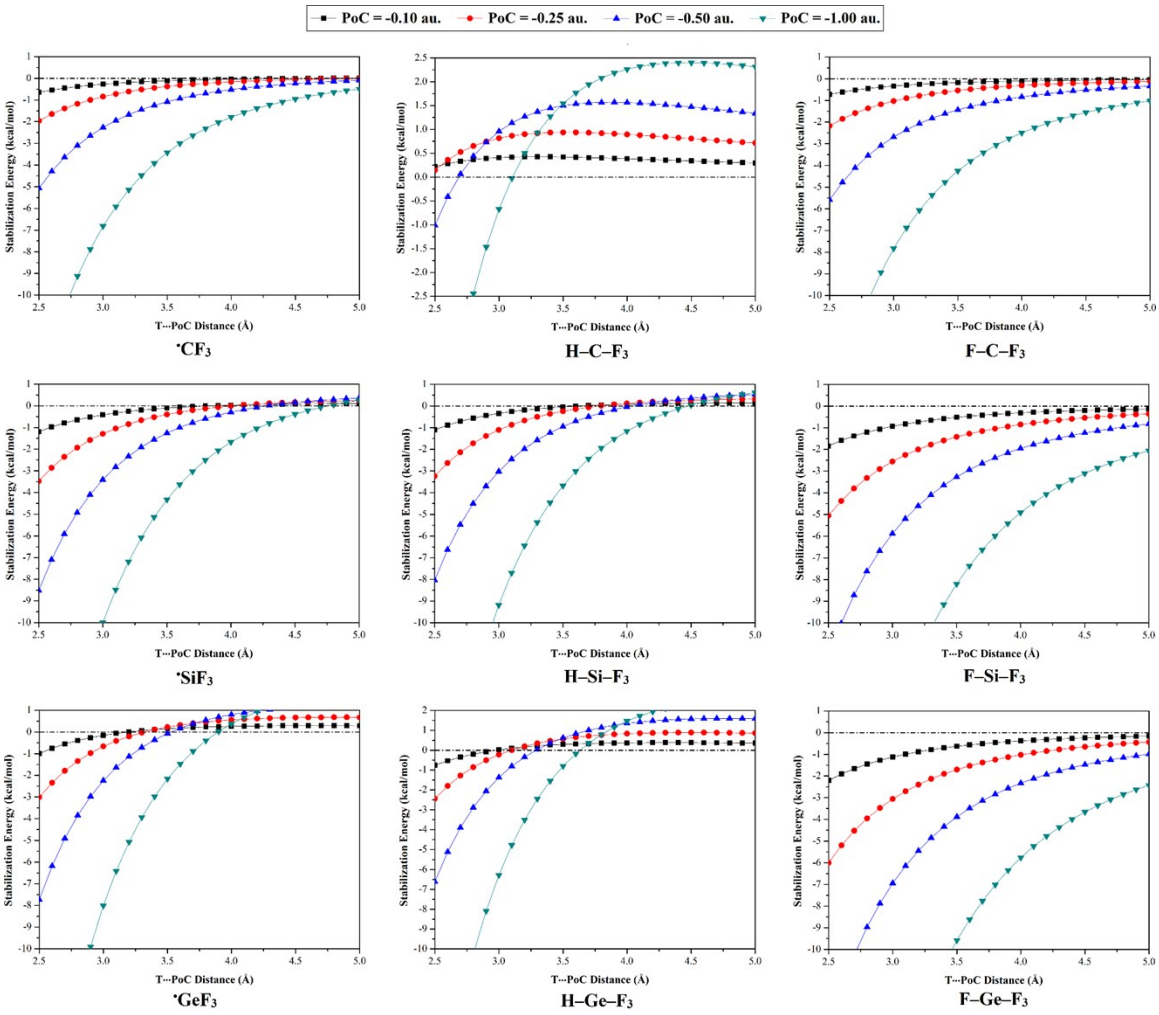


**Figure S1:** Generated molecular stabilization energy curves for the $^{\bullet}TF_3$ and W–T–$F_3$ systems (where T = C, Si, and Ge, and W = H and F) in the presence of −0.10, −0.25, −0.50, and −1.00 au PoCs at T···PoC distances ranging from 2.5 Å to 5.0 Å.

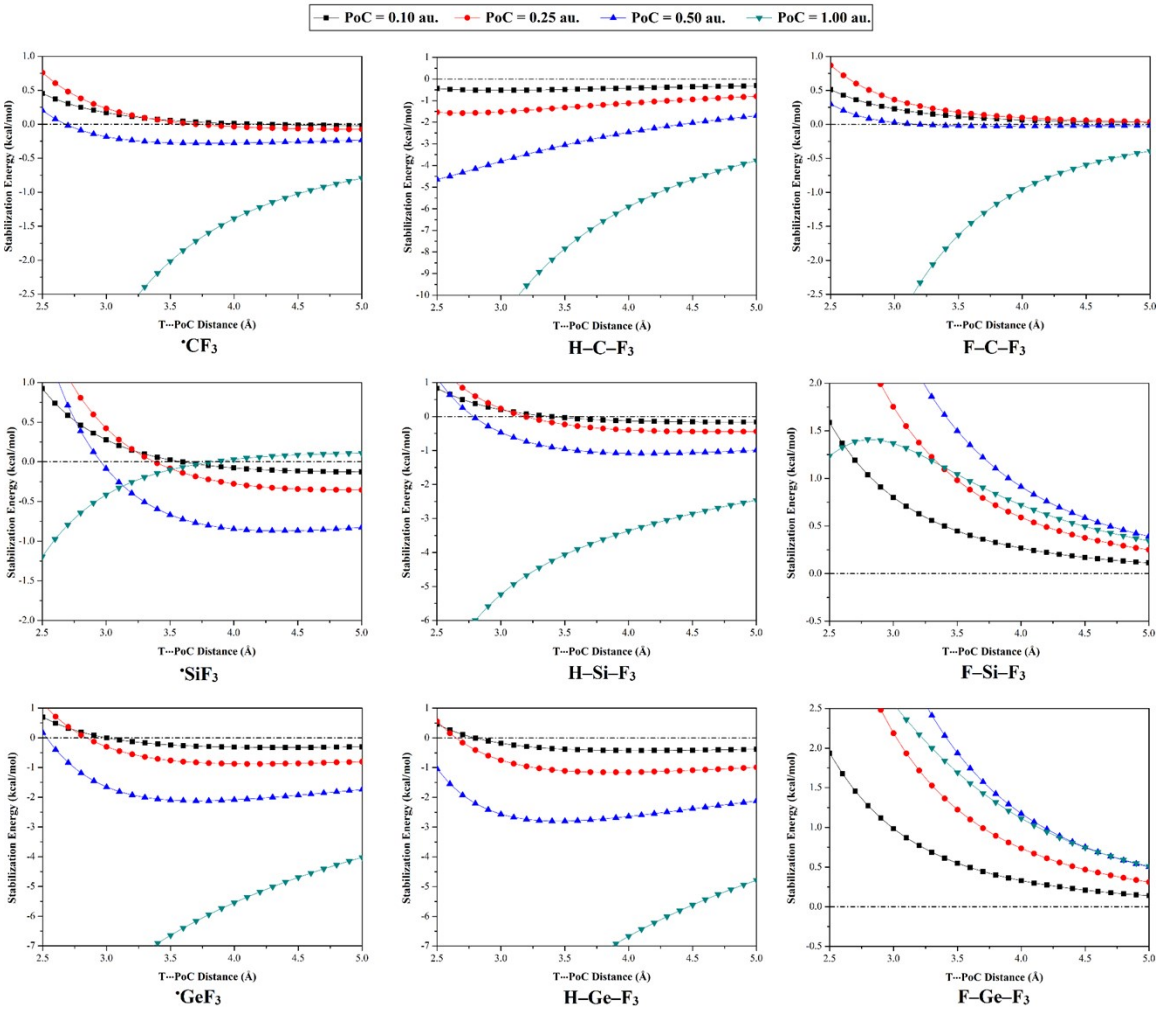


**Figure S2:** Generated molecular stabilization energy curves for the $^{\bullet}TF_3$ and W–T–$F_3$ systems (where T = C, Si, and Ge, and W = H and F) in the presence of 0.10, 0.25, 0.50, and 1.00 au PoCs at T···PoC distances ranging from 2.5 Å to 5.0 Å.

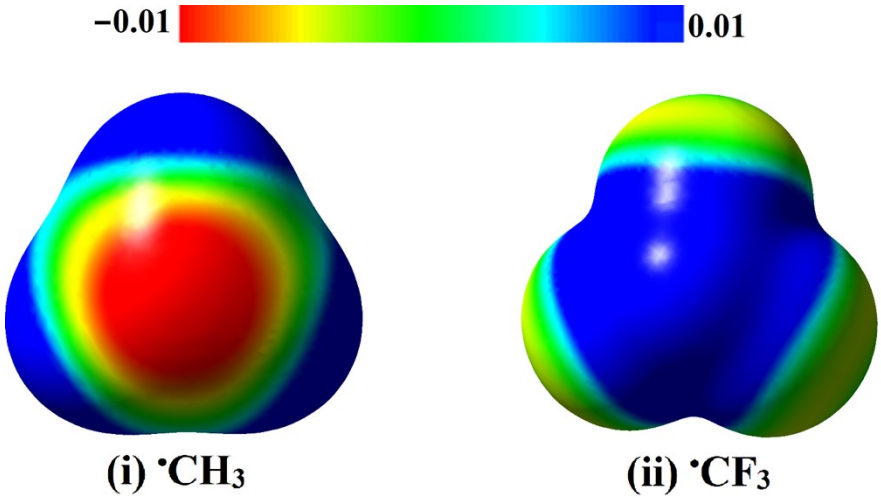


**Figure S3:** The generated molecular electrostatic potential (MEP) maps of the (i) $^{\bullet}CH_3$ and (ii) $^{\bullet}CF_3$ molecules at the MP2/aug-cc-pVTZ level of theory. The MEP maps were plotted at 0.002 au electron density contours, and the electrostatic potentials vary from −0.01 au (red) to 0.01 au (blue).

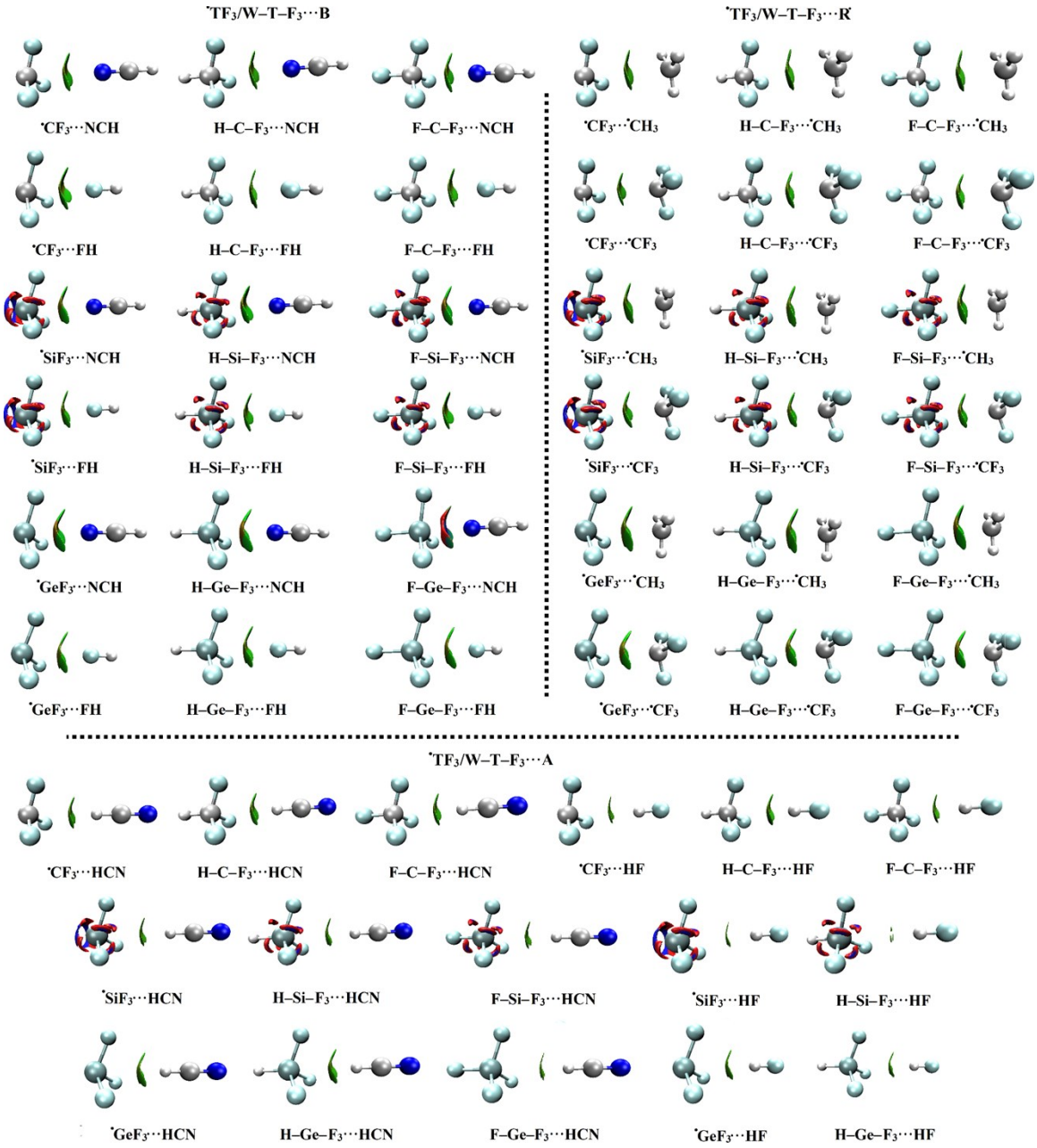


**Figure S4:** NCI isosurfaces for the studied $^{\bullet}TF_3\cdots$ and W–T–$F_3\cdots$ B/R$^{\bullet}$/A complexes (where T = C, Si, and Ge, W = H and F, B = Lewis bases, R$^{\bullet}$ = free radicals, and A = Lewis acids).

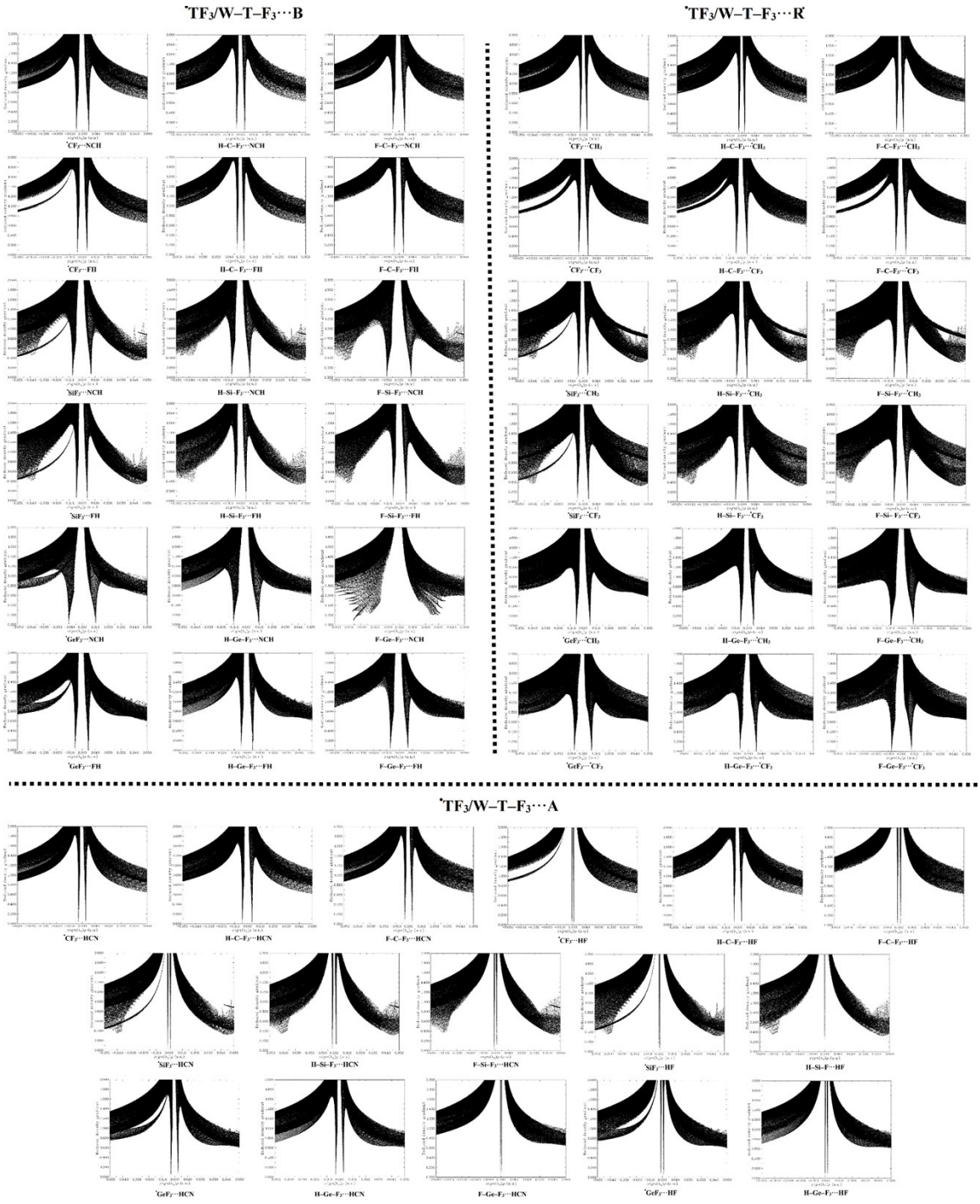


**Figure S5:** Plots of the electron density and its reduced gradient for the studied $^{\bullet}TF_3\cdots$ and $W–T–F_3\cdots$ B/ R$^{\bullet}$/A complexes (where T = C, Si, and Ge, W = H and F, B = Lewis bases, R$^{\bullet}$ = free radicals, and A = Lewis acids).